

FunctionalDiagrams

Functional derivatives and Feynman diagrams

a Mathematica package for diagrammatic many-body theory



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FunctionalDiagrams is built on an engine for functional derivatives. Its expressions are sums of integrals, over labels standing for space, time and spin, of products of commuting or Grassmann-odd functions; the engine differentiates them with respect to bosonic and Grassmann sources and brings every term to a canonical form, in which equal diagrams are recognized. Generating functionals, Wick's theorem and perturbation theory are built on it: Feynman diagrams are derived as on paper, with the signs and symmetry factors that come out of the algebra, and then classified, differentiated with respect to the propagator, compared and drawn, in Mathematica or as TikZ code. Every formula, picture and number in this document was produced by the package; the code shown is the core of the script that made them.

$\delta/\delta J$

functional calculus

Bosonic and Grassmann sources, chain rule, implicit dependence, canonical form.

exact

signs and weights

Fermion signs from the Grassmann algebra, symmetry factors from the derivatives.

0

residuals

Dyson, Ward, Bethe–Salpeter and parquet equations, checked order by order.

TikZ

for papers

Diagrams in a standard style and formulas, exported as $\text{\LaTeX}$ code.

How it works. Section 1 shows the engine alone. A theory is then given by its free generating functional — $Z_0[J] = e^{\frac{1}{2}J \cdot D_0 \cdot J}$ for bosons, $Z_0[\eta, \bar{\eta}] = e^{-\bar{\eta} \cdot G_0 \cdot \eta}$ for fermions — and by its interaction, written with the fields. The first part, many-body theory, goes from Wick's theorem to the effective actions (the map is on the next page), the vertices and the response functions, roughly in the order of a course [1], each step worked out for the electron gas and for ϕ^4 theory; the second evaluates the diagrams of field theory in dimensional regularization (ϕ^4 to two loops, QED at one loop) and draws the vertices of QCD; the third is about pictures for papers and the inner workings of the package. Every identity marked ✓ was checked by the package. The methods are those of the textbooks of many-body theory [2, 3, 4, 5, 6, 7, 8, 9, 1] and of quantum field theory [10, 11, 12, 13, 14], going back to Feynman, Dyson and Schwinger [15, 16, 17, 18].

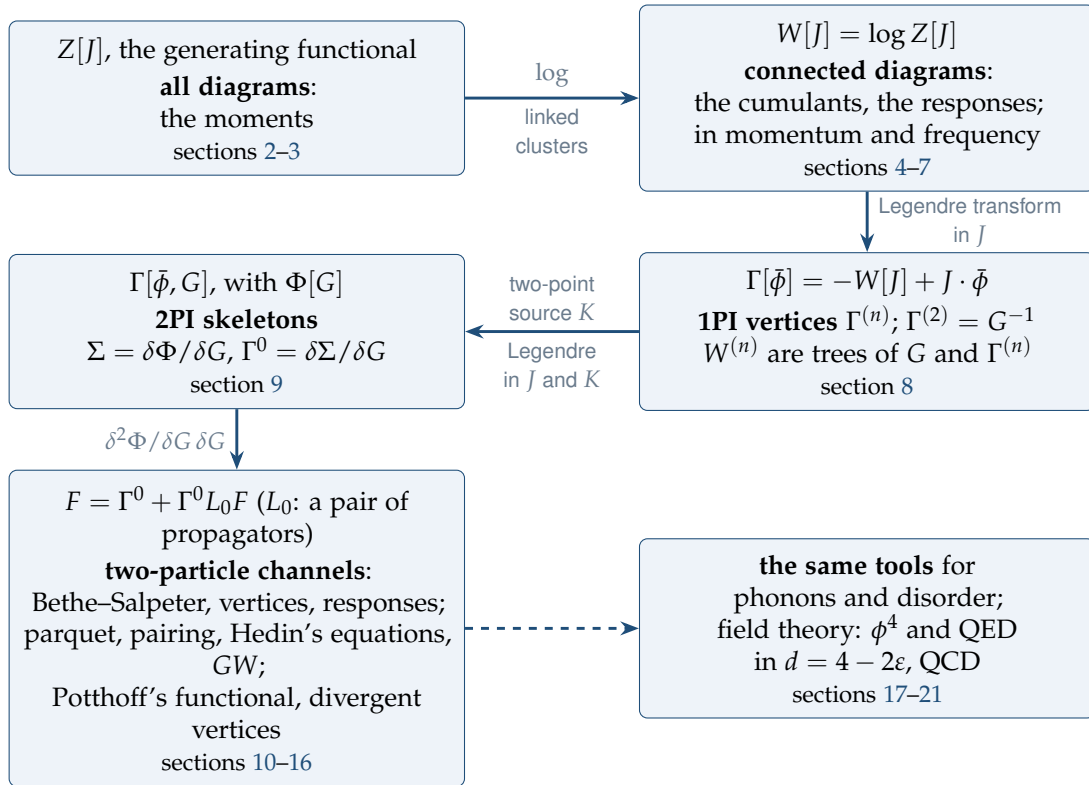
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Getting started. Needs["FunctionalDiagrams"] after
 PacletDirectoryLoad["/path/to/FunctionalDiagrams"] (Mathematica 12.1 or later). Guided tour:
 Examples.nb; reference manual: Documentation/FunctionalDiagrams_Manual.pdf; tests:
 Tests/RunTests.wl.

The road map

Correlation functions are derivatives of a generating functional with respect to its sources; each step below is a change of functional that keeps fewer diagrams, obtained from the previous one by a logarithm or a Legendre transform; the two-particle channels come from the second derivative of the last one. Every step is exact: the logarithm and the Legendre transforms are definitions, at any strength of the interaction, and the diagrams are their expansion in it, the form in which the package computes them. In every section the object is first obtained as a functional derivative (FunctionalDerivative) of a functional written by the user — Z , $W = \log Z$, $\Gamma[\bar{\phi}]$, $\Gamma[\bar{\phi}, G]$, $\Phi[G]$, $\Phi[G]$ — with respect to sources, means and propagators; the functions of the package that compute it directly (SelfEnergy, IrreducibleVertex, PerturbativeFullVertex, the option "Channel", ...) are shortcuts for these derivatives, and serve as checks. Each step is shown on two examples, both computed and checked to third order (drawn to the second where the third runs to dozens of diagrams): ϕ^4 theory (a real boson with a local four-point interaction) and the electron gas (fermions with a two-body interaction V).



- $Z[J]$ **generates the moments**: its derivatives with respect to the sources, at zero source, are the correlation functions. For a free theory they are given by Wick’s theorem; with an interaction, expanding $e^{-S_{\text{int}}}$ gives perturbation theory, whose vacuum bubbles cancel in the normalized correlation functions.
- $W = \log Z$ **generates the cumulants**, the connected correlation functions, sums of connected diagrams only (linked-cluster theorem). The connected two-point function is the full propagator G (for fermions $G = -\langle T\psi\bar{\psi} \rangle_c$); its one-particle-irreducible part, with the legs removed (amputated), is the self-energy, and the Dyson equation $G = G_0 + G_0\Sigma G$ rebuilds G .

- **From diagrams to numbers:** in momentum and Matsubara frequency the sums over the internal frequencies are done by residues, and the continued self-energy obeys the optical theorem.
- The **1PI effective action** $\Gamma[\bar{\phi}]$ of the mean field $\bar{\phi} = \langle \phi \rangle$ is the Legendre transform of W in the source. Its pieces are the classical action $S[\bar{\phi}]$, the one loop $\frac{1}{2} \text{Tr} \ln S''[\bar{\phi}]$ and the 1PI vacuum diagrams in the background; its derivatives are the one-particle-irreducible vertices, and every connected function is a tree of full propagators and 1PI vertices.
- The **2PI effective action** adds to J a two-point source $K(x, y)$, coupled to $\frac{1}{2} \phi(x) \phi(y)$ (to $\bar{\psi}(x) \psi(y)$ for fermions), and is the Legendre transform of $W[J, K]$ in both sources: the mean field $\bar{\phi}$ and the full propagator G become the variables. The rest, $\Gamma_2[\bar{\phi}, G]$ ($\Phi[G]$, the Luttinger–Ward functional, at zero mean field), is defined exactly; expanded, it is minus the two-particle-irreducible skeleton diagrams. Its derivatives are the self-energy $\Sigma[G]$ and the irreducible vertex Γ^0 ; truncating Φ gives conserving approximations.
- The response of G to a one-body source, $L = \delta G / \delta U$, obeys by the chain rule the **Bethe–Salpeter equation**, with Γ^0 as its kernel. The **vertex of a one-body operator** (density, current) is the response of G^{-1} to an external field coupled to that operator; it gives the response functions and the self-energy by the equation of motion.
- The **parquet equations** sort the four-point vertex by the channel in which it is two-particle reducible: given the fully irreducible vertex, $\delta^4 \Gamma[\bar{\phi}, G] / \delta \bar{\phi}^4$ at fixed G , they determine the vertex and, with the Schwinger–Dyson equation for Σ , the propagator together.
- For fermions the Nambu propagator of the **superfield** $(\psi, \bar{\psi})$, with its pairing blocks, as the variable gives the gap equation of BCS theory and the kernels of all three channels.
- With the screened interaction W , the vertex gives **Hedin’s equations**. A Hubbard–Stratonovich field makes W a propagator: the 2PI functional of G and W starts with the GW approximation.
- **Without the series:** one more Legendre transform, from G to Σ , gives Potthoff’s functional; where the irreducible vertex diverges, the functional becomes multivalued and the skeleton series can converge to the wrong branch. For **phonons and disorder**, functionals of two propagators, or of the averaged one, give the self-energies as derivatives.

Other names

The most common other names, in textbooks and papers, of the objects of Part I, in the order of the sections; signs and normalizations vary from book to book.

here	also called
$Z[J]$, generating functional	partition function in an external field; vacuum-to-vacuum amplitude
$W = \log Z$	generating functional of the connected functions; at zero source, $-\Omega/T$
connected diagrams	linked diagrams; their sums are the cumulants
G , full propagator	Green function, two-point function
F , full vertex	reducible vertex, two-particle scattering amplitude
Σ , self-energy	mass operator, proper self-energy
skeleton diagrams	bold or dressed diagrams
χ , density response	density–density correlation function, susceptibility
L_0 , χ_0	particle–hole propagator; closed, the bubble (with free lines, Lindhard)
bubble chain	random-phase approximation (RPA), ring diagrams
P , polarization	irreducible polarization or polarizability; for photons, the vacuum polarization
imaginary time	Matsubara formalism, finite-temperature field theory
$\bar{\phi} = \langle \phi \rangle$, mean field	classical or background field; for bosons below T_c , the condensate
$\Gamma[\bar{\phi}]$, 1PI effective action	quantum effective action; at constant $\bar{\phi}$, the effective potential
$\Gamma^{(n)}$, 1PI vertices	proper vertices, vertex functions
$\Gamma[\bar{\phi}, G]$, 2PI effective action	Cornwall–Jackiw–Tomboulis (CJT) effective action

here	also called
$\Phi[G]$, Luttinger–Ward functional	Baym’s Φ , Γ_2 ; truncated, a Φ -derivable (conserving) approximation
$\Gamma^0 = \delta\Sigma/\delta G$	particle–hole irreducible vertex, Bethe–Salpeter kernel
Λ , vertex of the density	three-point vertex; its proper part $\tilde{\Lambda}$ is Hedin’s Γ
Γ_{irr}	fully irreducible vertex, often written Λ
Schwinger–Dyson equation	Dyson–Schwinger equation, equation of motion of G
$\psi = (\psi, \bar{\psi})$, superfield	Nambu spinor
$\mathcal{G}$, Nambu propagator	Nambu–Gor’kov Green function, with normal and anomalous blocks
Δ , gap function	anomalous self-energy, pairing field
W , screened interaction (not $W = \log Z$)	effective or dressed interaction
Hubbard–Stratonovich field	auxiliary field
$\mathcal{F}[\Sigma]$, Potthoff’s functional	universal functional; $\Omega[\Sigma]$, the self-energy functional
Migdal’s self-energy	Migdal–Eliashberg approximation; for disorder, the SCBA (self-consistent Born approximation)

PART I Many-body theory

1 The engine: functional derivatives

Everything in the package is built on a symbolic calculus of functional derivatives, which can be used on its own. Its objects are sums of terms

$$c \int_{z_1 \dots z_n} f(x, \dots; z_1, \dots, z_n) \theta_1 \theta_2 \dots \theta_k,$$

a coefficient times an integral — `IntegralOver[... , {z1, ...}]` — of a product of commuting factors f and of Grassmann-odd factors θ_i in a definite order (written with `**`). A label such as x stands for whatever the problem needs: position, imaginary time, spin, orbital; the integral is the integral or sum over it. Functions are arbitrary symbols, declared symmetric or antisymmetric if they are; sources are declared, commuting or Grassmann; nothing else needs to be said about them. Every result is returned in a canonical form, described first.

1.1 Expressions and their canonical form

Delta functions are integrated as soon as they meet an integration variable; between two external labels they are kept, and used to simplify. The integration variables of a result are renamed $z_1, z_2, \dots$ ($w_1, w_2, \dots$ in nested integrals) by a canonical rule, so that two terms that differ only by the names of their integration variables, or by the order of the arguments of symmetric functions, become identical and are added:

```
SimplifyDiagrams[IntegralOver[M[x, u] DeltaFunction[u, v] M[v, y], {u, v}]]
SimplifyDiagrams[DeltaFunction[a, b] M[a, b] M[b, c]]
DeclareSymmetric[Q];
SimplifyDiagrams[IntegralOver[M[x, u] Q[u, v] M[v, y], {u, v}] +
  IntegralOver[M[x, s] Q[t, s] M[t, y], {s, t}]]
```

$$\int_{z_1} M(x, z_1) M(z_1, y), \quad \delta(a, b) M(a, a) M(a, c), \quad 2 \int_{z_1 z_2} M(x, z_2) M(z_1, y) Q(z_1, z_2)$$

A term that changes sign under a symmetry of its own vanishes: here Q is symmetric and the product of the two Grassmann sources antisymmetric. The odd factors of a canonical term are sorted, with the sign of the permutation.

```
DeclareGrassmannSource[eta, etabar];
SimplifyDiagrams[IntegralOver[Q[u, v] etabar[u] ** etabar[v], {u, v}]]
```

$$0$$

`DiagramTerms` lists the distinct terms with their weights, and `SimplifyDiagrams[a - b]` is 0 exactly when a and b are equal: this is how every identity in this document is checked. Recognizing equal terms is what makes the weights come out right; the algorithm, a colour refinement of the integration variables as in graph-isomorphism programs, is described in section 23.

1.2 Derivatives with respect to commuting sources

`FunctionalDerivative[F, s1, s2, ...]` is $\delta/\delta s_1 \delta/\delta s_2 \dots F$, the rightmost derivative acting first. A functional of a source J , with a symmetric kernel Q and a totally symmetric three-point kernel Q_3 :

```

DeclareSource[J]; DeclareSymmetric[Q, Q3];
W = 1/2 IntegralOver[Q[x, y] J[x] J[y], {x, y}] +
    1/6 IntegralOver[Q3[x, y, z] J[x] J[y] J[z], {x, y, z}];
FunctionalDerivative[W, J[a]]
FunctionalDerivative[W, J[a], J[b]]

```

$$\frac{\delta W}{\delta J(a)} = \int_{z_1} J(z_1) Q(a, z_1) + \frac{1}{2} \int_{z_1 z_2} J(z_1) J(z_2) Q_3(a, z_1, z_2)$$

$$\frac{\delta^2 W}{\delta J(a) \delta J(b)} = \int_{z_1} J(z_1) Q_3(a, b, z_1) + Q(a, b)$$

The product rule gives three terms from the cubic part; since Q_3 is symmetric they are the same term, and their weights add up to $\frac{1}{2}$. Any function of the sources is differentiated by the chain rule — powers, exponentials, logarithms, the elementary functions, and functions left unspecified, whose derivatives are written f' , f'' :

```

FunctionalDerivative[f[IntegralOver[g[x] J[x], {x}]], J[a], J[b]]
FunctionalDerivative[Log[1 + IntegralOver[g[x] J[x], {x}]], J[a], J[b]]
FunctionalDerivative[Sqrt[IntegralOver[g[x] J[x]^2, {x}]], J[a]]

```

$$g(a) g(b) f''\left(\int_{w_1} g(w_1) J(w_1)\right), \quad -\frac{g(a) g(b)}{\left(1 + \int_{w_1} g(w_1) J(w_1)\right)^2}, \quad \frac{g(a) J(a)}{\sqrt{\int_{w_1} g(w_1) J(w_1)^2}}$$

A source can have several arguments, and an argument can run over discrete values, such as a spin projection: $\delta J(x, s) / \delta J(y, t) = \delta(x, y) \delta(s, t)$, with $\delta(\uparrow, \uparrow) = 1$ and $\delta(\uparrow, \downarrow) = 0$.

```

DeclareDiscreteIndexValues[{up, down}]; DeclareSymmetric[U];
spinFunctional = 1/2 IntegralOver[U[x, y] J[x, s] J[y, s], {x, y, s}];
FunctionalDerivative[spinFunctional, J[a, up], J[b, up]]
FunctionalDerivative[spinFunctional, J[a, up], J[b, down]]

```

$$U(a, b) \quad \text{and} \quad 0$$

1.3 Grassmann sources

For anticommuting sources the derivatives anticommute, and a left derivative that passes k odd factors to reach its source picks up the sign $(-1)^k$:

```

bilinear = IntegralOver[M[x, y] etabar[x] ** eta[y], {x, y}];
FunctionalDerivative[bilinear, etabar[a], eta[b]]
FunctionalDerivative[bilinear, eta[b], etabar[a]]
FunctionalDerivative[Exp[bilinear], etabar[a], eta[b]]

```

$$\begin{aligned}\frac{\delta^2 B}{\delta \bar{\eta}(a) \delta \eta(b)} &= -M(a, b), & \frac{\delta^2 B}{\delta \eta(b) \delta \bar{\eta}(a)} &= M(a, b) & \left(B = \int_{x,y} M(x, y) \bar{\eta}(x) \eta(y) \right) \\ \frac{\delta^2 e^B}{\delta \bar{\eta}(a) \delta \eta(b)} &= -e^{-\int_{w_1 w_2} M(w_2, w_1) \eta(w_1) \bar{\eta}(w_2)} \int_{z_1 z_2} M(a, z_1) M(z_2, b) \eta(z_1) \bar{\eta}(z_2) \\ &\quad - e^{-\int_{w_1 w_2} M(w_2, w_1) \eta(w_1) \bar{\eta}(w_2)} M(a, b)\end{aligned}$$

In the canonical form the odd factors are sorted: $\bar{\eta}(x)\eta(y) = -\eta(y)\bar{\eta}(x)$. Grassmann-odd quantities that are not sources, such as fermion fields written explicitly, are declared with `DeclareGrassmannOdd`.

1.4 Implicit dependence

Objects that depend on the sources only implicitly are differentiated by rules declared once with `DeclareFunctionalDerivative`; the rules are then used everywhere, inside integrals and functions. A propagator in a local source, $G = (G_0^{-1} - J)^{-1}$, obeys $\delta G(a, b) / \delta J(c) = G(a, c) G(c, b)$, and its second derivative follows:

```
DeclareSymmetric[PropagatorOfJ];
DeclareFunctionalDerivative[PropagatorOfJ[p_, q_], J[r_],
  PropagatorOfJ[p, r] PropagatorOfJ[r, q]];
FunctionalDerivative[PropagatorOfJ[x, y], J[u], J[v]]
```

$$\frac{\delta^2 G(x, y)}{\delta J(u) \delta J(v)} = G(u, v) G(u, y) G(v, x) + G(u, v) G(u, x) G(v, y)$$

The rules that generate the connected functions as trees of vertex functions (the tree expansion, section 8.3) are rules of this kind.

1.5 Derivatives with respect to a propagator

A source can be any function of any number of labels — in particular a propagator. The Hartree–Fock functional $\Phi = \frac{1}{2} \int V(u, v) G(u, u) G(v, v) - \frac{1}{2} \int V(u, v) G(u, v) G(v, u)$, differentiated once and twice with respect to G , gives the Hartree–Fock self-energy $\Sigma(x, y) = \delta \Phi / \delta G(y, x)$ and the bare vertex, direct and exchange:

```
DeclareSource[G]; DeclareSymmetric[V];
phiHF = 1/2 IntegralOver[V[u, v] G[u, u] G[v, v], {u, v}] -
  1/2 IntegralOver[V[u, v] G[u, v] G[v, u], {u, v}];
FunctionalDerivative[phiHF, G[y, x]]
FunctionalDerivative[phiHF, G[x4, x3], G[x2, x1]]
```

$$\begin{aligned}\Sigma(x, y) &= \delta(x, y) \int_{z_1} G(z_1, z_1) V(x, z_1) - G(x, y) V(x, y) \\ \frac{\delta \Sigma(x_1, x_2)}{\delta G(x_4, x_3)} &= -\delta(x_1, x_4) \delta(x_2, x_3) V(x_1, x_2) + \delta(x_1, x_2) \delta(x_3, x_4) V(x_1, x_3)\end{aligned}$$

Differentiating a diagram with respect to G opens one of its lines, in all possible ways; diagrams with external legs follow in this way from the vacuum diagrams, as in the recursive graphical construction of Kleinert and coworkers [19, 20, 21]. This is how `SelfEnergy` and `IrreducibleVertex` work (section 9.4). The declaration is not even needed: `FunctionalDerivative[F, G[x, y]]` takes

any object with two labels that is not a source — a propagator, a self-energy, an interaction — as the variable, and differentiates through traces and logarithms of operators too (section 9.4).

1.6 Generating functionals

A field is attached to its source with `DeclareField`: `DeclareField[phi, J]` makes the field $\phi(x)$ stand for the derivative $\delta/\delta J(x)$. For any generating functional Z , `FieldDerivative[Z, {phi[a], ...}]` applies these derivatives, and `FieldExpectationValue`, with the same arguments, also divides by Z at zero source. With $Z = e^W$ and the cumulants W_1, W_2, W_3 of a non-Gaussian distribution, the third moment is expressed through the cumulants, and the derivatives of $\log Z$ at zero source give the cumulants back:

```
DeclareField[phi, J]; DeclareSymmetric[W2, W3];
Z = Exp[IntegralOver[W1[x] J[x], {x}] + 1/2 IntegralOver[W2[x, y] J[x] J[y], {x, y}] +
1/6 IntegralOver[W3[x, y, z] J[x] J[y] J[z], {x, y, z}]];
FieldExpectationValue[Z, {phi[a], phi[b], phi[c]}]
SetSourcesToZero[FunctionalDerivative[Log[Z], J[a], J[b], J[c]]]
```

$$\begin{aligned} \langle \phi(a)\phi(b)\phi(c) \rangle &= W_1(a) W_1(b) W_1(c) + W_1(c) W_2(a, b) \\ &\quad + W_1(b) W_2(a, c) + W_1(a) W_2(b, c) + W_3(a, b, c) \\ \frac{\delta^3 \log Z}{\delta J(a) \delta J(b) \delta J(c)} \Big|_{J=0} &= W_3(a, b, c) \end{aligned}$$

For a Gaussian Z_0 the expectation values are given by Wick's theorem, and the results are Feynman diagrams (section 2).

Every formula in the boxes above was written by `ExpressionToLaTeX`, which turns an expression of the package into $\text{\LaTeX}$ ("`Names`" $\rightarrow$ `{PropagatorOfJ}` $\rightarrow$ "`G`") gave G its name in the implicit derivative); `DiagramToTikZ` does the same for pictures (section 22). In Mathematica the results are displayed in a compact notation, $\int_{z_1 z_2} \delta_{xy}$, which remains valid input.

2 Generating functionals and Wick's theorem

From the path integral to derivatives. The generating functional of a field theory is the path integral $Z[J] = \int D\phi e^{-S[\phi] + J \cdot \phi}$, with $J \cdot \phi = \int_x J(x)\phi(x)$ — in statistical physics the partition function in an external field J , in real-time field theory the vacuum-to-vacuum amplitude (the other names of the objects of this document are collected on page 3). A derivative with respect to the source brings down a field, $\delta e^{J \cdot \phi} / \delta J(a) = \phi(a) e^{J \cdot \phi}$, so that the derivatives of Z at $J = 0$ are the expectation values — the moments of the distribution e^{-S} :

$$\langle \phi_a \phi_b \dots \rangle = \frac{1}{Z[0]} \frac{\delta^n Z}{\delta J_a \delta J_b \dots} \Big|_{J=0}, \quad \frac{\delta^n W}{\delta J_a \delta J_b \dots} \Big|_{J=0} = \langle \phi_a \phi_b \dots \rangle_c, \quad W = \log Z,$$

for n fields $\phi_a \phi_b \dots$, and, as for any probability distribution, the derivatives of the logarithm are the cumulants [22], the connected correlation functions: $\langle \phi_a \rangle_c = \langle \phi_a \rangle$, $\langle \phi_a \phi_b \rangle_c = \langle \phi_a \phi_b \rangle - \langle \phi_a \rangle \langle \phi_b \rangle$, and so on (section 4). At a non-zero source the same derivatives, with $Z[J]$ in place of $Z[0]$, are the expectation values in the presence of an external field J . Write the action as a quadratic part and an interaction, $S = \frac{1}{2} \phi \cdot D_0^{-1} \cdot \phi + S_{\text{int}}[\phi]$. Inside the integral a field is a derivative of the source term, $\phi(x) e^{J \cdot \phi} = \frac{\delta}{\delta J(x)} e^{J \cdot \phi}$, so that the interaction can be taken out of the integral as a differential operator, and what is left is a Gaussian integral, done once and for all:

$$Z[J] = e^{-S_{\text{int}}[\delta/\delta J]} \int D\phi e^{-\frac{1}{2} \phi \cdot D_0^{-1} \cdot \phi + J \cdot \phi} = \mathcal{N} e^{-S_{\text{int}}[\delta/\delta J]} e^{\frac{1}{2} J \cdot D_0 \cdot J}.$$

Perturbation theory as differentiation. From here on everything is differentiation. Each derivative acting on the Gaussian either brings down a factor $D_0 \cdot J$ or, acting on a factor brought down before, turns it into a propagator D_0 between two points — Wick's theorem — and expanding $e^{-S_{\text{int}}[\delta/\delta J]}$ in powers of the interaction generates every Feynman diagram, with its weight. For fermions the fields and the sources are Grassmann variables, and the same construction holds [23, 4] (paragraph *Free fields* below). The engine carries out these derivatives literally (for the path integral and its Gaussian integrals see [4, 12, 8, 11]).

The weights of the pictures. In the pictures an interaction line stands for $-V$ and a vertex for minus its coupling ($-\lambda$ in ϕ^4 theory): the minus sign comes from expanding $e^{-S_{\text{int}}}$. The number written in front of a picture, times the values of its lines and vertices, is the term, with the internal points integrated over.

Free fields. A Gaussian generating functional $Z_0[J] = \exp(\frac{1}{2} J \cdot D_0 \cdot J)$ generates the free correlation functions, $\langle \phi_a \phi_b \cdots \rangle_0 = \delta^n Z_0 / \delta J_a \delta J_b \cdots |_{J=0}$ [24, 4]. The product and chain rules produce all the terms, and at zero source only the complete pairings survive. The results are sums of diagrams, shown as pictures drawn by the package; the names of the functions are explicit in the input, and can be displayed as short symbols in the output (`DeclareDisplayName`).

```
DeclareSymmetric[FreePropagator];
FreeBosonGeneratingFunctional = Exp[1/2 IntegralOver[J[x] FreePropagator[x, y] J[y],
  {x, y}]];
fourPoint = SetSourcesToZero[FunctionalDerivative[FreeBosonGeneratingFunctional,
  J[a], J[b], J[c], J[d]]];
DiagramPlot[fourPoint, {a, b, c, d}]
```

$$\langle \phi_a \phi_b \phi_c \phi_d \rangle_0 = \begin{array}{c} a \text{---} d \\ b \text{---} c \end{array} + \begin{array}{c} a \text{---} c \\ b \text{---} d \end{array} + \begin{array}{c} a \text{---} b \\ c \text{---} d \end{array}$$

Fermions are described by Grassmann fields and sources. In many-body theory a label x includes the imaginary time $\tau_x \in [0, \beta)$ of the thermal path integral at the temperature $1/\beta$ (section 7), and T orders the fields by it, the latest on the left, with a factor -1 for each exchange of two fermion fields [3, 4]: the path integral gives these time-ordered products directly. With the convention $G_0(x, y) = -\langle T \psi(x) \bar{\psi}(y) \rangle_0$ the free generating functional is $Z_0[\eta, \bar{\eta}] = \exp(-\bar{\eta} \cdot G_0 \cdot \eta)$, and the fields stand for the derivatives $\psi \leftrightarrow \delta/\delta \bar{\eta}$, $\bar{\psi} \leftrightarrow -\delta/\delta \eta$. The sign of the exchange term is not put in by hand: it comes out of the Grassmann algebra.

```
DeclareGrassmannSource[eta, etabar];
DeclareField[psi, etabar]; DeclareField[psibar, eta, -1];
FreeFermionGeneratingFunctional = Exp[-IntegralOver[
  BareGreenFunction[x, y] etabar[x] ** eta[y], {x, y}]];
GaussianExpectationValue[FreeFermionGeneratingFunctional,
  {psi[a], psi[b], psibar[c], psibar[d]}]
```

$$\langle \psi_a \psi_b \bar{\psi}_c \bar{\psi}_d \rangle_0 = \begin{array}{c} a \text{---} d \\ b \text{---} c \end{array} - \begin{array}{c} a \text{---} c \\ b \text{---} d \end{array}$$

The fermionic six-point function $\langle \psi \psi \psi \bar{\psi} \bar{\psi} \bar{\psi} \rangle_0$ is a 3×3 determinant, $3! = 6$ terms; the bosonic $\langle \phi^6 \rangle_0$ has 15 pairings. For Gaussian functionals `GaussianExpectationValue` uses Wick's theorem as a sum over pairings, which is much faster; literal differentiation ("Method" -> "Differentiation") gives the same results, as the test suite checks, and works for any generating functional.

What a label is. Nothing in the diagrams depends on what a label is (section 1): the same diagrams hold in any dimension, for a lattice or the continuum, at zero or finite temperature in imaginary time [25] (the Matsubara formalism, thermal or Euclidean field theory in particle physics), and, with factors of i in the weights from e^{iS} in place of e^{-S} , in real time and out of equilibrium, where the times run on the closed Schwinger–Keldysh contour [26, 27, 28, 29]; only the meaning of the contracted labels changes. A propagator at equal labels, $G(z, z)$, stands for $G(z, z^+)$, the density; an instantaneous interaction is $V(x, y) = v(\mathbf{r}_x - \mathbf{r}_y) \delta(\tau_x - \tau_y)$ (in momentum space v_q , the Fourier transform of v , with $v_q = 4\pi e^2/q^2$ for the Coulomb interaction), a retarded one (phonons) is just another function; for a spin-independent interaction spin need not appear, and each closed fermion loop then carries the factor $2s + 1$ on evaluation. The results are exact symbolic expressions, with their signs and weights, ready for any representation. Throughout, $\hbar = k_B = 1$; the electron gas is written in Gaussian units, QED (section 20) in Heaviside–Lorentz units. Section 7 turns the diagrams into momentum and Matsubara frequency.

3 Interactions: vacuum bubbles and the linked-cluster theorem

With an interaction the generating functional is $Z[J] = e^{-S_{\text{int}}[\delta/\delta J]} Z_0[J]$ (section 2), up to a constant. For ϕ^4 theory, $S_{\text{int}} = \frac{\lambda}{4!} \int_z \phi^4$, the package applies this operator as it stands, one order at a time. In this document ϕ^4 theory is worked out to third order in λ and the electron gas to third order in V :

```
DeclareField[phi, J];
Phi4Vertex = lambda/24 IntegralOver[phi[z]^4, {z}]; (* S_int, used below *)
DeclareCoupling[lambda]; (* in the pictures each vertex stands for -lambda *)
applyInteraction[F_] := SimplifyDiagrams[
  -lambda/24 IntegralOver[FunctionalDerivative[F, J[z], J[z], J[z], J[z]], {z}];
firstOrder = applyInteraction[FreeBosonGeneratingFunctional];
secondOrder = applyInteraction[firstOrder]; thirdOrder =
  applyInteraction[secondOrder];
SetSourcesToZero[FreeBosonGeneratingFunctional + firstOrder + secondOrder/2 +
  thirdOrder/6]
```

At zero source $Z/Z_0 = \langle e^{-S_{\text{int}}} \rangle_0$ is the sum of all the vacuum diagrams, disconnected ones included, each with its symmetry factor [11, 30]. Here and below, a sum of several orders is written order by order, in coloured bands with the order in the interaction on the left:

$$\frac{Z}{Z_0} =$$

$$\begin{aligned}
& \lambda^0 \quad 1 \\
& \lambda \quad + \frac{1}{8} \infty \\
& \lambda^2 \quad + \frac{1}{48} \ominus + \frac{1}{16} \infty \infty + \frac{1}{128} \infty \infty \\
& \lambda^3 \quad + \frac{1}{48} \triangle + \frac{1}{32} \infty \infty \infty + \frac{1}{384} \infty \ominus + \frac{1}{24} \text{bubble} + \frac{1}{48} \text{bubble} + \frac{1}{128} \infty \infty \\
& \quad + \frac{1}{3072} \infty \infty \infty
\end{aligned}$$

Symmetry factors. The coefficient of a diagram is what the expansion puts in front, at order n $(-\lambda)^n / (n! (4!)^n)$, times the number of Wick contractions that give the same picture. It is $(-\lambda)^n / S$,

and the weight written with the picture, each vertex standing for $-\lambda$, is $1/S$, where the symmetry factor S is the number of permutations of the vertices and of the lines that leave the diagram unchanged [11, 30]: the figure eight has $S = 2 \cdot 2 \cdot 2 = 8$ (its two loops can be reversed and exchanged), the two vertices joined by four lines (the first diagram at λ^2) $S = 2 \cdot 4! = 48$, the tadpole on a propagator $S = 2$, the sunset $S = 3! = 6$. The package does not use this rule: it counts the contractions as derivatives, and the canonical form adds up the copies of each diagram.

Products of connected pieces: the linked-cluster theorem. Most of these diagrams are disconnected, and a disconnected diagram is the product of its connected pieces: the pieces share no line, so the integrals over their vertices are independent. The weights multiply too. At order n the exponential brings $1/n!$, and a diagram whose pieces have $n_1, n_2, \dots$ vertices arises from the $n!/(n_1! n_2! \dots)$ ways of choosing which vertices go to which piece, each with the contractions of every piece: the $n!$ cancels, and each piece keeps the $1/n_i!$ of its own order — its own weight. The one exception is a piece that occurs k times: two choices that differ only by exchanging the vertices of two identical pieces give the same contractions, one term and not two, so k identical pieces carry an extra $1/k!$. This is how the exponential series counts: $\exp(c_1 + c_2 + \dots)$ of the connected vacuum diagrams c_i , expanded, contains every collection of them once, with the product of their weights and $1/k!$ for a diagram repeated k times. Hence

$$\frac{Z}{Z_0} = \exp\left(\sum \text{connected vacuum diagrams}\right), \quad \log \frac{Z}{Z_0} = \sum \text{connected vacuum diagrams},$$

the linked-cluster theorem [31, 32, 2] (Goldstone's linked-diagram theorem). With c_n the connected diagrams of order λ^n , $Z/Z_0 = 1 + c_1 + (c_2 + \frac{1}{2!}c_1^2) + (c_3 + c_1c_2 + \frac{1}{3!}c_1^3) + \dots$; in pictures, the rows λ^2 and λ^3 of the sum above are

$$\begin{aligned} \frac{Z}{Z_0} \Big|_{\lambda^2} &= \left(\frac{1}{48} \ominus + \frac{1}{16} \infty \infty \right) + \frac{1}{2!} \left(\frac{1}{8} \infty \right)^2, \\ \frac{Z}{Z_0} \Big|_{\lambda^3} &= \left(\frac{1}{48} \triangle + \frac{1}{32} \infty \infty \infty + \frac{1}{24} \text{tadpole} + \frac{1}{48} \text{bubble} \right) + \frac{1}{8} \infty \left(\frac{1}{48} \ominus + \frac{1}{16} \infty \infty \right) + \frac{1}{3!} \left(\frac{1}{8} \infty \right)^3. \end{aligned}$$

Counted by hand: a vertex closes its four lines into a figure eight in 3 ways, so the eight has the weight $3/4! = \frac{1}{8}$, and two vertices are joined by four lines in $4!$ ways, with the weight $\frac{1}{2!} 4!/(4!)^2 = \frac{1}{48}$. Two figure eights come from the $3 \cdot 3$ contractions in which each vertex closes on itself: the two pieces are identical, there is no choice of which vertex makes which eight, and the $\frac{1}{2!}$ of the exponential stays. The eight beside the two vertices joined by four lines has 3 choices of the vertex of the eight, which turn the $\frac{1}{3!}$ of the exponential into the $\frac{1}{2!}$ of the piece of second order:

$$\frac{1}{2!} \frac{3 \cdot 3}{(4!)^2} = \frac{1}{128} = \frac{1}{2!} \left(\frac{1}{8} \right)^2, \quad \frac{1}{3!} \frac{3 \cdot 3 \cdot 4!}{(4!)^3} = \frac{1}{384} = \frac{1}{8} \cdot \frac{1}{48},$$

in the same way the eight beside the other diagram of second order has $\frac{1}{128} = \frac{1}{8} \cdot \frac{1}{16}$, and three eights $\frac{1}{3072} = \frac{1}{3!} \left(\frac{1}{8} \right)^3$. The package checks the theorem on the series computed above by derivatives: with z_n the vacuum diagrams of order λ^n (vacuum1, vacuum2, vacuum3 in the code), the logarithm of $1 + z_1 + z_2 + z_3$, expanded to λ^3 , is the sum of the connected diagrams among them, which ConnectedDiagrams picks out:

```
{vacuum1, vacuum2, vacuum3} = {SetSourcesToZero[firstOrder],
  SetSourcesToZero[secondOrder]/2, SetSourcesToZero[thirdOrder]/6};
connectedVacuum = ConnectedDiagrams[vacuum1 + vacuum2 + vacuum3, {}];
SimplifyDiagrams[vacuum1 + vacuum2 + vacuum3 - vacuum1^2/2 - vacuum1 vacuum2
  + vacuum1^3/3 - connectedVacuum]
```

$$\log \frac{Z}{Z_0} =$$

$$\lambda \quad \frac{1}{8} \infty$$

$$\lambda^2 \quad + \frac{1}{48} \ominus + \frac{1}{16} \infty \infty$$

$$\lambda^3 \quad + \frac{1}{48} \triangle + \frac{1}{32} \infty \infty \infty + \frac{1}{24} \text{tadpole} + \frac{1}{48} \text{bubble}$$

ConnectedVacuumDiagrams[FreeBosonGeneratingFunctional, Phi4Vertex, 3] computes the same sum directly.

$\log(1 + z_1 + z_2 + z_3)$ minus the connected diagrams of Z/Z_0 , to λ^3 : 0 ✓
 $\exp(c_1 + c_2 + c_3) - Z/Z_0$, to λ^3 : 0 ✓
 ConnectedVacuumDiagrams minus the connected diagrams of Z/Z_0 : 0 ✓

External points: the bubbles cancel. A correlation function is normalized by Z . Its numerator $\langle \phi_a \phi_b e^{-S_{\text{int}}} \rangle_0$, the second derivative of Z/Z_0 at $J = 0$, contains the vacuum diagrams as factors — the figure eight beside the free propagator and beside the tadpole, and so on:

$$\langle \phi_a \phi_b e^{-S_{\text{int}}} \rangle_0 =$$

$$\lambda^0 \quad a \text{---} b$$

$$\lambda \quad + \frac{1}{2} a \text{---} \text{bubble} \text{---} b + \frac{1}{8} a \text{---} \infty \infty$$

$$\lambda^2 \quad + \frac{1}{4} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} b + \frac{1}{6} a \text{---} \text{triangle} \text{---} b + \frac{1}{48} a \text{---} \infty \infty \infty + \frac{1}{16} a \text{---} \text{bubble} \text{---} \infty \infty + \frac{1}{4} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} b$$

$$+ \frac{1}{16} a \text{---} \infty \infty \infty + \frac{1}{128} a \text{---} \infty \infty \infty \infty$$

$$\lambda^3 \quad + \frac{1}{12} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \text{bubble} \text{---} b + \frac{1}{4} a \text{---} \text{triangle} \text{---} \text{triangle} \text{---} b + \frac{1}{8} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \infty \infty + \frac{1}{8} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \text{bubble} \text{---} b + \frac{1}{8} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \text{bubble} \text{---} b + \frac{1}{48} a \text{---} \infty \infty \infty \infty$$

$$+ \frac{1}{32} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \infty \infty + \frac{1}{32} a \text{---} \infty \infty \infty \infty + \frac{1}{48} a \text{---} \text{triangle} \text{---} \infty \infty + \frac{1}{384} a \text{---} \infty \infty \infty \infty \infty$$

$$+ \frac{1}{96} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \infty \infty + \frac{1}{32} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \infty \infty \infty + \frac{1}{256} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \infty \infty \infty + \frac{1}{8} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \text{bubble} \text{---} b + \frac{1}{12} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \text{triangle} \text{---} b$$

$$+ \frac{1}{12} a \text{---} \text{triangle} \text{---} \text{bubble} \text{---} b + \frac{1}{4} a \text{---} \text{triangle} \text{---} \text{triangle} \text{---} \text{bubble} \text{---} b + \frac{1}{24} a \text{---} \infty \infty \text{tadpole} + \frac{1}{32} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \infty + \frac{1}{8} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \text{bubble} \text{---} b$$

$$+ \frac{1}{48} a \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \text{bubble} \text{---} \text{bubble} \text{---} b + \frac{1}{128} a \text{---} \infty \infty \infty \infty + \frac{1}{3072} a \text{---} \infty \infty \infty \infty \infty$$

The counting is the same: a diagram of the numerator is a part joined to the external points times vacuum pieces. At order n , the $n!/(m!(n-m)!)$ ways of choosing which m vertices go to the part joined to a and b turn the $1/n!$ of the exponential into $1/m!$ for that part and $1/(n-m)!$ for the vacuum pieces, and the sum of all the diagrams is a product,

$$\langle \phi_a \phi_b e^{-S_{\text{int}}} \rangle_0 = \left(a \text{---} b + \frac{1}{2} a \text{---} \text{bubble} \text{---} b + \dots \right) \left(1 + \frac{1}{8} \infty + \dots \right) = \langle \phi_a \phi_b \rangle \frac{Z}{Z_0},$$

so the bubbles cancel against the normalization: $\langle \phi_a \phi_b \rangle = \langle \phi_a \phi_b e^{-S_{\text{int}}} \rangle_0 / \langle e^{-S_{\text{int}}} \rangle_0$ is the sum of the diagrams without vacuum bubbles. The package checks the product order by order; `PerturbativeCorrelationFunction` computes $\langle \phi_a \phi_b \rangle$ directly, and never generates the bubbles:

```
numerator = SetSourcesToZero[FunctionalDerivative[FreeBosonGeneratingFunctional +
  firstOrder + secondOrder/2 + thirdOrder/6, J[a], J[b]]];
SimplifyDiagrams[numerator - DropVacuumBubbles[numerator, {a, b}]
  (1 + vacuum1 + vacuum2 + vacuum3)]
phi4Propagator = PerturbativeCorrelationFunction[FreeBosonGeneratingFunctional,
  {phi[a], phi[b]}, Phi4Vertex, 3]
```

$\langle \phi_a \phi_b \rangle =$

$$\begin{aligned}
 \lambda^0 & \quad a \circ \text{---} \circ b \\
 \lambda & \quad + \frac{1}{2} a \circ \text{---} \text{---} \circ b \\
 \lambda^2 & \quad + \frac{1}{4} a \circ \text{---} \text{---} \text{---} \circ b + \frac{1}{6} a \circ \text{---} \text{---} \text{---} \circ b + \frac{1}{4} a \circ \text{---} \text{---} \text{---} \circ b \\
 \lambda^3 & \quad + \frac{1}{12} a \circ \text{---} \text{---} \text{---} \text{---} \circ b + \frac{1}{4} a \circ \text{---} \text{---} \text{---} \text{---} \circ b + \frac{1}{8} a \circ \text{---} \text{---} \text{---} \text{---} \circ b + \frac{1}{8} a \circ \text{---} \text{---} \text{---} \text{---} \circ b + \frac{1}{8} a \circ \text{---} \text{---} \text{---} \text{---} \circ b + \frac{1}{8} a \circ \text{---} \text{---} \text{---} \text{---} \circ b \\
 & \quad + \frac{1}{12} a \circ \text{---} \text{---} \text{---} \text{---} \circ b + \frac{1}{12} a \circ \text{---} \text{---} \text{---} \text{---} \circ b + \frac{1}{4} a \circ \text{---} \text{---} \text{---} \text{---} \circ b + \frac{1}{8} a \circ \text{---} \text{---} \text{---} \text{---} \circ b
 \end{aligned}$$

The numerator minus its diagrams without bubbles times Z/Z_0 , orders $\lambda^0, \dots, \lambda^3$: $\{0, 0, 0, 0\}$ ✓
 PerturbativeCorrelationFunction minus the diagrams of the numerator without bubbles: 0 ✓

Fermions: the electron gas. Electrons with a two-body interaction $V(x, y)$ between densities — the Coulomb interaction or any other — have the interaction

$$S_{\text{int}} = \frac{1}{2} \int_{x,y} V(x, y) \bar{\psi}(x) \bar{\psi}(y) \psi(y) \psi(x).$$

The same steps as for ϕ^4 theory, with $e^{-S_{\text{int}}[-\delta/\delta\eta, \delta/\delta\bar{\eta}]}$ applied to $Z_0[\eta, \bar{\eta}]$, give the vacuum diagrams, disconnected ones included: 2, 8 and 34 at orders V , V^2 and V^3 , every closed fermion loop with a factor -1 :

```
DeclareSymmetric[InteractionPotential]; DeclareInteractionLine[InteractionPotential];
DeclareDirectedPropagator[BareGreenFunction];
CoulombVertex = 1/2 IntegralOver[InteractionPotential[x, y]
  psibar[x] ** psibar[y] ** psi[y] ** psi[x], {x, y}]; (* S_int, used below *)
applyInteraction[F_] := SimplifyDiagrams[-1/2 IntegralOver[InteractionPotential[u, v]
  FunctionalDerivative[F, eta[u], eta[v], etabar[v], etabar[u]], {u, v}]];
```

$$\frac{Z}{Z_0} =$$

$$V^0 \quad 1$$

$$V = -\frac{1}{2} \text{ (Hartree bubble)} + \frac{1}{2} \text{ (Fock bubble)}$$

$$V^2 = -\frac{1}{4} \text{ (Hartree-Hartree)} - \frac{1}{2} \text{ (Hartree-Fock)} + \frac{1}{4} \text{ (Fock-Fock)} - \frac{1}{2} \text{ (Hartree-Fock)} + \frac{1}{8} \text{ (Hartree-Hartree)} - \frac{1}{4} \text{ (Hartree-Fock)} + \frac{1}{8} \text{ (Fock-Fock)}$$

$$V^3 = -\frac{1}{6} \text{ (Hartree-Hartree-Hartree)} + \frac{1}{2} \text{ (Hartree-Hartree-Fock)} - \frac{1}{2} \text{ (Hartree-Fock-Fock)} + \frac{1}{6} \text{ (Fock-Fock-Fock)} - \frac{1}{2} \text{ (Hartree-Hartree-Fock)} - \frac{1}{2} \text{ (Hartree-Fock-Fock)} + \frac{1}{6} \text{ (Fock-Fock-Fock)} + \frac{1}{3} \text{ (Hartree-Hartree-Hartree)} + \frac{1}{2} \text{ (Hartree-Hartree-Fock)} + \frac{1}{8} \text{ (Hartree-Fock-Fock)} - \frac{1}{8} \text{ (Hartree-Fock-Fock)} + \frac{1}{8} \text{ (Hartree-Fock-Fock)} - \frac{1}{6} \text{ (Hartree-Hartree-Fock)} - \frac{1}{3} \text{ (Hartree-Fock-Fock)} + \frac{1}{4} \text{ (Hartree-Hartree-Fock)} - \frac{1}{4} \text{ (Hartree-Fock-Fock)} + \frac{1}{8} \text{ (Hartree-Fock-Fock)} - \frac{1}{8} \text{ (Hartree-Fock-Fock)} + \frac{1}{8} \text{ (Hartree-Fock-Fock)} + \frac{1}{8} \text{ (Hartree-Fock-Fock)} - \frac{1}{4} \text{ (Hartree-Hartree-Fock)} + \frac{1}{2} \text{ (Hartree-Hartree-Fock)} - \frac{1}{2} \text{ (Hartree-Fock-Fock)} + \frac{1}{2} \text{ (Hartree-Fock-Fock)} - \frac{1}{4} \text{ (Hartree-Hartree-Fock)} + \frac{1}{4} \text{ (Hartree-Hartree-Fock)} + \frac{1}{8} \text{ (Hartree-Fock-Fock)} - \frac{1}{8} \text{ (Hartree-Fock-Fock)} + \frac{1}{2} \text{ (Hartree-Fock-Fock)} - \frac{1}{2} \text{ (Hartree-Fock-Fock)} - \frac{1}{48} \text{ (Hartree-Hartree-Fock)} + \frac{1}{16} \text{ (Hartree-Hartree-Fock)} - \frac{1}{16} \text{ (Hartree-Fock-Fock)} + \frac{1}{48} \text{ (Hartree-Fock-Fock)}$$

The interaction lines carry two different points, so most weights are ± 1 ; the vacuum diagrams keep factors such as $\frac{1}{2}$ (Hartree and Fock): the symmetry of the diagram under the exchange of the two ends of its interaction line. The counting is that of ϕ^4 theory, and so are the theorem and the cancellation of the bubbles; the signs do not spoil the products. A vacuum piece contains an even number of Grassmann fields — four at each vertex, contracted in pairs within the piece — so the pieces commute with each other, and the sign of a diagram is the product of the signs of its pieces, $(-1)^{n_L} = \prod_i (-1)^{n_{L,i}}$ for pieces with $n_{L,i}$ closed loops: the sign of a loop belongs to its connected piece. At second order, the products of the Fock and Hartree diagrams of first order:

$$\frac{1}{8} \text{ (Hartree-Hartree)} = \frac{1}{2!} \left(-\frac{1}{2} \text{ (Hartree)} \right)^2, \quad -\frac{1}{4} \text{ (Hartree-Fock)} = \left(-\frac{1}{2} \text{ (Hartree)} \right) \left(\frac{1}{2} \text{ (Fock)} \right),$$

$$\frac{1}{8} \text{ (Fock-Fock)} = \frac{1}{2!} \left(\frac{1}{2} \text{ (Fock)} \right)^2.$$

So the logarithm keeps the connected vacuum diagrams, $\log(Z/Z_0) = -\beta(\Omega - \Omega_0)$, where $Z = \text{tr} e^{-\beta(H - \mu N)}$ and $\Omega = -\beta^{-1} \log Z$ is the grand potential. With `vacuum1`, `vacuum2`, `vacuum3` now the vacuum diagrams of the electron gas, made with this `applyInteraction` as for ϕ^4 theory:

```
connectedVacuum = ConnectedDiagrams[vacuum1 + vacuum2 + vacuum3, {}];
vacuum = ConnectedVacuumDiagrams[FreeFermionGeneratingFunctional, CoulombVertex, 3];
```

$$\log \frac{Z}{Z_0} =$$

$$V = -\frac{1}{2} \text{ (bubble)} + \frac{1}{2} \text{ (two-bubble)}$$

$$V^2 = -\frac{1}{4} \text{ (self-energy)} - \frac{1}{2} \text{ (bubble)} + \frac{1}{4} \text{ (two-bubble)} - \frac{1}{2} \text{ (three-bubble)} + \frac{1}{2} \text{ (four-bubble)}$$

$$V^3 = -\frac{1}{6} \text{ (self-energy)} + \text{ (two-bubble)} - \frac{1}{2} \text{ (bubble)} + \frac{1}{6} \text{ (three-bubble)} - \frac{1}{2} \text{ (four-bubble)} - \text{ (five-bubble)} + \frac{1}{6} \text{ (six-bubble)}$$

$$+ \frac{1}{3} \text{ (seven-bubble)} + \frac{1}{2} \text{ (eight-bubble)} + \text{ (nine-bubble)} - \frac{1}{6} \text{ (ten-bubble)} - \frac{1}{3} \text{ (eleven-bubble)} + \text{ (twelve-bubble)} - \text{ (thirteen-bubble)}$$

$$+ \frac{1}{2} \text{ (fourteen-bubble)} - \frac{1}{2} \text{ (fifteen-bubble)} + \frac{1}{2} \text{ (sixteen-bubble)} - \text{ (seventeen-bubble)} + \text{ (eighteen-bubble)} - \text{ (twenty-bubble)}$$

$\log(1 + z_1 + z_2 + z_3)$ minus the connected diagrams of Z/Z_0 , to V^3 : 0 ✓
 ConnectedVacuumDiagrams minus the same: 0 ✓

The numerator of the Green function, $-\langle T \psi_x \bar{\psi}_y e^{-S_{\text{int}}} \rangle_0$, contains the vacuum diagrams as factors (22 diagrams at second order, drawn here to that order):

$$-\langle T \psi_x \bar{\psi}_y e^{-S_{\text{int}}} \rangle_0 =$$

$$V^0 \quad x \longleftrightarrow y$$

$$V = -x \text{ (bubble)} \text{ } y + x \text{ (two-bubble)} \text{ } y - \frac{1}{2} x \text{ (bubble)} \text{ } y + \frac{1}{2} x \text{ (two-bubble)} \text{ } y$$

$$V^2 = -x \text{ (self-energy)} \text{ } y - \frac{1}{4} x \text{ (self-energy)} \text{ } y + x \text{ (two-bubble)} \text{ } y - x \text{ (three-bubble)} \text{ } y - \frac{1}{2} x \text{ (four-bubble)} \text{ } y$$

$$+ x \text{ (five-bubble)} \text{ } y + x \text{ (six-bubble)} \text{ } y + x \text{ (seven-bubble)} \text{ } y - x \text{ (eight-bubble)} \text{ } y + \frac{1}{4} x \text{ (nine-bubble)} \text{ } y$$

$$- \frac{1}{2} x \text{ (ten-bubble)} \text{ } y - \frac{1}{2} x \text{ (eleven-bubble)} \text{ } y - x \text{ (twelve-bubble)} \text{ } y + \frac{1}{2} x \text{ (thirteen-bubble)} \text{ } y + x \text{ (fourteen-bubble)} \text{ } y$$

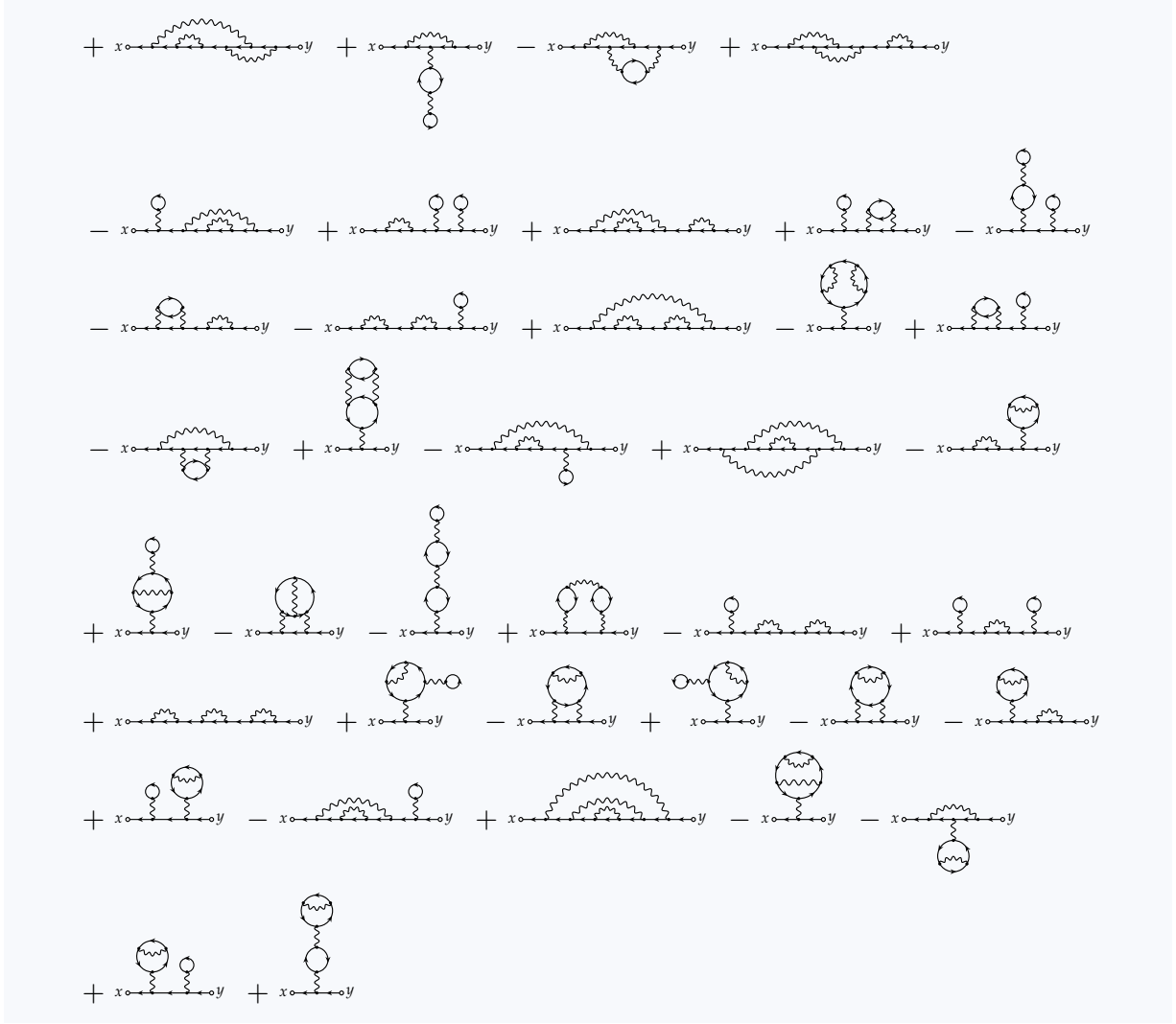
$$- x \text{ (fifteen-bubble)} \text{ } y + x \text{ (sixteen-bubble)} \text{ } y + \frac{1}{2} x \text{ (seventeen-bubble)} \text{ } y - \frac{1}{2} x \text{ (eighteen-bubble)} \text{ } y + \frac{1}{8} x \text{ (nineteen-bubble)} \text{ } y$$

$$- \frac{1}{4} x \text{ (twenty-bubble)} \text{ } y + \frac{1}{8} x \text{ (twenty-one-bubble)} \text{ } y$$

and is the Green function, without vacuum bubbles, times Z/Z_0 . So the Green function

$$G(x, y) = -\frac{\langle T \psi(x) \bar{\psi}(y) e^{-S_{\text{int}}} \rangle_0}{\langle e^{-S_{\text{int}}} \rangle_0},$$

here to third order, has no vacuum bubbles:



The numerator minus its diagrams without bubbles times Z/Z_0 , orders V^0, V, V^2 : $\{0, 0, 0\}$ ✓
 Its diagrams without bubbles minus G , to V^2 : 0 ✓

Diagrams at a non-zero source. The series can also be drawn before any derivative is taken, and the linked-cluster theorem holds at any source. For ϕ^4 theory write $Z[J] = Z_0[J] (1 + z_1[J] + z_2[J] + \dots)$, with $Z_0[J]$ set aside; a line is a free propagator D_0 and a crossed circle a source J , integrated over its position. To first order there is one diagram with no source, one with two sources and one with four:

$$z_1[J] = \frac{1}{8} \text{ (loop) } + \frac{1}{4} \text{ (line with bubble) } + \frac{1}{24} \text{ (cross) }$$

and to second order 14 diagrams, with zero to eight sources, many of them products of disconnected pieces:

$$z_2[J] = \frac{1}{48} \text{ (two loops) } + \frac{1}{16} \text{ (two bubbles on line) } + \frac{1}{128} \text{ (two loops on line) } + \frac{1}{12} \text{ (line with two bubbles) } + \frac{1}{8} \text{ (line with bubble and loop) } + \frac{1}{8} \text{ (line with two loops) } \\ + \frac{1}{32} \text{ (line with bubble and loop on line) } + \frac{1}{12} \text{ (line with bubble and loop on line) } + \frac{1}{16} \text{ (cross with bubble) } + \frac{1}{32} \text{ (line with two bubbles on line) } + \frac{1}{192} \text{ (cross with two loops) }$$

$$+ \frac{1}{96} \text{diagram} + \frac{1}{72} \text{diagram} + \frac{1}{1152} \text{diagram}$$

A derivative $\delta/\delta J(a)$ removes a source and leaves an external point a in its place; at $J = 0$ only the diagrams with as many sources as derivatives survive. So $\delta^2 Z/\delta J_a \delta J_b$ at $J = 0$ collects the diagrams with two sources — the other diagrams of the numerator above — and the free propagator times the diagrams with none, the vacuum bubbles; $\delta^4/\delta J^4$ the diagrams with four sources, and so on. Taking the logarithm, $W[J] = \log Z[J] = \frac{1}{2} J \cdot D_0 \cdot J + w_1[J] + w_2[J] + \dots$ with $w_1 = z_1$ and $w_2 = z_2 - \frac{1}{2} z_1^2$: the square of the first order removes exactly the products of disconnected pieces, and W keeps the 8 connected diagrams — the linked-cluster theorem, at any source:

$$w_2[J] = \frac{1}{48} \text{diagram} + \frac{1}{16} \text{diagram} + \frac{1}{12} \text{diagram} + \frac{1}{8} \text{diagram} + \frac{1}{8} \text{diagram} + \frac{1}{12} \text{diagram} + \frac{1}{16} \text{diagram} + \frac{1}{72} \text{diagram}$$

$w_2[J]$ minus its connected diagrams: 0 ✓

The same holds for the electron gas, with $Z[\eta, \bar{\eta}] = Z_0 (1 + z_1 + z_2 + \dots)$. A line is a free propagator G_0 , and a crossed circle a source: η where a line starts, $\bar{\eta}$ where it ends. To first order there are the two vacuum diagrams, Hartree and Fock, the same two opened into a line between two sources, and the interaction between two lines:

$$z_1[\eta, \bar{\eta}] = -\frac{1}{2} \text{diagram} + \frac{1}{2} \text{diagram} - \text{diagram} + \text{diagram} - \frac{1}{2} \text{diagram}$$

To second order there are 39 diagrams:

$$z_2[\eta, \bar{\eta}] = -\frac{1}{4} \text{diagram} - \frac{1}{2} \text{diagram} + \frac{1}{4} \text{diagram} - \frac{1}{2} \text{diagram} + \text{diagram} + \frac{1}{8} \text{diagram} - \frac{1}{4} \text{diagram} + \frac{1}{8} \text{diagram} + \text{diagram} - \frac{1}{2} \text{diagram} - \text{diagram} + \text{diagram} - \text{diagram} + \frac{1}{2} \text{diagram} - \text{diagram} + \frac{1}{2} \text{diagram} + \text{diagram} - \frac{1}{2} \text{diagram} - \frac{1}{2} \text{diagram} + \text{diagram} - \frac{1}{2} \text{diagram} - \text{diagram} + \text{diagram} - \frac{1}{2} \text{diagram} - \frac{1}{2} \text{diagram} + \text{diagram} - \frac{1}{2} \text{diagram} - \text{diagram} + \text{diagram} - \frac{1}{2} \text{diagram} - \frac{1}{2} \text{diagram} + \text{diagram} - \frac{1}{4} \text{diagram}$$

$$\begin{aligned}
& + \text{diagram} - \frac{1}{2} \text{diagram} - \text{diagram} + \frac{1}{4} \text{diagram} - \text{diagram} \\
& + \frac{1}{2} \text{diagram} - \frac{1}{2} \text{diagram} + \frac{1}{8} \text{diagram}
\end{aligned}$$

and $W = \log Z$ keeps the 24 connected ones:

$$\begin{aligned}
w_2[\eta, \bar{\eta}] = & -\frac{1}{4} \text{diagram} - \frac{1}{2} \text{diagram} + \frac{1}{4} \text{diagram} - \frac{1}{2} \text{diagram} + \text{diagram} + \text{diagram} \\
& - \text{diagram} + \text{diagram} - \text{diagram} + \text{diagram} + \text{diagram} \\
& - \text{diagram} - \text{diagram} + \text{diagram} - \text{diagram} + \text{diagram} - \frac{1}{2} \text{diagram} \\
& - \text{diagram} + \text{diagram} - \text{diagram} + \frac{1}{2} \text{diagram} - \frac{1}{2} \text{diagram} - \text{diagram} \\
& - \text{diagram}
\end{aligned}$$

$w_2[\eta, \bar{\eta}]$ minus its connected diagrams: 0 ✓

4 Moments and cumulants: $W = \log Z$

$Z[J]$ generates the moments, the full correlation functions; $W[J] = \log Z[J]$ (at zero source $-\Omega/T$, minus the grand potential over the temperature; in field theory the Schwinger functional, in probability the cumulant generating function) generates the cumulants, the *connected* correlation functions $W^{(n)} = \delta^n W / \delta J^n$, sums of connected diagrams only (section 1 shows the algebra on a non-Gaussian distribution).

Why the logarithm. The derivatives of $Z = e^W$ show it. $\delta e^W / \delta J_a = W_a e^W$, and every further derivative either acts on the exponential, bringing down W_b — a new block — or on a derivative of W already there, turning W_a into W_{ab} — the point b joins the block of a :

$$\frac{1}{Z} \frac{\delta^2 Z}{\delta J_a \delta J_b} = W_{ab} + W_a W_b, \quad \frac{1}{Z} \frac{\delta^3 Z}{\delta J_a \delta J_b \delta J_c} = W_{abc} + W_{ab} W_c + W_{ac} W_b + W_{bc} W_a + W_a W_b W_c.$$

After n derivatives, $\delta^n Z / Z$ is the sum over all the partitions of the n points into blocks, each block a cumulant: the moments in terms of the cumulants. It is the exponential series of section 3 again, with the cumulants in place of the connected pieces; the points are all different, so no two blocks are alike, and each partition comes once, with the coefficient 1 (no $1/k!$). Read backwards, $W^{(n)}$ is the moment minus every way of splitting its points into smaller blocks, and this removes exactly the disconnected diagrams. In ϕ^4 theory at zero source the odd cumulants vanish, and the four-point function is the connected four-point function $W^{(4)}$ plus the three pairings of full propagators $W^{(2)} = \langle \phi \phi \rangle$ (double lines); the package draws it from the derivatives of e^W :

```

DeclareSymmetric[ConnectedTwoPoint, ConnectedFourPoint];
DeclareLineStyle[ConnectedTwoPoint, "Double"]; DeclareBlob[ConnectedFourPoint,
  "W^{(4)}"];
expW = Exp[1/2 IntegralOver[ConnectedTwoPoint[x, y] J[x] J[y], {x, y}] +
  1/24 IntegralOver[ConnectedFourPoint[x, y, u, v] J[x] J[y] J[u] J[v],
    {x, y, u, v}]];
FieldExpectationValue[expW, {phi[a], phi[b], phi[c], phi[d]}]

```

$$\langle \phi_a \phi_b \phi_c \phi_d \rangle = \text{Diagram with a central blob labeled } W^{(4)} \text{ and four external lines } a, b, c, d + \text{Diagram with two horizontal double lines } a \text{ to } d \text{ and } b \text{ to } c + \text{Diagram with two crossing double lines } a \text{ to } d \text{ and } b \text{ to } c + \text{Diagram with two vertical double lines } a \text{ to } b \text{ and } d \text{ to } c$$

The package checks it by derivatives in J . With $Z[J] = Z_0[J] (1 + z_1[J] + z_2[J] + z_3[J])$, the series of section 3 at a non-zero source, $W[J] = \frac{1}{2} J \cdot D_0 \cdot J + \log(1 + z_1[J] + z_2[J] + z_3[J])$ expanded to λ^3 ; its fourth derivative at $J = 0$ is compared with the fourth moment, the fourth derivative of Z without its vacuum bubbles:

```

(* Z = Z0[J] (1 + z1[J] + z2[J] + z3[J]), the series of section 3 at a source, and
  W = 1/2 J.D0.J + log(1 + z1[J] + z2[J] + z3[J]), expanded to lambda^3 *)
W4 = SetSourcesToZero[FunctionalDerivative[W, J[a], J[b], J[c], J[d]]];
W2[p_, q_] := SetSourcesToZero[FunctionalDerivative[W, J[p], J[q]]];
moment = DropVacuumBubbles[SetSourcesToZero[
  FunctionalDerivative[Z, J[a], J[b], J[c], J[d]], {a, b, c, d}];
SimplifyDiagrams[W4 - ConnectedDiagrams[moment, {a, b, c, d}]]
SimplifyDiagrams[moment - (W4 + W2[a, b] W2[c, d] + W2[a, c] W2[b, d] + W2[a, d]
  W2[b, c])]

```

$W^{(4)}$ minus the connected diagrams of the fourth moment, to λ^3 : 0 ✓

The fourth moment minus $W^{(4)}$ and the three pairings of $W^{(2)}$, to λ^3 : 0 ✓

PerturbativeCorrelationFunction and ConnectedCorrelationFunction compute the moment and the cumulant directly (the same, 0 ✓ and 0 ✓). The four-point function has 3, 7, 28, 120 diagrams at orders $\lambda^0, \dots, \lambda^3$, most of them disconnected: up to first order, the three pairings of free propagators, the same with a tadpole on one line (the first-order part of one $W^{(2)}$), and one connected diagram. Below, all the diagrams to first order and the connected ones to third order:

```

PerturbativeCorrelationFunction[FreeBosonGeneratingFunctional,
  {phi[a], phi[b], phi[c], phi[d]}, Phi4Vertex, 3]
phi4FourPointConnected = ConnectedCorrelationFunction[FreeBosonGeneratingFunctional,
  {phi[a], phi[b], phi[c], phi[d]}, Phi4Vertex, 3]

```

$$\langle \phi_a \phi_b \phi_c \phi_d \rangle =$$

$$\lambda^0 \quad \text{Diagram with two horizontal double lines } a \text{ to } d \text{ and } b \text{ to } c + \text{Diagram with two crossing double lines } a \text{ to } d \text{ and } b \text{ to } c + \text{Diagram with two vertical double lines } a \text{ to } b \text{ and } d \text{ to } c$$

$$\lambda \quad + \text{Diagram with two crossing double lines } a \text{ to } d \text{ and } b \text{ to } c + \frac{1}{2} \text{Diagram with a tadpole on line } a \text{ and a vertical double line } b \text{ to } c + \frac{1}{2} \text{Diagram with a tadpole on line } b \text{ and a vertical double line } a \text{ to } c + \frac{1}{2} \text{Diagram with a tadpole on line } c \text{ and a vertical double line } a \text{ to } b + \frac{1}{2} \text{Diagram with a tadpole on line } d \text{ and a vertical double line } a \text{ to } b + \frac{1}{2} \text{Diagram with a tadpole on line } a \text{ and a vertical double line } c \text{ to } b + \frac{1}{2} \text{Diagram with a tadpole on line } b \text{ and a vertical double line } c \text{ to } d$$

λ

λ^2

λ^3

```
twoParticle = PerturbativeCorrelationFunction[FreeFermionGeneratingFunctional,
  {psi[x1], psibar[x2], psibar[x4], psi[x3]}, CoulombVertex, 1];
```

$$V^0 = \begin{array}{c} x_1 \longleftarrow x_4 \\ x_2 \longrightarrow x_3 \end{array} - \begin{array}{c} x_1 \quad x_4 \\ | \quad | \\ x_2 \quad x_3 \end{array}$$

$$\langle \psi_1 \bar{\psi}_2 \bar{\psi}_4 \psi_3 \rangle = \begin{array}{c} x_1 \longleftarrow x_4 \\ x_2 \longrightarrow x_3 \end{array} - \begin{array}{c} x_1 \\ \downarrow \\ x_2 \end{array} \begin{array}{c} x_4 \\ \downarrow \\ x_3 \end{array} + \langle \psi_1 \bar{\psi}_2 \bar{\psi}_4 \psi_3 \rangle_c$$

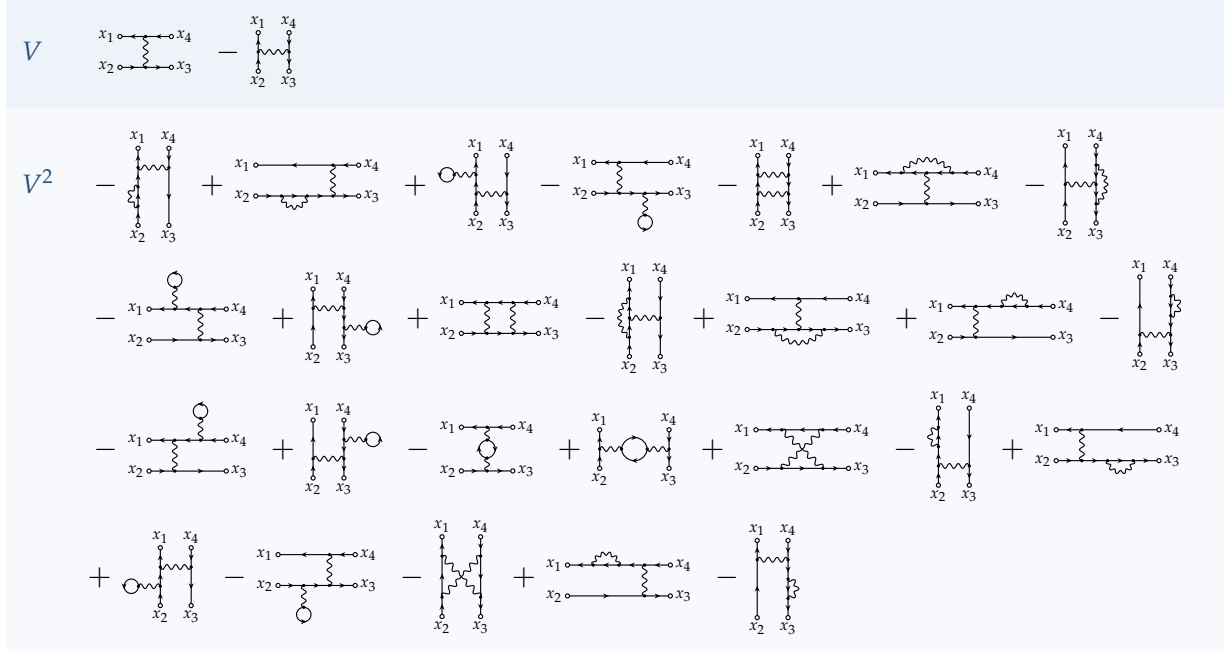
The same derivatives, in η and $\bar{\eta}$, check it to second order, and `ConnectedCorrelationFunction` computes the cumulant directly:

The cumulant minus the connected diagrams of the moment, to V^2 : 0 ✓
 The moment minus the cumulant and the two pairs, to V^2 : 0 ✓
`ConnectedCorrelationFunction` minus the fourth derivative of W , to V^2 : 0 ✓

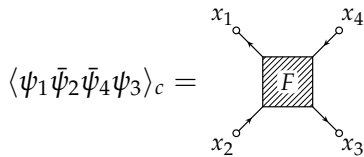
`ConnectedCorrelationFunction` keeps the connected diagrams alone, 2, 26 and 330 at orders V , V^2 and V^3 , drawn here to second order; the free four-point function, the product of two propagators, is not connected and disappears:

```
ConnectedCorrelationFunction[FreeFermionGeneratingFunctional,
  {psi[x1], psibar[x2], psibar[x4], psi[x3]}, CoulombVertex, 3]
```

$$\langle \psi_1 \bar{\psi}_2 \bar{\psi}_4 \psi_3 \rangle_c =$$



The connected part defines the full vertex F (the reducible vertex, or two-particle scattering amplitude), drawn as a hatched square: the connected function is F with its four legs, full propagators G , attached at the corners x_1 (out), x_2 (in), x_3 (out), x_4 (in), counterclockwise from the top left,



F is the connected four-point function with its legs removed: a one-particle-irreducible vertex (section 8.3).

5 The propagator: self-energy and Dyson equation

The connected two-point function is the full propagator G , the Green function (for fermions $G = -\langle T\psi\bar{\psi} \rangle_c$). Its one-particle-irreducible diagrams — those that stay connected when any one propagator line is cut (interaction lines are never cut) — with the external legs removed are the

self-energy Σ (also called the mass operator, or the proper self-energy Σ^* [3]), and the Dyson equation $G = G_0 + G_0 \Sigma G$, that is $G = G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 + \dots$, builds all the diagrams of G from those of Σ . Drawn for fermions, with G as a double line, G_0 as a single line and Σ as a hatched blob (DeclareBlob), the Dyson equation [17, 18] reads

$$x \longleftrightarrow y = x \longrightarrow y + x \longrightarrow \text{hatched blob } \Sigma \longleftarrow y$$

The double line is needed only where G and G_0 appear together: in the relations that contain full propagators alone (the pairs of section 4, the exact equations from section 10 on) G is a plain line. Here Σ is found by cutting the diagrams of G , the textbook definition. The package also generates it as a derivative, and checks it against these diagrams: of the 1PI action, $\Gamma^{(2)} = D_0^{-1} - \Sigma$ for ϕ^4 (section 8.3, checked there against the diagrams below), and, as a functional of the full propagator, of the Luttinger–Ward functional, $\Sigma[G] = \delta\Phi/\delta G$ (section 9.4). For ϕ^4 theory, to third order:

```
phi4SelfEnergy = AmputateExternalLegs[ParticleIrreducibleDiagrams[phi4Propagator, 1,
  {a, b}, {FreePropagator}], {a, b}, {FreePropagator}]
```

$$\Sigma(a, b) =$$

$$\lambda \quad \frac{1}{2} a \text{---} \bigcirc \text{---} b$$

$$\lambda^2 \quad + \frac{1}{6} a \text{---} \bigcirc \text{---} b + \frac{1}{4} a \text{---} \bigcirc \text{---} b$$

$$\lambda^3 \quad + \frac{1}{4} a \text{---} \bigcirc \text{---} b + \frac{1}{4} a \text{---} \bigcirc \text{---} b + \frac{1}{8} a \text{---} \bigcirc \text{---} b + \frac{1}{12} a \text{---} \bigcirc \text{---} b + \frac{1}{8} a \text{---} \bigcirc \text{---} b$$

$$G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 + \dots = G, \text{ to } \lambda^3: 0 \checkmark$$

Fermions. Self-energies and vertices are drawn with short external legs: the fermion enters at y and leaves at x , and the Hartree term, proportional to $\delta(x, y)$, sits on the single point $x = y$.

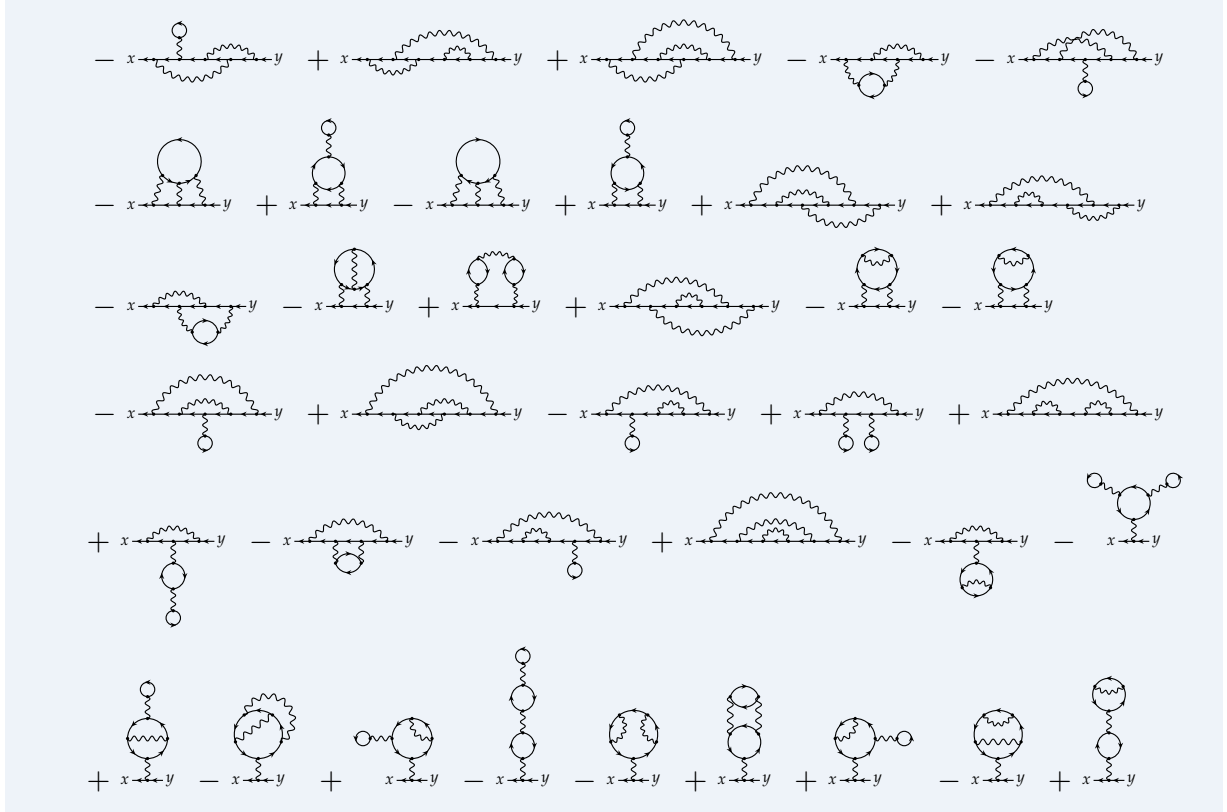
```
selfEnergyPerturbative = AmputateExternalLegs[
  ParticleIrreducibleDiagrams[greenFunction, 1, {x, y}, {BareGreenFunction}],
  {x, y}, {BareGreenFunction}];
```

$$\Sigma(x, y) =$$

$$V \quad x \text{---} \text{wavy line} \text{---} y \quad - \quad x \text{---} \text{wavy line} \text{---} y$$

$$V^2 \quad + \quad x \text{---} \text{wavy line} \text{---} y \quad - \quad x \text{---} \text{wavy line} \text{---} y \quad - \quad x \text{---} \text{wavy line} \text{---} y \quad + \quad x \text{---} \text{wavy line} \text{---} y \quad + \quad x \text{---} \text{wavy line} \text{---} y \quad - \quad x \text{---} \text{wavy line} \text{---} y$$

$$V^3 \quad - \quad x \text{---} \text{wavy line} \text{---} y \quad + \quad x \text{---} \text{wavy line} \text{---} y \quad + \quad x \text{---} \text{wavy line} \text{---} y \quad + \quad x \text{---} \text{wavy line} \text{---} y \quad - \quad x \text{---} \text{wavy line} \text{---} y$$



$G_0 + G_0 \Sigma G_0 + \dots - G$ (DysonSeries), to V^3 : 0 ✓

Of these 2, 6 and 42 diagrams, only 2, 2 and 10 are skeleton diagrams (bold, or dressed, diagrams), without self-energy insertions (SkeletonDiagrams). With the bare lines replaced by the dressed propagator G , they are the self-energy $\Sigma[G]$ of self-consistent approximations, which section 9.4 derives from the Luttinger–Ward functional.

6 Linear response

A weak external field U coupled to the density, $H \rightarrow H + \int d^3r U(\mathbf{r}, t) \rho(\mathbf{r})$, changes the density by $\delta\langle\rho(x)\rangle = \int d^4y \chi^R(x, y) U(y)$ to first order in U , with the retarded response function

$$\chi^R(x, y) = -i\Theta(t_x - t_y) \langle [\rho(x), \rho(y)] \rangle,$$

a correlation function of the unperturbed system (Kubo formula [33, 7, 6]); the current gives in the same way the conductivity, the spin density the magnetic susceptibility. Diagrams compute its imaginary-time version, $\chi(x, y) = \delta\langle\rho(x)\rangle / \delta U(y) = -\langle T\rho(x)\rho(y) \rangle_c$, from which χ^R follows by analytic continuation (section 7). The correlation functions of the package are the time-ordered products themselves: $\langle\rho\rho\rangle_c = -\chi$. The potential enters the bare propagator, $G_0^{-1} \rightarrow G_0^{-1} - U$, so that $\delta G_0(p, q) / \delta U(z) = G_0(p, z) G_0(z, q)$, a rule declared once; FunctionalDerivative then inserts the potential into every line of every diagram of G (section 5), and with the density $\langle\rho(a)\rangle = G(a, a)$, $\langle\rho_a\rho_b\rangle_c = -\delta G(a, a) / \delta U(b)$. The density $\rho(x) = \bar{\psi}(x)\psi(x)$ is a composite operator, and the same function is the connected four-point function with the fields taken pairwise at the same point, which ConnectedCorrelationFunction computes directly (0 ✓). The density vertices are drawn as the crossed circles of the insertion of an external field, and the bubble of two propagators between them as a circle.

```

DeclareSource[LocalPotential]; (* U(z), coupled to the density *)
DeclareFunctionalDerivative[BareGreenFunction[p_, q_], LocalPotential[z_],
  BareGreenFunction[p, z] BareGreenFunction[z, q]];
densityCorrelation = -FunctionalDerivative[OrderPart[greenFunction,
  InteractionPotential, {0, 1}] /. {x -> a, y -> a}, LocalPotential[b]];
(* the same: ConnectedCorrelationFunction[FreeFermionGeneratingFunctional,
  {psibar[a], psi[a], psibar[b], psi[b]}, CoulombVertex, 1] *)
properPart = IrreducibleDiagrams[densityCorrelation, {{a}, {b}}, 1,
  {InteractionPotential}];

```

$$\langle \rho_a \rho_b \rangle_c =$$

$$V^0 \quad - \quad \text{bubble diagram}$$

$$V \quad - \quad \text{Hartree diagram} + \text{Fock diagram} - \text{RPA diagram} + \text{Lindhard diagram} + \text{polarization diagram} - \text{proper part diagram}$$

To zeroth order the correlation function is minus the bubble, $-\chi_0$; to first order it has the vertex correction, the Hartree and Fock self-energy insertions on each of the two lines, and two bubbles joined by an interaction line. This last diagram falls apart, with a and b on different sides, when the interaction line is cut: it is the first term of the RPA series (below), whose bubble χ_0 is, with bare lines, the Lindhard function [34] (section 7). The others form the proper part of $\langle \rho \rho \rangle_c$, that is $-P$, minus the polarization (below), which `IrreducibleDiagrams` selects by cutting interaction lines instead of propagators.

Proper and improper response, and the dielectric function. The distinction has a simple physical meaning. The full, or improper, χ is the response to the external potential U . But the induced density $\delta\rho$ has its own Hartree potential $V\delta\rho$, so the electrons feel the total potential $U_{\text{tot}} = U + V\delta\rho$, and the proper response P is the response to it: $\delta\rho = P U_{\text{tot}}$. In the diagrams, every diagram of χ is a chain of proper parts joined by single interaction lines, each line carrying the Hartree potential of the charge induced on its left; the chain is the equation $\chi = P + PV\chi$, whose last term has the sign $-$ in the picture, where the wavy line stands for $-V$:

$$x \text{---} \chi \text{---} y = x \text{---} P \text{---} y - x \text{---} P \text{---} \chi \text{---} y$$

In momentum space, for a homogeneous system, the chain is a geometric series; with $v_q = 4\pi e^2/q^2$ for the Coulomb interaction (section 2),

$$\chi(q, \omega) = \frac{P(q, \omega)}{1 - v_q P(q, \omega)}, \quad U_{\text{tot}} = \frac{U}{\varepsilon},$$

$$\varepsilon(q, \omega) = 1 - v_q P(q, \omega), \quad \frac{1}{\varepsilon(q, \omega)} = 1 + v_q \chi(q, \omega).$$

ε is the longitudinal dielectric function: an external charge is screened by the charge it induces, and two electrons interact through the screened interaction $v_q/\varepsilon(q, \omega)$ (the W of Hedin's equations, section 14: W is the screened interaction in sections 11, 14 and 15, where it is called so, and $W = \log Z$ everywhere else). Two limits show what it contains. Static and at long wavelength the proper response is minus the compressibility, $P(q \rightarrow 0, 0) = -\partial n/\partial\mu$ ($-N(0)$, the density of states at the Fermi level, for free electrons), so that $\varepsilon = 1 + k_{\text{TF}}^2/q^2$ with $k_{\text{TF}}^2 = 4\pi e^2 \partial n/\partial\mu$: the potential of a charge is screened over the Thomas–Fermi length $1/k_{\text{TF}}$. At long wavelength and finite frequency

$P \rightarrow nq^2/(m\omega^2)$ (see below), so that $\varepsilon = 1 - \omega_p^2/\omega^2$ with $\omega_p^2 = 4\pi ne^2/m$: ε vanishes at the plasma frequency, and the zeros of $\varepsilon(q, \omega)$ are the plasmons, the collective oscillations of the charge. The random-phase approximation (RPA) replaces P by the bubble χ_0 [35, 7, 3]; the diagrams of order V above are its first corrections, exchange and self-energy.

Gauge invariance: density and current response. (Background: nothing in this paragraph is computed; the package checks the Ward identity it rests on in section 9.6.) A scalar potential couples to the density, a vector potential $\mathbf{A}$ to the current. A gauge transformation, $U \rightarrow U - \partial_t \theta$ and $\mathbf{A} \rightarrow \mathbf{A} + \nabla \theta$, does not change the physics, so a pure-gauge field induces neither density nor current; equivalently, the charge is conserved, $\partial_t \rho + \nabla \cdot \mathbf{j} = 0$. Applied to the induced density and current, this fixes the density response by the longitudinal current response [7, 36, 5]:

$$\chi(q, \omega) = \frac{q^2}{\omega^2} \chi_{\parallel}(q, \omega), \quad \chi_{\parallel} = \frac{n}{m} + \chi_{j_{\parallel}j_{\parallel}}^{\text{para}},$$

where $\chi_{\parallel}$, the response of the longitudinal current to a longitudinal $\mathbf{A}$, is the sum of a diamagnetic term n/m , from the $\mathbf{A}^2$ of the kinetic energy, and of the paramagnetic current–current correlation function. Three consequences follow. A static longitudinal $\mathbf{A}$ is a pure gauge, so $\chi_{\parallel}(q, 0) = 0$: the paramagnetic term cancels the diamagnetic one. In a translation-invariant system the total current is the total momentum divided by m , which a two-body interaction conserves, so the paramagnetic term vanishes at long wavelength: $P \rightarrow nq^2/(m\omega^2)$, and the plasma frequency at $q \rightarrow 0$ is exact, not an artefact of the RPA. And the spectrum obeys the f-sum rule $\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \text{Im} \chi^R(q, \omega) = -nq^2/m$. The current response to the total electric field is the conductivity, $\sigma = ie^2 P_{\parallel}/\omega$ for the proper part $P_{\parallel}$ of $\chi_{\parallel}$, so that $\varepsilon = 1 + 4\pi i\sigma/\omega$; for free electrons $\sigma = ine^2/(m\omega)$, Drude’s without collisions. In the diagrams, the continuity equation is a Ward identity (section 9.6): it holds when self-energy insertions and vertex corrections come together, as they do at every order of the expansion above (the Hartree and Fock insertions with the vertex correction) and in the conserving approximations of section 11.2; a bubble of dressed propagators without its vertex corrections violates it, and with it the f-sum rule [37, 38].

ϕ^2 in ϕ^4 theory. In ϕ^4 theory the simplest composite operator is ϕ^2 . Its correlation function is the response to a source coupled to $\frac{1}{2}\phi^2$, a local change of the mass; near a critical point, where m^2 measures the distance from the critical temperature, it is the response to the temperature, and its integral over space gives the specific heat. Section 19 uses the same insertion of $\frac{1}{2}\phi^2$ to renormalize the mass. The source U of $\frac{1}{2}\phi^2$ enters the bare line as $D_0^{-1} \rightarrow D_0^{-1} + U$, so that $\delta D_0(p, q)/\delta U(z) = -D_0(p, z)D_0(z, q)$; since $\delta\langle\phi_a\phi_a\rangle/\delta U(b) = -\frac{1}{2}\langle\phi_a^2\phi_b^2\rangle_c$, the correlation function is $-2\delta G(a, a)/\delta U(b)$, with the propagator `phi4Propagator` of section 3 (and again `ConnectedCorrelationFunction` directly, 0 ✓). It has 2 diagrams at first order — the vertex joining the two bubbles, the first term of a bubble chain, and the tadpole on a line — and 8 at second:

```
DeclareSource[MassSource]; (* U(z), coupled to phi^2/2 *)
DeclareFunctionalDerivative[FreePropagator[p_, q_], MassSource[z_],
  -FreePropagator[p, z] FreePropagator[z, q]];
-2 FunctionalDerivative[OrderPart[phi4Propagator, lambda, {0, 1, 2}] /. b -> a,
  MassSource[b]]
(* the same: ConnectedCorrelationFunction[FreeBosonGeneratingFunctional,
  {phi[a], phi[a], phi[b], phi[b]}, Phi4Vertex, 2] *)
```

$$\langle \phi_a^2 \phi_b^2 \rangle_c =$$

$$\lambda^0 \quad 2 \text{ } a \text{ } \text{---} \text{ } b$$

$$\lambda \quad + \text{ } a \text{ } \text{---} \text{ } b \quad + 2 \text{ } a \text{ } \text{---} \text{ } b$$

$$\lambda^2 \quad + \text{ } a \text{ } \text{---} \text{ } b \quad + \text{ } a \text{ } \text{---} \text{ } b \quad + \text{ } a \text{ } \text{---} \text{ } b \quad + \frac{1}{2} \text{ } a \text{ } \text{---} \text{ } b \quad + \text{ } a \text{ } \text{---} \text{ } b \quad + \frac{2}{3} \text{ } a \text{ } \text{---} \text{ } b \quad + \frac{1}{2} \text{ } a \text{ } \text{---} \text{ } b$$

7 From diagrams to numbers: Matsubara sums and the optical theorem

Every result so far is a sum of integrals over labels. For a system invariant under translations in space and in imaginary time, at a temperature T , the same diagrams become integrals over loop momenta and sums over Matsubara frequencies [25, 2, 3, 5, 6]. The package takes this step too: it routes momenta and frequencies through the lines and carries out the frequency sums, leaving the momentum integrals symbolic.

Imaginary time. At the temperature $T = 1/\beta$ ($\hbar = k_B = 1$, section 2) the thermal averages $\text{tr}[e^{-\beta(H-\mu N)} \dots]/Z$ are path integrals over fields of an imaginary time $\tau \in [0, \beta)$: $e^{-\beta(H-\mu N)}$ evolves the system over the imaginary time β , and the trace closes the path, periodically for bosons, $\phi(\beta) = \phi(0)$, and antiperiodically for fermions, $\psi(\beta) = -\psi(0)$ [4, 8]. The propagators are periodic or antiperiodic too, $G(\tau + \beta) = \pm G(\tau)$, and their Fourier series have discrete frequencies, odd multiples of πT for fermions and even ones for bosons:

$$G(\tau) = T \sum_n e^{-i\omega_n \tau} G(i\omega_n), \quad G(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} G(\tau), \quad \omega_n = (2n+1)\pi T, \quad \nu_m = 2m\pi T.$$

A free electron of energy $\xi_k = \epsilon_k - \mu$, measured from the chemical potential, has $G_0(k, i\omega_n) = 1/(i\omega_n - \xi_k)$. Momentum and frequency are conserved at every vertex, so that every loop of a diagram carries one free momentum, summed as $\sum_p$ (that is $\frac{1}{\mathcal{V}} \sum_p$ for a volume $\mathcal{V}$, or $\int d^d p / (2\pi)^d$ in an infinite system), and one free frequency, summed over n ; the sums give the Fermi and Bose functions $n_F(x) = 1/(e^{\beta x} + 1)$ and $n_B(x) = 1/(e^{\beta x} - 1)$.

Frequency sums. The function $n_F(z)$ has simple poles at $z = i\omega_n$, with residue $-T$, and $n_B(z)$ at $z = i\nu_m$, with residue T . A contour around these poles, opened onto the poles z_j of the summand g , turns the sums into residues [5, 6, 39, 40],

$$T \sum_n g(i\omega_n) = \sum_j \text{Res}_{z=z_j} [g(z) n_F(z)], \quad T \sum_m g(i\nu_m) = - \sum_j \text{Res}_{z=z_j} [g(z) n_B(z)],$$

when g decays faster than $1/|z|$. A single line, $g = 1/(z - \xi)$, decays only as $1/z$, and its sum converges only conditionally. A line closed on itself, or inside the instantaneous vertex, is a propagator at equal times, $G(\tau = 0^-) = \langle \psi^\dagger \psi \rangle$, and the limit $\tau \rightarrow 0^-$ gives the convergence factor $e^{i\omega_n 0^+}$, which makes $g(z) n_F(z) e^{z 0^+}$ decay on both sides of the imaginary axis: $T \sum_n e^{i\omega_n 0^+} / (i\omega_n - \xi) = n_F(\xi)$, the occupation of the level.

`EvaluateMatsubara` routes momenta and frequencies along the lines and sums the loop frequencies one after the other by these formulas. The summand is a rational function: its poles are read from the linear factors of the denominators (a boson propagator with a quadratic denominator is split into two), and its residues, of any order, are Laurent coefficients computed by differentiation.

After each sum the statistical factors are freed of the frequencies still to be summed by periodicity, $n_F(E + i\nu_m) = n_F(E)$ and $n_F(E + i\omega_n) = -n_B(E)$, so that the next summand is again rational. When no line fixes the convergence factor the symmetric sum is taken, with a message; the momentum sums are left as they are. Rules say what the lines are: G_0 for the fermion lines and v_q for the instantaneous interaction (section 2). For electrons of spin $\frac{1}{2}$ the option "SpinDegeneracy" $\rightarrow 2$ gives each closed fermion loop the factor 2 of the sum over spin.

```
DeclareMatsubaraFrequency[w, "Fermion"]; DeclareMatsubaraFrequency[nu, "Boson"];
gasRules = {BareGreenFunction -> {"Fermion", xi},
  InteractionPotential -> {"Instantaneous", v}};
twoPoint = {y -> {k, I w}, x -> {-k, -I w}}; (* k, i w enter at y *)
```

Three orderings. The convergence factor is the ordering of the two operators at equal times [4]. The limit $\tau \rightarrow 0^+$ puts ψ to the left, $G(0^+) = -\langle\psi\psi^\dagger\rangle$, with the factor $e^{-i\omega_n 0^+}$; the mean of the two limits is the symmetric sum, with no factor at all:

$$T \sum_n \frac{e^{i\omega_n 0^+}}{i\omega_n - \xi} = n_F(\xi) = \langle\psi^\dagger\psi\rangle, \quad T \sum_n \frac{e^{-i\omega_n 0^+}}{i\omega_n - \xi} = n_F(\xi) - 1 = -\langle\psi\psi^\dagger\rangle,$$

$$T \sum_n \frac{1}{i\omega_n - \xi} = n_F(\xi) - \frac{1}{2} = \frac{1}{2}\langle[\psi^\dagger, \psi]\rangle,$$

and for bosons, with $1/(i\nu_m - \xi)$, $-n_B(\xi)$, $-n_B(\xi) - 1$ and $-n_B(\xi) - \frac{1}{2} = -\frac{1}{2}\langle\{b^\dagger, b\}\rangle$. A Hamiltonian with every $\psi^\dagger$ to the left, as the interaction $\frac{1}{2} \int V \psi^\dagger \psi^\dagger \psi \psi$ of the electron gas, gives the first. The third belongs to densities written as $\frac{1}{2}[\psi^\dagger, \psi] = n - \frac{1}{2}$, as in the particle-hole symmetric interaction $U(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})$ of a lattice model, where it is the natural choice: the difference, $\frac{1}{2}$ per state, is a shift of the chemical potential. In the continuum the sum over states of that $\frac{1}{2}$ diverges, and $e^{i\omega_n 0^+}$ is the default; the option "ConvergenceFactor" $\rightarrow 1, -1$ or $\emptyset$ of EvaluateMatsubara chooses the ordering of all the lines at equal times. With the symmetric sum the Hartree-Fock self-energy is $\Sigma_{\text{HF}}(k) = \sum_p (2v_0 - v_{k-p})(n_F(\xi_p) - \frac{1}{2})$, a constant away from the one with $n_F(\xi_p)$.

The Lindhard function. The zeroth order of $\langle\rho\rho\rangle_c$ of section 6, minus the bubble χ_0 , with the momentum q and the frequency $i\nu_m$ entering at b :

```
lindhard = EvaluateMatsubara[OrderPart[densityCorrelation, InteractionPotential, \emptyset],
  {b -> {q, I nu}, a -> {-q, -I nu}}, gasRules, "SpinDegeneracy" -> 2,
  "LoopMomenta" -> {p}]
```

$$\langle\rho\rho\rangle_c(q, i\nu_m) = -2 \sum_p \frac{n_F(\xi_p) - n_F(\xi_{p+q})}{i\nu_m + \xi_p - \xi_{p+q}}$$

Since $\langle\rho\rho\rangle_c = -\chi$ (section 6), this is minus the Lindhard function [34], the response of free electrons, $\chi_0(q, i\nu_m) = 2 \sum_p (n_F(\xi_p) - n_F(\xi_{p+q})) / (i\nu_m + \xi_p - \xi_{p+q})$ (0 ✓).

The retarded function $\chi^R(q, \omega)$ that is measured follows from it by analytic continuation. Inserting a complete set of eigenstates (the Lehmann representation) shows that both are values of one function $\chi(z)$, analytic off the real axis: $\chi(i\nu_m)$ at the Matsubara frequencies, and $\chi^R(\omega) = \chi(\omega + i0^+)$ just above the real axis [3, 5, 6]. The values at the Matsubara frequencies determine the function that vanishes at large $|z|$ uniquely [41], but the continuation needs a formula valid off them: $n_F(\xi + i\nu_m) = n_F(\xi)$ holds only at $i\nu_m$. AnalyticContinuation ($i\nu_m \rightarrow \omega$) is therefore applied after the sums, whose statistical factors are already free of the external frequency. RetardedImaginaryPart

then sets $\omega \rightarrow \omega + i0^+$ and takes the imaginary part of every pole,

$$\frac{1}{x + i0^+} = \text{P} \frac{1}{x} - i\pi \delta(x), \quad \text{Im} \frac{1}{(x + i0^+)^k} = -\pi \frac{(-1)^{k-1}}{(k-1)!} \delta^{(k-1)}(x),$$

and `ZeroTemperatureLimit` replaces $n_F(E) \rightarrow \Theta(-E)$ and $n_B(E) \rightarrow -\Theta(-E)$. The imaginary part of a response function is the absorption of energy from the field; here it is the continuum of particle-hole pairs:

```
RetardedImaginaryPart[AnalyticContinuation[lindhard, nu -> omega], omega]
ZeroTemperatureLimit[lindhard]
```

$$\text{Im} \langle \rho \rho \rangle_c^R(q, \omega) = 2\pi \sum_p \delta(\omega + \xi_p - \xi_{p+q}) (n_F(\xi_p) - n_F(\xi_{p+q}))$$

$$\langle \rho \rho \rangle_c(q, i\nu_m) \big|_{T=0} = -2 \sum_p \frac{\Theta(-\xi_p) - \Theta(-\xi_{p+q})}{i\nu_m + \xi_p - \xi_{p+q}}$$

and at $T = 0$, in one dimension and at $\nu_m = 0$, for $\xi_p = (p^2 - k_F^2)/2m$, the integral over p gives minus the static Lindhard function, $-\chi_0(q, 0) = \frac{2m}{\pi q} \log \left| \frac{2k_F + q}{2k_F - q} \right|$, positive since $\chi_0(q, 0) < 0$ (for $k_F = m = 1$ and $q = 0.8$: 0 ✓).

The second-order self-energy. The two skeleton diagrams of the self-energy at order V^2 (section 5), those without self-energy insertions:

```
sigmaSkeleton = SkeletonDiagrams[selfEnergyPerturbative, {x, y}, {BareGreenFunction}];
sigma2 = EvaluateMatsubara[OrderPart[sigmaSkeleton, InteractionPotential, 2],
  twoPoint, gasRules, "SpinDegeneracy" -> 2, "LoopMomenta" -> {p1, p2}]
```

$$\Sigma^{(2)}(k, i\omega_n) = - \sum_{p_1, p_2} \frac{((1 - n_1) n_2 (1 - n_3) + n_1 (1 - n_2) n_3) v_{k-p_1} v_{p_1-p_2}}{i\omega_n - \xi_1 + \xi_2 - \xi_3}$$

$$+ 2 \sum_{p_1, p_2} \frac{((1 - n_1) n_2 (1 - n_3) + n_1 (1 - n_2) n_3) v_{p_1-p_2}^2}{i\omega_n - \xi_1 + \xi_2 - \xi_3}$$

with $\xi_1 = \xi_{p_1}$, $\xi_2 = \xi_{p_2}$, $\xi_3 = \xi_{k-p_1+p_2}$ and $n_i = n_F(\xi_i)$ (option "Names" of `ExpressionToLaTeX`). The first term is the exchange diagram, the second the direct one, whose closed loop gives the factor 2 of spin. Both have the same denominator, the energy of the intermediate state, and the statistical factors come out as a sum over processes: the particle of momentum k goes into two particles (p_1 and $k - p_1 + p_2$, the factors $1 - n_1$ and $1 - n_3$) and a hole (p_2 , the factor n_2), or the reverse ($n_1 n_3 (1 - n_2)$).

The optical theorem. The continued self-energy has $\text{Im} \Sigma^R \leq 0$, and on shell $-2 \text{Im} \Sigma^R$ is the rate at which the particle decays (at $T > 0$, plus the rate of the inverse process): by Fermi's golden rule, 2π times the sum, over the final states of the same energy, of the squared matrix elements of the transitions. For the self-energy above,

$$-2 \text{Im} \Sigma^{(2)R}(k, \omega) = 2\pi \sum_{p_1, p_2} (2v_{p_1-p_2}^2 - v_{k-p_1} v_{p_1-p_2}) \delta(\omega - \xi_1 + \xi_2 - \xi_3)$$

$$\times [(1 - n_1) n_2 (1 - n_3) + n_1 (1 - n_2) n_3],$$

the squared matrix element, direct and exchange, summed over spins, times the factors of the decay into two particles and a hole and of the inverse process. This is the optical theorem, and the

diagrams carry it in the *cutting rules*: cutting a diagram into two parts through lines put on shell gives its imaginary part [42]. At finite temperature every cut line carries the factor of its emission ($1 - n_F$, $1 + n_B$) or absorption (n_F , n_B), and the inverse process, $e^{-\omega/T}$ times as frequent, multiplies the decay rate by $1 + e^{-\omega/T}$ (fermions) [43, 44, 45, 46, 39, 40].

The package computes the imaginary part both ways: from the Matsubara sums, by continuation, and from the cutting rules, which it derives in imaginary time without any frequency sum. The points joined by instantaneous interactions are at one imaginary time and form a *time vertex*; the lines between two time vertices propagate, those inside one are static (at equal times). For $0 < \tau < \beta$ the propagating lines between the time vertex where the external frequency enters, at τ , and the one where it leaves, at 0, form chains, and the diagram is a product of chains, $\mathcal{D}(\tau) = c \prod_k C_k(\tau)$. A chain whose propagators, as a function of the frequency x that flows through it, are $C(x) = \sum_j r_j / (x - E_j)$ is in imaginary time $C(\tau) = -\sum_j r_j (1 \mp n(E_j)) e^{-E_j \tau}$: each line on shell with its emission factor $1 - n_F$ or $1 + n_B$ (a static Hartree or Fock insertion makes a double pole, and a derivative with respect to E_j). The product is a sum of exponentials $e^{-E\tau}$, E the energy of the cut lines; written as $\mathcal{D}(\tau) = -\int dE \mathcal{D}^>(E) e^{-E\tau}$, it gives the rate of the decay, $\mathcal{D}^>(\omega)$, a sum of $\delta(\omega - E)$ times residues and emission factors, and

$$\text{Im } \mathcal{D}^R(\omega) = -\pi \mathcal{D}^>(\omega) (1 \pm e^{-\beta\omega}),$$

the second term (upper sign for fermions) being the inverse process, by detailed balance. The two ways give the same expression,

```
RetardedImaginaryPart[AnalyticContinuation[sigma2, w -> omega], omega]
CuttingRuleImaginaryPart[OrderPart[sigmaSkeleton, InteractionPotential, 2], twoPoint,
  gasRules, w -> omega, "SpinDegeneracy" -> 2, "LoopMomenta" -> {p1, p2}]
```

$$\begin{aligned} \text{Im } \Sigma^{(2)R}(k, \omega) = \\ \pi \sum_{p_1, p_2} \delta(\omega - \xi_1 + \xi_2 - \xi_3) ((1 - n_1) n_2 (1 - n_3) + n_1 (1 - n_2) n_3) v_{k-p_1} v_{p_1-p_2} \\ - 2\pi \sum_{p_1, p_2} \delta(\omega - \xi_1 + \xi_2 - \xi_3) ((1 - n_1) n_2 (1 - n_3) + n_1 (1 - n_2) n_3) v_{p_1-p_2}^2 \end{aligned}$$

residues minus cutting rules, delta function by delta function (CheckCuttingRules), and the two expressions compared: {0, 0} ✓

The cutting rules are implemented for two-point functions whose propagating lines form chains between the time vertex where the external frequency enters and the one where it leaves, with static insertions (Hartree, Fock) on their lines: of the 6 diagrams of $\langle \rho \rho \rangle_c$ at first order they apply to 4, of the perturbative self-energy to all 6 at second order and to 32 of the 42 at third order, 12 of which, sunsets with Hartree and Fock insertions, have an imaginary part. The diagrams left out have a time vertex, besides the two external ones, with four propagating lines: of $\langle \rho \rho \rangle_c$, the vertex correction and the two bubbles joined by an interaction line; of the self-energy at third order, exactly the 10 skeleton diagrams (0 ✓). In a chain every time vertex other than the external ones carries a Hartree or Fock insertion, so no skeleton diagram beyond second order is of the implemented kind. These diagrams need the general circling rules of real-time thermal field theory [45], which are not implemented.

of all these diagrams, those in which the residues and the cutting rules differ: 0 ✓

Double poles. A self-energy insertion on a line puts two equal propagators in a row, a double pole, and the sum gives the derivative of the Fermi function: the residue of $f(z) n_F(z) / (z - \xi)^2$ at ξ is

$f'(\xi) n_F(\xi) + f(\xi) n'_F(\xi)$. The diagrams of the perturbative self-energy at second order that are not skeletons, Hartree and Fock insertions on the lines of the Hartree and Fock diagrams,

```
insertions2 = SimplifyDiagrams[OrderPart[selfEnergyPerturbative - sigmaSkeleton,
    InteractionPotential, 2]];
EvaluateMatsubara[insertions2, twoPoint, gasRules, "SpinDegeneracy" -> 2,
    "LoopMomenta" -> {p1, p2}]
```

$$\Sigma^{(2)} - \Sigma_{\text{skeleton}}^{(2)} = - \text{diagram 1} + \text{diagram 2} + \text{diagram 3} - \text{diagram 4}$$

give

$$\begin{aligned} \Sigma^{(2)}(k, i\omega_n) - \Sigma_{\text{skeleton}}^{(2)} = & \sum_{p_1, p_2} n_2 v_{k-p_1} v_{p_1-p_2} n'_F(\xi_1) - 2 v_0 \sum_{p_1, p_2} n_2 v_{p_1-p_2} n'_F(\xi_1) \\ & - 2 v_0 \sum_{p_1, p_2} n_1 v_{k-p_2} n'_F(\xi_2) + 4 v_0^2 \sum_{p_1, p_2} n_1 n'_F(\xi_2) \end{aligned}$$

the first-order change of the occupations in the Hartree and Fock terms, $n_F(\xi + \Sigma^{(1)}) = n_F(\xi) + \Sigma^{(1)} n'_F(\xi) + \dots$, which the skeleton expansion in the dressed G (section 9.4) takes into account. They are static; in the bubble the same insertions make the imaginary part a sum of derivatives of delta functions, $\delta'(\omega - \epsilon)$ (0 ✓), and the cutting rules follow them.

Numbers. Each of the evaluations of this section is checked against the brute-force sum of its integrand: `DiagramIntegrand` gives the integrand before the sums, a function of the loop frequencies, which is summed over up to 2×40000 frequencies (800×16000 for two frequency sums), with the convergence factors and a Richardson extrapolation in their number (a sum truncated at N frequencies has an error of order $1/N$, which $2S(2N) - S(N)$ removes), at $T = 0.37$, for $\xi_p = p^2/2 - 0.35$, $v_q = 1/(q^2 + 0.6)$ and given momenta:

```
DiagramIntegrand[OrderPart[sigmaSkeleton, InteractionPotential, 2], twoPoint,
    gasRules]
```

relative errors: Lindhard 2×10^{-13} , $\Sigma^{(2)}$ (two frequency sums) 7×10^{-8} , insertions 3×10^{-9} ; errors above 10^{-5} : 0 ✓

8 The 1PI effective action $\Gamma[\bar{\phi}]$

Why a Legendre transform removes diagrams. The logarithm removed the disconnected diagrams: a product of connected pieces is not a new cumulant. A Legendre transform goes one step further. In $\Gamma[\bar{\phi}] = -W[J] + J \cdot \bar{\phi}$ the source is no longer given: it is the function of $\bar{\phi}$ that makes the mean field $\langle \phi \rangle$ equal to $\bar{\phi}$, whatever the interaction does. A one-particle-reducible diagram — two parts joined by a single line — is a part that acts as a source for the other through one propagator, a correction to the mean field; with the mean field fixed, the self-consistent source cancels these parts, and Γ keeps only the one-particle-irreducible diagrams. The same holds one level up: a two-point source K coupled to $\frac{1}{2}\phi\phi$ and chosen so that the connected two-point function equals a prescribed G cancels every self-energy insertion, the parts joined to the rest by two lines, and what is left is the sum of the two-particle-irreducible skeletons, with G on the lines [47, 48, 49, 14]. In general,

once a moment or a cumulant has become a variable, the diagrams that would renormalize it disappear, and its value is fixed by a stationarity condition — the equation of state $\delta\Gamma/\delta\bar{\phi} = J$, the Dyson equation $\delta\Gamma/\delta G = 0$ at zero two-point source K . This section and the next show the two levels, each for ϕ^4 theory and for the electron gas; section 15 adds a third variable, the screened interaction.

The definition. This Legendre transform of W , with the mean field $\bar{\phi} = \delta W/\delta J = \langle\phi\rangle$, is the 1PI effective action [50, 47] [12, sections 7.5 and 7.8] [13, section 16.1] — the quantum effective action, or generating functional of the vertex functions; in statistical physics, the free energy as a function of the order parameter. Like W , it is defined exactly, at any strength of the interaction; the diagrams are its expansion in the interaction, one way of evaluating it. The expectation value of the field at zero source is a stationary point of the effective action, $\delta\Gamma/\delta\bar{\phi} = J = 0$, not of the action S , whose stationary point is the classical field, and its value there is $-\log Z$. Its second derivative is the inverse full propagator, $\Gamma^{(2)} = G^{-1} = G_0^{-1} - \Sigma$ — the Dyson equation — and its higher derivatives $\Gamma^{(n)}$ are the one-particle-irreducible vertices (section 8.3).

Its pieces. Shifting the field by the mean field, $\phi \rightarrow \bar{\phi} + \phi$, turns S_{int} into vertices of every degree in the fluctuation ϕ : the number $S_{\text{int}}[\bar{\phi}]$; a linear vertex, cancelled by the source; a vertex of degree two, which adds to the inverse propagator, $D^{-1}[\bar{\phi}] = D_0^{-1} + S''_{\text{int}}[\bar{\phi}] = S''[\bar{\phi}]$, the fluctuation operator in the background; and the vertices of degree three or more. Then

$$\Gamma[\bar{\phi}] = S[\bar{\phi}] + \frac{1}{2}\text{Tr} \ln D^{-1}[\bar{\phi}] - (\text{1PI vacuum diagrams in the background}),$$

with the lines $D[\bar{\phi}]$ and the vertices of degree three or more. The three pieces are the orders of the loop expansion, the number of loops ℓ being the power of $\hbar$: the tree $\Gamma^{[0]} = S[\bar{\phi}]$, the classical action; the one loop $\Gamma^{[1]} = \frac{1}{2}\text{Tr} \ln D^{-1}[\bar{\phi}]$, at constant $\bar{\phi}$ the volume times the effective potential of Coleman and Weinberg [51]; and the vacuum diagrams, $\Gamma^{[\ell]}$ with $\ell \geq 2$. `EffectiveAction1PI` writes it with the lines $D[\bar{\phi}]$ (double lines), whose derivative $\delta D/\delta\bar{\phi} = -D S'''_{\text{int}}[\bar{\phi}] D$ is declared, so that the vertex functions follow by differentiation; for ϕ^4 (computed to third order, shown here to the second):

```
gamma1PI = EffectiveAction1PI[FreeBosonGeneratingFunctional, Phi4Vertex, 3,
  phi -> phiMean, FreePropagator -> BackgroundPropagator];
```

$$\begin{aligned} \Gamma[\bar{\phi}] = & \frac{1}{8} \lambda \int_{z_1} D(z_1, z_1)^2 - \frac{1}{48} \lambda^2 \int_{z_1 z_2} D(z_1, z_2)^4 - \frac{1}{16} \lambda^2 \int_{z_1 z_2} D(z_1, z_1) D(z_1, z_2)^2 D(z_2, z_2) \\ & + \frac{1}{24} \lambda \int_{z_1} \bar{\phi}(z_1)^4 - \frac{1}{12} \lambda^2 \int_{z_1 z_2} D(z_1, z_2)^3 \bar{\phi}(z_1) \bar{\phi}(z_2) + \frac{1}{2} \int_{z_1 z_2} \bar{\phi}(z_1) \bar{\phi}(z_2) D_0^{-1}(z_1, z_2) \\ & + \frac{1}{2} \text{Tr} \ln (D^{-1}) \end{aligned}$$

8.1 ϕ^4 theory to λ^3

In ϕ^4 theory the shift turns $S_{\text{int}} = \frac{\lambda}{24} \int \phi^4$ into $S_{\text{int}}[\bar{\phi}]$, the linear vertex, the mass $\lambda\bar{\phi}^2\phi^2/4$ in the background, $D^{-1}[\bar{\phi}] = D_0^{-1} + \lambda\bar{\phi}^2/2$, and the vertices $\lambda\bar{\phi}\phi^3/6$ and $\lambda\phi^4/24$. In the pictures the mean field is a crossed circle at the end of a short line, and every vertex stands for $-\lambda$. Expanded in the bare propagator D_0 , the logarithm is a series of rings and every line $D[\bar{\phi}]$ a chain of mass insertions:

```
ExpandTrace[gamma1PI /. BackgroundPropagator -> Power[Power[FreePropagator, -1] -
  LabelFunction[-lambda/2 phiMean[a]^2 DeltaFunction[a, b], {a, b}], -1],
  FreePropagator, 3, "MaximumOrder" -> {lambda, 3}]
```

The same series comes directly with bare lines, `FreePropagator -> FreePropagator`: the mass insertion then stays a vertex of degree two. At the orders λ , λ^2 and λ^3 there are 3, 5, 13 diagrams. A mass insertion does not change the number of loops, so that grouping the diagrams by L gives the pieces: the tree, $S[\bar{\phi}] = \frac{1}{2} \int \bar{\phi} D_0^{-1} \bar{\phi} + S_{\text{int}}[\bar{\phi}]$, the one loop, the rings of insertions $\bar{\phi}^2$, and the 1PI vacuum diagrams with two, three and four loops in the background:

$$S_{\text{int}}[\bar{\phi}] = -\frac{1}{24} \text{diagram}$$

$$\frac{1}{2} \text{Tr} \ln D^{-1}[\bar{\phi}] - \frac{1}{2} \text{Tr} \ln D_0^{-1} = -\frac{1}{4} \text{diagram} - \frac{1}{16} \text{diagram} - \frac{1}{48} \text{diagram}$$

$$\Gamma^{[2]} =$$

$$\lambda \quad -\frac{1}{8} \text{diagram}$$

$$\lambda^2 \quad -\frac{1}{12} \text{diagram} - \frac{1}{8} \text{diagram}$$

$$\lambda^3 \quad -\frac{1}{8} \text{diagram} - \frac{1}{32} \text{diagram} - \frac{1}{16} \text{diagram}$$

$$\Gamma^{[3]} =$$

$$\lambda^2 \quad -\frac{1}{48} \text{diagram} - \frac{1}{16} \text{diagram}$$

$$\lambda^3 \quad -\frac{1}{8} \text{diagram} - \frac{1}{8} \text{diagram} - \frac{1}{24} \text{diagram} - \frac{1}{16} \text{diagram} - \frac{1}{16} \text{diagram}$$

$$\Gamma^{[4]} =$$

$$\lambda^3 \quad -\frac{1}{48} \text{diagram} - \frac{1}{32} \text{diagram} - \frac{1}{24} \text{diagram} - \frac{1}{48} \text{diagram}$$

Up to the overall sign, the orders λ and λ^2 are Fig. 2 of Eckhardt, Kappl, Kauch and Held [52], whose Λ_1 is $-\Gamma[\bar{\phi}]$. Of the three-loop diagrams at λ^2 the basketball is 2PI, the chain of three bubbles only 1PI: the 2PI action of section 9 has the first among its diagrams and generates the second by dressing its lines (section 9.3).

in zero dimensions ($D_0 = 1$): $\Gamma[\bar{\phi}] + \log Z(J) - J\bar{\phi}$, $Z(J) = \int \frac{d\phi}{\sqrt{2\pi}} e^{-\phi^2/2 - \lambda\phi^4/24 + J\phi}$ 0 ✓
 the diagrams minus their 1PI part; $\Gamma^{[1]}$ minus the rings of $\frac{1}{2} \text{Tr} \ln(D_0^{-1} + \lambda\bar{\phi}^2/2)$ {0, 0} ✓
 the bare lines D_0 minus the lines $D[\bar{\phi}]$ expanded in D_0 , orders 0 to 3 {0, 0, 0, 0} ✓

8.2 The electron gas to V^3

For fermions the sources $\bar{\eta}$, η couple to ψ and $\bar{\psi}$, and the means $\Psi = \langle \psi \rangle$ and $\bar{\Psi} = \langle \bar{\psi} \rangle$ are Grassmann-odd. The action is even in the fields, so that an odd expectation value vanishes at

zero source: the means are variables to be differentiated, and the physical point is $\Psi = \bar{\Psi} = 0$, where $\Gamma = -\log Z$. The shift $\psi \rightarrow \Psi + \psi$, $\bar{\psi} \rightarrow \bar{\Psi} + \bar{\psi}$ turns $S_{\text{int}} = \frac{1}{2} \int V \bar{\psi} \psi \psi \psi$ into $S_{\text{int}}[\bar{\Psi}, \Psi]$, four means on one interaction line, vertices with three means and one fluctuation (cancelled by the source), vertices of degree two, and vertices of degree three (one mean) and four. The vertices of degree two are of two kinds: normal, $V \bar{\Psi} \Psi \bar{\psi} \psi$, the Hartree and Fock potentials of the means, and anomalous, $V \Psi \Psi \bar{\psi} \bar{\psi}$ and $V \bar{\Psi} \bar{\Psi} \psi \psi$, which create or destroy two fermions. Because of these the fluctuation operator in the background mixes ψ and $\bar{\psi}$, as in the Nambu–Gor’kov formalism, and its inverse is not one directed line but a Nambu matrix, with anomalous parts (section 13). `EffectiveAction1PI` therefore keeps the bare lines and the vertices of degree two:

$$\Gamma[\bar{\Psi}, \Psi] = -\bar{\Psi} G_0^{-1} \Psi + S_{\text{int}}[\bar{\Psi}, \Psi] - \text{Tr} \ln(-G_0^{-1}) - (\text{1PI vacuum diagrams}),$$

with the lines G_0 and the vertices of degree two or more: the form of the ϕ^4 series with bare lines.

```
gammaPsi1PI = EffectiveAction1PI[FreeFermionGeneratingFunctional, CoulombVertex, 3,
  {psi -> MeanPsi, psibar -> MeanPsibar}, BareGreenFunction -> BareGreenFunction];
```

The pieces are again the orders in the loops, $\ell = (\text{fermion lines}) - (\text{interaction lines}) + 1$: the tree $-\bar{\Psi} G_0^{-1} \Psi + S_{\text{int}}[\bar{\Psi}, \Psi]$; the one loop, the logarithm of the fluctuation operator in the background (a supertrace over its Nambu components), which expanded in G_0 is $-\text{Tr} \ln(-G_0^{-1})$ and the rings of the vertices of degree two, normal and anomalous; and the 1PI vacuum diagrams with two or more loops. A mean is a crossed circle at the end of a short fermion line, the means taken in the canonical order of section 1, every Ψ before every $\bar{\Psi}$ (so that $S_{\text{int}}[\bar{\Psi}, \Psi] = \frac{1}{2} \int_{x,y} V(x,y) \bar{\Psi}(x) \bar{\Psi}(y) \Psi(y) \Psi(x) - \frac{1}{2} \int_{x,y} V(x,y) \Psi(x) \Psi(y) \bar{\Psi}(x) \bar{\Psi}(y)$), and every interaction line stands for $-V$:

$$S_{\text{int}}[\bar{\Psi}, \Psi] = \frac{1}{2} \text{diagram}$$

$$\Gamma^{[1]} + \text{Tr} \ln(-G_0^{-1}) =$$

$$V - \text{diagram} + \text{diagram}$$

$$V^2 + \frac{1}{2} \text{diagram} + \text{diagram} - \frac{1}{2} \text{diagram} + \frac{1}{2} \text{diagram}$$

$$V^3 + \text{diagram} + \frac{1}{3} \text{diagram} + \text{diagram} - \frac{1}{3} \text{diagram} + \text{diagram} + \text{diagram}$$

$$\Gamma^{[2]} =$$

$$V \frac{1}{2} \text{diagram} - \frac{1}{2} \text{diagram}$$

$$V^2 - \text{diagram} + \text{diagram} - \text{diagram} + \text{diagram} + \text{diagram} - \text{diagram}$$

$\Gamma^{[3]} =$

$$V^2 \quad \frac{1}{4} \text{ (Hartree)} + \frac{1}{2} \text{ (Fock)} - \frac{1}{4} \text{ (ring)} + \frac{1}{2} \text{ (particle-particle pair)} - \text{ (vacuum diagram)}$$

At V the two-loop diagrams are the Hartree and Fock vacuum diagrams, without means; at V^2 the ring with two anomalous vertices is the particle–particle pair of the means. At V^3 the four pieces with one to four loops have 6, 35, 42 and 20 diagrams, 103 in all (5 at V , 15 at V^2). At zero means only the vacuum diagrams without means are left, and they are all the connected vacuum diagrams: a fermion line cannot be a bridge, since it would carry one fermion from one part to the other. With a single Grassmann pair the interaction vanishes, so there is no zero-dimensional check; the checks are the vertex functions of section 8.3:

the diagrams minus their 1PI part	0 ✓
$\Gamma[0,0] + \text{Tr} \ln(-G_0^{-1}) + (\text{connected vacuum diagrams})$	0 ✓
$\delta^2 \Gamma / \delta \bar{\Psi}(x) \delta \Psi(y) _0 - G_0^{-1} + \Sigma$, the perturbative Σ of section 5, orders 0 to 3	{0, 0, 0, 0} ✓
$\delta^4 \Gamma / \delta \bar{\Psi}(x_1) \delta \Psi(x_2) \delta \bar{\Psi}(x_3) \delta \Psi(x_4) _0 - F$, bare lines, orders 1 and 2	{0, 0} ✓

8.3 The vertex functions and the trees

The derivatives of $\Gamma[\bar{\phi}]$ with respect to the mean field are the vertex functions. The first, at zero source, is the equation of the mean field; differentiating the lines $D[\bar{\phi}]$ through their declared derivative, for ϕ^4 :

$$\frac{\delta \Gamma}{\delta \bar{\phi}(a)} - \frac{\delta S}{\delta \bar{\phi}(a)} =$$

$$\lambda - \frac{1}{2} a \text{ (self-energy)}$$

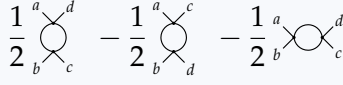
$$\lambda^2 - \frac{1}{6} a \text{ (triangle)} - \frac{1}{4} a \text{ (bubble)}$$

At $\bar{\phi} = 0$, where the lines $D[\bar{\phi}]$ are D_0 , the second derivative is $\Gamma^{(2)} = D_0^{-1} - \Sigma$, and the fourth the 1PI four-point vertex; to λ^3 (a derivative of the lines brings a coupling, so that the derivatives hold terms of higher orders, not all of them complete):

```
atZero[e_] := ExpandTrace[SetSourcesToZero[e]] /.
  BackgroundPropagator -> FreePropagator;
sigma1PI = OrderPart[OperatorKernel[Power[FreePropagator, -1]][a, b] - atZero[
  FunctionalDerivative[gamma1PI, phiMean[a], phiMean[b]]], lambda, {1, 2, 3}];
gamma4 = atZero[OrderPart[FunctionalDerivative[gamma1PI, phiMean[a], phiMean[b],
  phiMean[c], phiMean[d]], lambda, {1, 2, 3}]];
```

$$\Gamma^{(4)} =$$

$$\lambda -$$


$$\lambda^2 - \frac{1}{2} \text{ (diagram)} - \frac{1}{2} \text{ (diagram)} - \frac{1}{2} \text{ (diagram)}$$


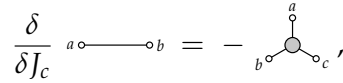
$\Gamma^{(2)} = D_0^{-1} - \Sigma$, Σ cut out of the propagator (section 5), orders 0 to 3	$\{0, 0, 0, 0\}$ ✓
$\Gamma^{(4)} = -(\text{amputated 1PI part of the connected four-point function})$, orders 1 to 3	$\{0, 0, 0\}$ ✓

For the electron gas the second derivative at zero means, $\delta^2 \Gamma / \delta \bar{\Psi} \delta \Psi$ (the rightmost derivative first), is $G_0^{-1} - \Sigma$ and the fourth the full vertex F (section 8.2).

Conversely, the connected functions are *trees* of full propagators and 1PI vertices: the tree expansion. Three differentiation rules, which follow from the Legendre transform, generate the trees one leg at a time, by differentiating with respect to the source (in graphical form, e.g. [53], section 5.6). At any source, let $\bar{\phi} = \delta W / \delta J$ be the mean field, $G = \delta^2 W / \delta J \delta J$ the full propagator and $\Gamma^{(n)} = \delta^n \Gamma / \delta \bar{\phi}^n$ the vertices, at $\bar{\phi} = \bar{\phi}[J]$; with a sum over repeated labels,

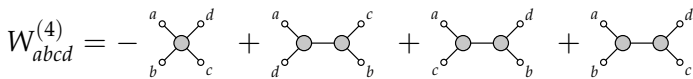
$$(R1) \quad \frac{\delta \bar{\phi}_a}{\delta J_b} = G_{ab}, \quad (R2) \quad \frac{\delta G_{ab}}{\delta J_c} = -G_{aa'} G_{bb'} G_{cc'} \Gamma_{a'b'c'}^{(3)}, \quad (R3) \quad \frac{\delta \Gamma_{a_1 \dots a_n}^{(n)}}{\delta J_b} = \Gamma_{a_1 \dots a_n c}^{(n+1)} G_{cb}.$$

(R1) is the definition of G ; (R3) is the chain rule together with (R1); (R2) follows from $\delta G = -G \delta(G^{-1}) G$, since $G^{-1} = \Gamma^{(2)}$, and (R3). In pictures, with lines G and grey blobs $\Gamma^{(n)}$: differentiating a line inserts a three-vertex that carries the new leg (R2),

$$\frac{\delta}{\delta J_c} a \text{---} b = - \text{ (diagram) },$$


and differentiating a vertex adds the new leg to it (R3). The rules are declared to the engine once, and the trees follow by differentiating the propagator:

```
DeclareSource[ExternalSource]; DeclareSymmetric[FullPropagator, VertexFunction];
DeclareFunctionalDerivative[MeanField[a_], ExternalSource[b_], FullPropagator[a, b]];
DeclareFunctionalDerivative[FullPropagator[a_, b_], ExternalSource[c_],
  -IntegralOver[FullPropagator[a, x] FullPropagator[b, y] FullPropagator[c, z]
    VertexFunction[x, y, z], {x, y, z}]];
DeclareFunctionalDerivative[VertexFunction[as_], ExternalSource[b_],
  IntegralOver[VertexFunction[as, x] FullPropagator[x, b], {x}]];
FunctionalDerivative[FullPropagator[c, d], ExternalSource[a], ExternalSource[b]]
```

$$W_{abcd}^{(4)} = - \text{ (diagram)} + \text{ (diagram)} + \text{ (diagram)} + \text{ (diagram)}$$


The first tree comes from (R3) applied to the vertex of $W^{(3)}$, the other three from (R2) applied to its three lines; they are the three two-particle channels, the three ways of dividing the four legs into two pairs (section 8.4). Every tree is generated exactly once — removing the last leaf of a tree with $n + 1$ leaves gives a unique tree with n leaves, from which (R2) or (R3) recovers it — so that all the weights are ± 1 , the sign being $(-1)^{\text{number of vertices}}$, and there are no symmetry factors.

All the trees up to six points. Integrating over the external labels identifies the trees that differ only by their labels, and the canonical form counts them:

```
W6 = FunctionalDerivative[FullPropagator[x5, x6], ExternalSource[x1],
  ExternalSource[x2],
  ExternalSource[x3], ExternalSource[x4]];
SimplifyDiagrams[IntegralOver[W6, {x1, x2, x3, x4, x5, x6}]]
```

Each picture stands for the sum over the inequivalent ways of attaching the labels to its legs, and the number in front counts them:

$W^{(n)} =$

$$n = 3 - \text{diagram}$$

$$n = 4 - \text{diagram} + 3 \text{diagram}$$

$$n = 5 - \text{diagram} + 10 \text{diagram} - 15 \text{diagram}$$

$$n = 6 - \text{diagram} + 10 \text{diagram} + 15 \text{diagram} - 45 \text{diagram} - 60 \text{diagram} + 90 \text{diagram} + 15 \text{diagram}$$

In all, $W^{(3)}, \dots, W^{(6)}$ have 1, 4, 26 and 236 trees: the trees with n labelled leaves and no vertex of two lines, whose numbers are the terms $a(n-1)$ of Schröder's fourth problem [54, 55]. For $n = 6$: $\Gamma^{(6)}$ itself, $\binom{6}{2} = 15$ choices of the two legs of $\Gamma^{(3)}$ in $\Gamma^{(5)}\Gamma^{(3)}$, $\frac{1}{2}\binom{6}{3} = 10$ splittings into two triples, 45 and 60 trees of three vertices with $\Gamma^{(4)}$ in the middle or at one end, 90 chains and 15 stars of four $\Gamma^{(3)}$: $1 + 15 + 10 + 45 + 60 + 90 + 15 = 236$. In zero dimensions, where $W^{(n)} = (G d/d\bar{\phi})^{n-2} G$ with $G = 1/\Gamma^{(2)}(\bar{\phi})$, forgetting the labels gives

$$W^{(6)} = 105 G^9 \Gamma^{(3)4} - 105 G^8 \Gamma^{(3)2} \Gamma^{(4)} + 10 G^7 \Gamma^{(4)2} + 15 G^7 \Gamma^{(3)} \Gamma^{(5)} - G^6 \Gamma^{(6)},$$

and the package checks that the trees reproduce these derivatives for $n = 3, \dots, 6$:

residuals of $W^{(n)} - (G d/d\bar{\phi})^{n-2} G$ in zero dimensions, $n = 3, \dots, 6$: $\{0, 0, 0, 0\}$ ✓

ConnectedFunctionFromVertices[{x1, ..., xn}] declares these rules and returns the same trees (0 ✓).

A check against perturbation theory. In ϕ^4 theory $\Gamma^{(3)} = \Gamma^{(5)} = 0$ by symmetry and $\Gamma^{(4)} = \lambda + O(\lambda^2)$, a point vertex: the trees of $W^{(6)}$ made of two $\Gamma^{(4)}$ are of order λ^2 , and at this order there is no one-particle-irreducible six-point diagram. The 10 diagrams of the connected six-point function at order λ^2 are exactly these ten trees:

$W^{(6)}$ of ϕ^4 theory at λ^2 , minus the trees $G^7 \Gamma^{(4)} \Gamma^{(4)}$ with $G = D_0$, $\Gamma^{(4)} = \lambda$: 0 ✓

Fermion lines. For fermions the same trees are made of directed lines, the propagator $G = -\langle \psi \bar{\psi} \rangle$, and of vertices with as many outgoing as incoming legs, $\Gamma^{(2n)}(\text{out}_1 \dots \text{out}_n; \text{in}_1 \dots \text{in}_n)$, antisymmetric in each group. They are obtained from the trees of a superfield $\psi = (\psi, \bar{\psi})$ [56, 57] — graded rules, antisymmetric propagator and vertices, "Fermion" — by projecting every line and every vertex on the components ψ and $\bar{\psi}$, with the signs of the permutations:

```
ConnectedFunctionFromVertices[{x1, x2, x3, x4, x5, x6}, "FermionLines"]
```

gives $\langle \psi_1 \bar{\psi}_2 \psi_3 \bar{\psi}_4 \psi_5 \bar{\psi}_6 \rangle_c$. $W^{(4)}$ is one tree and $W^{(6)}$ has 10: $\Gamma^{(6)}$, and nine trees of two $\Gamma^{(4)}$ joined by a fermion line, each with the sign of the permutation of its legs:

$$W^{(4)} = \text{Diagram: A central vertex with four legs labeled } x_1, x_2, x_3, x_4 \text{ in a cross pattern.}$$

$$W^{(6)} = - \text{Diagram 1} + \text{Diagram 2} - \text{Diagram 3} + \text{Diagram 4} - \text{Diagram 5} + \text{Diagram 6} \\ - \text{Diagram 7} + \text{Diagram 8} - \text{Diagram 9} + \text{Diagram 10}$$

The diagrams represent various permutations of two four-point vertices connected by a fermion line. Each diagram has six external legs labeled x_1 through x_6 .

In the electron gas $\Gamma^{(4)}$ is, at first order, the bare vertex (direct minus exchange), and the 36 diagrams of the connected six-point function at second order are exactly the nine trees:

$W^{(6)}$ of the electron gas at V^2 , minus the trees $G^7 \Gamma^{(4)} \Gamma^{(4)}$ with $G = G_0$ and the bare $\Gamma^{(4)}$: 0 ✓

8.4 The four-point vertex

The four legs of a four-point function can be divided into two pairs in three ways, the two-particle channels; a diagram belongs to a channel when two of its lines join one pair of legs to the other (section 12 makes this precise). For bosons the channels are s ($ab|cd$), t ($ac|bd$) and u ($ad|bc$), named after the Mandelstam variables, the squared momenta $(p_a + p_b)^2$, $(p_a + p_c)^2$ and $(p_a + p_d)^2$ that flow through the two lines (all momenta incoming). For fermions, with x_1, x_3 outgoing and x_2, x_4 incoming, they are named after what the two lines carry: the particle-hole channel ph ($x_1 x_2 | x_3 x_4$), the transverse particle-hole channel $\bar{ph}$ ($x_1 x_4 | x_3 x_2$) and the particle-particle channel pp ($x_1 x_3 | x_2 x_4$); with the legs in the order x_1, x_2, x_3, x_4 the pairings of s, t, u are those of $ph, pp, \bar{ph}$, the correspondence that the superfield of section 13 uses. Each has its physics [58]: for an interaction between densities the bubble chains of ph screen it and carry the plasmons (the random-phase approximation; with exchange, time-dependent Hartree-Fock, section 11.2), the ladders of $\bar{ph}$ describe a particle and a hole that scatter repeatedly (bound into excitons in an insulator), and those of pp two particles that scatter repeatedly (the T -matrix) or bind into Cooper pairs.

The four-point vertex is the fourth derivative of Γ at zero means (sections 8.2 and 8.3): $\Gamma^{(4)} = \delta^4 \Gamma / \delta \phi^4$ for real bosons, and for fermions the full vertex $F = \delta^4 \Gamma / \delta \bar{\Psi} \delta \Psi \delta \bar{\Psi} \delta \Psi$. Written with the dressed propagator, it is the sum of the skeleton diagrams of these derivatives, with $G_0 \rightarrow G$ (SkeletonDiagrams). For ϕ^4 theory, to two loops, $\Gamma^{(4)}$ has one bubble in each of the channels s, t and u at one loop and 9 diagrams at two loops:

```
vertexPhi4 = SkeletonDiagrams[gamma4, {a, b, c, d}, {FreePropagator}] /.
  FreePropagator -> DressedPropagator;
(* the same: PerturbativeFullVertex[FreeBosonGeneratingFunctional, Phi4Vertex, 3,
  {phi}, {a, b, c, d}, FreePropagator -> DressedPropagator] *)
```

$\Gamma^{(4)} =$

$$\begin{aligned}
\lambda & - \text{diagram: } \begin{array}{c} a \\ \diagup \quad \diagdown \\ b \quad c \end{array} \\
\lambda^2 & - \frac{1}{2} \text{diagram: } \begin{array}{c} a \quad d \\ \diagup \quad \diagdown \\ b \quad c \end{array} - \frac{1}{2} \text{diagram: } \begin{array}{c} a \quad c \\ \diagup \quad \diagdown \\ b \quad d \end{array} - \frac{1}{2} \text{diagram: } \begin{array}{c} a \quad d \\ \diagup \quad \diagdown \\ b \quad c \end{array} \\
\lambda^3 & - \frac{1}{2} \text{diagram: } \begin{array}{c} a \quad d \\ \diagup \quad \diagdown \\ b \quad c \end{array} - \frac{1}{2} \text{diagram: } \begin{array}{c} a \quad c \\ \diagup \quad \diagdown \\ b \quad d \end{array} - \frac{1}{2} \text{diagram: } \begin{array}{c} a \quad d \\ \diagup \quad \diagdown \\ b \quad c \end{array} - \frac{1}{2} \text{diagram: } \begin{array}{c} a \quad d \\ \diagup \quad \diagdown \\ b \quad c \end{array} - \frac{1}{2} \text{diagram: } \begin{array}{c} a \quad c \\ \diagup \quad \diagdown \\ b \quad d \end{array} - \frac{1}{2} \text{diagram: } \begin{array}{c} a \quad d \\ \diagup \quad \diagdown \\ b \quad c \end{array} - \frac{1}{4} \text{diagram: } \begin{array}{c} a \quad d \\ \diagup \quad \diagdown \\ b \quad c \end{array} - \frac{1}{4} \text{diagram: } \begin{array}{c} a \quad c \\ \diagup \quad \diagdown \\ b \quad d \end{array} \\
& - \frac{1}{4} \text{diagram: } \begin{array}{c} a \quad d \\ \diagup \quad \diagdown \\ b \quad c \end{array}
\end{aligned}$$

For fermions it is the full vertex F of section 4, the fourth derivative of the action $\Gamma[\bar{\Psi}, \Psi]$ of section 8.2 (the rightmost derivative first), with the dressed propagator, here to second order (section 10 checks the Bethe–Salpeter equation with it to the third, where it has 82 diagrams):

```

fullVertex = SkeletonDiagrams[SetSourcesToZero[FunctionalDerivative[gammaPsi1PI,
  MeanPsiBar[x1], MeanPsi[x2], MeanPsiBar[x3], MeanPsi[x4]]], {x1, x2, x3, x4},
  {BareGreenFunction}] /. BareGreenFunction -> DressedGreenFunction;
(* the same: PerturbativeFullVertex[FreeFermionGeneratingFunctional, CoulombVertex, 3,
  {psi, psiBar}, {x1, x2, x3, x4}, BareGreenFunction -> DressedGreenFunction] *)

```

 $F =$

$$\begin{aligned}
V & \text{diagram: } \begin{array}{c} x_1 \quad x_4 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} \\
V^2 & - \text{diagram: } \begin{array}{c} x_1 \quad x_4 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} + \text{diagram: } \begin{array}{c} x_1 \quad x_4 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} - \text{diagram: } \begin{array}{c} x_1 \quad x_4 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} + \text{diagram: } \begin{array}{c} x_1 \quad x_4 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} - \text{diagram: } \begin{array}{c} x_1 \quad x_4 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} + \text{diagram: } \begin{array}{c} x_1 \quad x_4 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} + \text{diagram: } \begin{array}{c} x_1 \quad x_4 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} \\
& - \text{diagram: } \begin{array}{c} x_1 \quad x_4 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} - \text{diagram: } \begin{array}{c} x_1 \quad x_4 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} + \text{diagram: } \begin{array}{c} x_1 \quad x_4 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array}
\end{aligned}$$

Since the derivatives of W are trees of G and of these vertices, the same objects are the connected four-point functions with their legs removed ($\Gamma^{(4)} = -(\text{amputated connected four-point function})$ for real bosons; for fermions, whose tree rules come with the signs of the Grassmann derivatives, section 8.3, F is the amputated connected function itself), which is how `PerturbativeFullVertex` computes them, directly from the generating functional:

`PerturbativeFullVertex` minus these skeletons, ϕ^4 to λ^3 and electrons to V^3 : 0 ✓, 0 ✓

9 The 2PI effective action $\Gamma[\bar{\phi}, G]$

The definition. A two-point source $K(x, y)$ coupled to $\frac{1}{2}\phi(x)\phi(y)$, added to the one-point source J , and the Legendre transform of $W[J, K]$ with respect to both make the full propagator itself a variable (the conjugate of K is $\frac{1}{2}\langle\phi\phi\rangle = \frac{1}{2}(G + \bar{\phi}\bar{\phi})$, so that the variables are $\bar{\phi}$ and the connected G):

$$\Gamma[\bar{\phi}, G] = S[\bar{\phi}] + \frac{1}{2}\text{Tr} \ln G^{-1} + \frac{1}{2}\text{Tr}(D^{-1}[\bar{\phi}] G - 1) + \Gamma_2[\bar{\phi}, G],$$

with $D^{-1}[\bar{\phi}] = S''[\bar{\phi}]$ the fluctuation operator of section 8. Like the transform in J alone, this is an exact definition, made without diagrams and at any strength of the interaction: at zero sources $\Gamma[\bar{\phi}, G]$ is stationary at the exact mean field and the exact propagator, where its value is $-\log Z$, and the equation defines Γ_2 . Expanding in the interaction is one way of evaluating it (section 16 follows the exact functional where the expansion fails): Γ_2 is then minus the sum of the two-particle-irreducible vacuum diagrams — those that stay connected when any two propagator lines are cut — with full propagators on the lines, the skeleton diagrams [47, 48, 49, 59], and the vertices of $S_{\text{int}}[\bar{\phi} + \phi]$ of degree three or more in the fluctuation ϕ .

Its pieces. The pieces carry the diagrams of $\Gamma[\bar{\phi}]$ in this way: $S[\bar{\phi}]$ the tree, as before; $\frac{1}{2}\text{Tr} \ln G^{-1} + \frac{1}{2}\text{Tr}(D_0^{-1}G - 1)$ the one loop, with the full G ; $\frac{1}{2}\text{Tr}(S''_{\text{int}}[\bar{\phi}] G)$, the vertex of degree two closed by one line G (the diagram $\langle S_{\text{int}}^{(2)} \rangle_G$); and Γ_2 the rest, with lines G . The vertex of degree two is not a vertex of Γ_2 : it is in the trace, and the rings of section 8 come back when G is dressed with it (section 9.3).

Fermions. The two-point source $K(x, y)$ couples to $\bar{\psi}(x)\psi(y)$, the variables are the Grassmann-odd means and $G = -\langle T\psi\bar{\psi} \rangle_c$, and the signs of the trace terms are those of a Grassmann integral:

$$\Gamma[\bar{\Psi}, \Psi, G] = -\bar{\Psi}G_0^{-1}\Psi + S_{\text{int}}[\bar{\Psi}, \Psi] - \text{Tr} \ln(-G^{-1}) - \text{Tr}(G_0^{-1}G - 1) + \langle S_{\text{int}}^{(2)} \rangle_G + \Gamma_2[\bar{\Psi}, \Psi, G],$$

with $\langle S_{\text{int}}^{(2)} \rangle_G$ the normal vertices of degree two, the Hartree and Fock potentials of the means, closed by one line G , and Γ_2 minus the 2PI vacuum diagrams with lines G and the vertices of degree three or more, which carry one mean each. The anomalous vertices of degree two, $V\Psi\Psi\bar{\psi}\bar{\psi}$ and $V\bar{\Psi}\bar{\Psi}\psi\psi$, are not in this form: a normal source cannot absorb them. `EffectiveAction2PI` with the means returns this form, which is exact at zero means in the normal state, where its derivatives are the self-energy and the irreducible vertex (section 9.5); at finite means, where the anomalous propagator $-\langle T\psi\bar{\psi} \rangle$ is of order $V\Psi\Psi$ (section 9.3), and in a paired state, the variable is the whole Nambu propagator, with the anomalous sources coupled to $\psi\psi$ and $\bar{\psi}\bar{\psi}$ (section 13).

9.1 ϕ^4 theory to λ^3

In ϕ^4 theory the vertices of Γ_2 are $\lambda\bar{\phi}\phi^3/6$, the mean field a crossed circle at the end of a short line, and $\lambda\phi^4/24$:

```
gammaPhiG = EffectiveAction2PI[FreeBosonGeneratingFunctional, Phi4Vertex, 3,
  FreePropagator -> DressedPropagator, "Statistics" -> "Boson",
  "MeanFields" -> {phi -> phiMean}];
```

To first order, with the traces as inert objects (`TraceLog`, `OperatorTrace`),

$$\begin{aligned} \Gamma[\bar{\phi}, G] = & \frac{1}{8} \lambda \int_{z_1} G(z_1, z_1)^2 + \frac{1}{4} \lambda \int_{z_1} G(z_1, z_1) \bar{\phi}(z_1)^2 + \frac{1}{24} \lambda \int_{z_1} \bar{\phi}(z_1)^4 \\ & + \frac{1}{2} \int_{z_1 z_2} \bar{\phi}(z_1) \bar{\phi}(z_2) D_0^{-1}(z_1, z_2) + \frac{1}{2} \text{Tr} \left(-1 + D_0^{-1} G \right) + \frac{1}{2} \text{Tr} \ln \left(G^{-1} \right) \end{aligned}$$

With $S[\bar{\phi}] = \frac{1}{2} \int \bar{\phi} D_0^{-1} \bar{\phi} + S_{\text{int}}[\bar{\phi}]$ and $\frac{1}{2}\text{Tr}(D^{-1}[\bar{\phi}] G - 1) = \frac{1}{2}\text{Tr}(D_0^{-1}G - 1) + \frac{1}{2}\text{Tr}(S''_{\text{int}}[\bar{\phi}] G)$, the pieces with vertices are

$$S_{\text{int}}[\bar{\phi}] = -\frac{1}{24} \star\star, \quad \frac{1}{2}\text{Tr}(S''_{\text{int}}[\bar{\phi}] G) = -\frac{1}{4} \star\infty,$$

and Γ_2 , to λ^3 :

$$\Gamma_2[\bar{\phi}, G] =$$

$$\lambda \quad -\frac{1}{8} \infty$$

$$\lambda^2 \quad -\frac{1}{48} \ominus \quad -\frac{1}{12} \bullet \text{---} \bigcirc \text{---} \bullet$$

$$\lambda^3 \quad -\frac{1}{48} \triangle \quad -\frac{1}{8} \bullet \text{---} \bigcirc \text{---} \bullet$$

The functional Λ_2^{int} drawn by Eckhardt, Kappl, Kauch and Held (their Fig. 5) [52], obtained by transforming also the free part of the two-point source, is $-\Gamma_2$ plus the classical interaction and the mass shift in the background (checked below).

$\Gamma_2[\bar{\phi}, G]$ minus its 2PI part; its vertices with two or more mean fields	$\{0, 0\}$ ✓
$\Lambda_2^{\text{int}} + \frac{\lambda}{24} \int \bar{\phi}^4 + \frac{\lambda}{4} \int \bar{\phi}^2 G + \Gamma_2[\bar{\phi}, G]$ at $\lambda, \lambda^2, \lambda^3$	$\{0, 0, 0\}$ ✓

9.2 The electron gas to V^3

```
DeclareDirectedPropagator[DressedGreenFunction];
gammaPsiG = EffectiveAction2PI[FreeFermionGeneratingFunctional, CoulombVertex, 3,
  BareGreenFunction -> DressedGreenFunction,
  "MeanFields" -> {psi -> MeanPsi, psibar -> MeanPsibar}];
```

To first order,

$$\begin{aligned} \Gamma[\bar{\Psi}, \Psi, G] = & -\frac{1}{2} \int_{z_1 z_2} G(z_1, z_2) G(z_2, z_1) V(z_1, z_2) + \frac{1}{2} \int_{z_1 z_2} G(z_1, z_1) G(z_2, z_2) V(z_1, z_2) \\ & + \int_{z_1 z_2} G(z_1, z_2) V(z_1, z_2) \Psi(z_2) \bar{\Psi}(z_1) - \int_{z_1 z_2} G(z_1, z_1) V(z_1, z_2) \Psi(z_2) \bar{\Psi}(z_2) \\ & - \frac{1}{2} \int_{z_1 z_2} V(z_1, z_2) \Psi(z_1) \Psi(z_2) \bar{\Psi}(z_1) \bar{\Psi}(z_2) + \int_{z_1 z_2} G_0^{-1}(z_2, z_1) \Psi(z_1) \bar{\Psi}(z_2) \\ & - \text{Tr} \left(-1 + G_0^{-1} G \right) - \text{Tr} \ln \left(-G^{-1} \right) \end{aligned}$$

The pieces with vertices are the classical interaction and the Hartree and Fock potentials of the means closed by G ,

$$S_{\text{int}}[\bar{\Psi}, \Psi] = \frac{1}{2} \text{---} \text{---} \text{---}, \quad \langle S_{\text{int}}^{(2)} \rangle_G = - \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---},$$

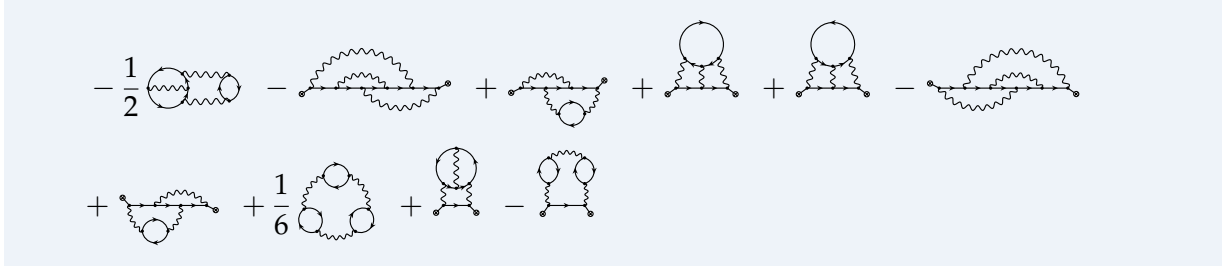
and Γ_2 . A vacuum diagram has the vertices with one mean in pairs, one with Ψ and one with $\bar{\Psi}$, so that the means enter Γ_2 from the second order; to V^3 it has 2, 4, 16 diagrams:

$$\Gamma_2[\bar{\Psi}, \Psi, G] =$$

$$V \quad \frac{1}{2} \text{---} \text{---} \text{---} \quad -\frac{1}{2} \text{---} \text{---} \text{---}$$

$$V^2 \quad +\frac{1}{4} \text{---} \text{---} \text{---} \quad - \text{---} \text{---} \text{---} \quad -\frac{1}{4} \text{---} \text{---} \text{---} \quad + \text{---} \text{---} \text{---}$$

$$V^3 \quad - \text{---} \text{---} \text{---} \quad - \text{---} \text{---} \text{---} \quad +\frac{1}{6} \text{---} \text{---} \text{---} \quad +\frac{1}{2} \text{---} \text{---} \text{---} \quad -\frac{1}{6} \text{---} \text{---} \text{---} \quad -\frac{1}{6} \text{---} \text{---} \text{---}$$



$\Gamma_2[\bar{\Psi}, \Psi, G]$ minus its 2PI part; its vertices with two or more means: $\{0, 0\}$ ✓

9.3 At the stationary G : back to the 1PI action

At its stationary point in G , the full propagator in the background $G[\bar{\phi}] = (\delta^2 \Gamma[\bar{\phi}] / \delta \bar{\phi} \delta \phi)^{-1} = D[\bar{\phi}] + O(\lambda)$, $\Gamma[\bar{\phi}, G]$ is the 1PI action $\Gamma[\bar{\phi}]$ of section 8, whose diagrams are these pieces with G dressed: at $G = D[\bar{\phi}]$ the traces are the one loop $\frac{1}{2} \text{Tr} \ln D^{-1}[\bar{\phi}]$ (the term $\frac{1}{2} \text{Tr}(D^{-1}[\bar{\phi}] G - 1)$ vanishes) and Γ_2 gives the diagrams of $\Gamma^{[2]}$, $\Gamma^{[3]}$ and $\Gamma^{[4]}$ that are 2PI in the lines $D[\bar{\phi}]$; the others, 1PI but two-particle reducible like the chain of three bubbles, come from the self-energy insertions in $G[\bar{\phi}] - D[\bar{\phi}]$, at second order in them since Γ is stationary in G .

For the electron gas the stationary G to first order is enough to V^3 (its error, of order V^2 , changes Γ at order V^4 , by stationarity). With the normal G alone it gives the diagrams of $\Gamma[\bar{\Psi}, \Psi]$ of section 8.2 except those with an anomalous vertex, 1 at V^2 and 11 at V^3 , which a normal propagator cannot generate; at V^2 it is the particle–particle pair of the means,

$$\frac{1}{2} \begin{array}{c} \bullet \\ \diagup \quad \diagdown \\ \bullet \end{array} \begin{array}{c} \bullet \\ \diagdown \quad \diagup \\ \bullet \end{array}$$

They come from the anomalous propagator, of order $V\Psi\Psi$ at the stationary point: with the Nambu propagator as the variable the functional at its stationary point is $\Gamma[\bar{\Psi}, \Psi]$ with all its diagrams (checked in section 13, paragraph *At finite means*).

ϕ^4 : $\Gamma[\bar{\phi}, G[\bar{\phi}]] - \Gamma[\bar{\phi}]$, expanded in D_0 , orders 0 to 3	$\{0, 0, 0, 0\}$ ✓
electron gas, G : $\Gamma[\bar{\Psi}, \Psi, G[\bar{\Psi}, \Psi]] - \Gamma[\bar{\Psi}, \Psi] + (\text{anomalous diagrams})$, orders 0 to 3	$\{0, 0, 0, 0\}$ ✓

9.4 At zero mean field: the Luttinger–Ward functional

At zero mean field — in the symmetric phase of ϕ^4 theory, and for fermions at zero source — only the diagrams without means are left: Γ_2 at zero means, $\Gamma_2[G]$ for ϕ^4 and $\Phi[G]$ for fermions, the Luttinger–Ward functional or Baym’s Φ [60, 38], is minus the 2PI skeleton vacuum diagrams. The package writes the whole action as an object:

$$\begin{aligned} \Gamma[G] &= \Phi[G] - \text{Tr} \left(-1 + G_0^{-1} G \right) - \text{Tr} \ln \left(-G^{-1} \right) & (\text{fermions}), \\ \Gamma[G] &= \Gamma_2[G] + \frac{1}{2} \text{Tr} \left(-1 + D_0^{-1} G \right) + \frac{1}{2} \text{Tr} \ln \left(G^{-1} \right) & (\phi^4). \end{aligned}$$

Its other names: the Luttinger–Ward or Baym–Kadanoff functional $\Omega[G]$ of the grand potential [60, 38], and the $\Gamma[\bar{\phi}, G]$ of Cornwall, Jackiw and Tomboulis [49] at $\bar{\phi} = 0$. A truncated Φ gives a Φ -derivable approximation, which is conserving (section 9.6).

```
luttingerWard = LuttingerWardFunctional[FreeFermionGeneratingFunctional,
  CoulombVertex, 3, BareGreenFunction -> DressedGreenFunction];
gamma = EffectiveAction2PI[luttingerWard, BareGreenFunction -> DressedGreenFunction];
FunctionalDerivative[gamma, DressedGreenFunction[y, x]]
```

FunctionalDerivative differentiates with respect to any object with two indices — here the propagator, which is not declared as a source — and through the traces, $\delta \text{Tr} \ln A = \text{Tr}(A^{-1} \delta A)$. To first order:

$$\frac{\delta \Gamma}{\delta G(y, x)} = \delta(x, y) \int_{z_1} G(z_1, z_1) V(x, z_1) - G(x, y) V(x, y) - G_0^{-1}(x, y) + G^{-1}(x, y).$$

The derivative is $\Sigma[G] + G^{-1} - G_0^{-1}$, which vanishes on the Dyson equation: the self-energy is $\Sigma(x, y) = \delta \Phi / \delta G(y, x)$ for fermions and $\Sigma = -2 \delta \Gamma_2 / \delta G$ for real bosons, a functional of the full propagator made of skeleton diagrams only. Differentiating with respect to G , which the package treats as a source, opens one line of a diagram in all possible ways (section 1). At the solution Γ is $-\log Z$, the grand potential over T . Written out at the perturbative $G = (G_0^{-1} - \Sigma)^{-1}$, the logarithm is a series of rings and the trace term a series of self-energy insertions, which cancel the reducible vacuum diagrams of Φ :

$$-\text{Tr} \ln(-(G_0^{-1} - \Sigma)) + \text{Tr} \ln(-G_0^{-1}) = \text{Diagram 1} + \frac{1}{2} \text{Diagram 2} + \frac{1}{3} \text{Diagram 3}$$

$$-\text{Tr}(G_0^{-1}(G_0^{-1} - \Sigma)^{-1} - 1) = - \text{Diagram 1} - \text{Diagram 2} - \text{Diagram 3}$$

$$\frac{1}{2} \text{Tr} \ln(D_0^{-1} - \Sigma) - \frac{1}{2} \text{Tr} \ln D_0^{-1} = -\frac{1}{2} \text{Diagram 1} - \frac{1}{4} \text{Diagram 2} - \frac{1}{6} \text{Diagram 3}$$

$$\frac{1}{2} \text{Tr}(D_0^{-1}(D_0^{-1} - \Sigma)^{-1} - 1) = \frac{1}{2} \text{Diagram 1} + \frac{1}{2} \text{Diagram 2} + \frac{1}{2} \text{Diagram 3}$$

For ϕ^4 theory, $\Gamma_2[G]$ and its self-energy to third order, $\Sigma = -2 \delta \Gamma_2 / \delta G$; **SelfEnergy** is a shortcut for this derivative:

```
gamma2 = LuttingerWardFunctional[FreeBosonGeneratingFunctional, Phi4Vertex, 3,
  FreePropagator -> DressedPropagator];
-2 FunctionalDerivative[gamma2, DressedPropagator[a, b]]
(* the same: SelfEnergy[gamma2, DressedPropagator, {a, b}, "Statistics" -> "Boson"] *)
```

$\Gamma_2[G] =$

$$\lambda - \frac{1}{8} \infty$$

$$\lambda^2 = -\frac{1}{48} \text{ (diagram: circle with a horizontal line through the center)}$$

$$\lambda^3 = -\frac{1}{48} \text{ (diagram: circle with an inscribed triangle)}$$

$$\Sigma[G](a, b) =$$

$$\lambda = \frac{1}{2} \text{ (diagram: circle with a horizontal line through the center, labeled } a \text{ on the left and } b \text{ on the right)}$$

$$\lambda^2 = +\frac{1}{6} \text{ (diagram: circle with a horizontal line through the center, labeled } a \text{ on the left and } b \text{ on the right)}$$

$$\lambda^3 = +\frac{1}{4} \text{ (diagram: circle with a horizontal line through the center, labeled } a \text{ on the left and } b \text{ on the right)}$$

For the electron gas, $\Phi[G]$ and $\Sigma(x, y) = \delta\Phi/\delta G(y, x)$; every line in these pictures, and in those of the vertices below, is a dressed propagator:

```
selfEnergy = FunctionalDerivative[luttingerWard, DressedGreenFunction[y, x]];
(* the same: SelfEnergy[luttingerWard, DressedGreenFunction, {x, y}] *)
```

$$\Phi[G] =$$

$$V = \frac{1}{2} \text{ (diagram: circle with a horizontal line through the center)} - \frac{1}{2} \text{ (diagram: circle with a horizontal line through the center)}$$

$$V^2 = +\frac{1}{4} \text{ (diagram: circle with a horizontal line through the center)} - \frac{1}{4} \text{ (diagram: circle with a horizontal line through the center)}$$

$$V^3 = +\frac{1}{6} \text{ (diagram: circle with a horizontal line through the center)} + \frac{1}{2} \text{ (diagram: circle with a horizontal line through the center)} - \frac{1}{6} \text{ (diagram: circle with a horizontal line through the center)} - \frac{1}{6} \text{ (diagram: circle with a horizontal line through the center)} - \frac{1}{2} \text{ (diagram: circle with a horizontal line through the center)} + \frac{1}{6} \text{ (diagram: circle with a horizontal line through the center)}$$

$$\Sigma[G](x, y) =$$

$$V = \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)} - \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)}$$

$$V^2 = + \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)} - \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)}$$

$$V^3 = + \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)} + \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)} + \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)} - \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)} - \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)}$$

$$- \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)} + \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)} - \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)} - \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)} + \text{ (diagram: circle with a horizontal line through the center, labeled } x \text{ on the left and } y \text{ on the right)}$$

$\delta\Gamma/\delta G = \Sigma[G] + G^{-1} - G_0^{-1}$ (to V^3 ; for $\phi^4 - \frac{1}{2}$ of it, to λ^3)	$\{0, 0\}$ ✓
$\Gamma[G]$ at the perturbative G : $-\log Z_0 -$ (connected vacuum diagrams)	$\{\{0, 0, 0\}, \{0, 0, 0\}\}$ ✓
SelfEnergy minus the derivatives of $\Phi[G], \Gamma_2[G], \Gamma_2[G, D_\sigma]$ (§15)	$\{0, 0, 0\}$ ✓
$\int V \delta\Phi^{(m)}/\delta V = m \Phi^{(m)}$ and $\int G \delta\Phi^{(m)}/\delta G = 2m \Phi^{(m)}, m = 1, 2, 3$	$\{\{0, 0\}, \{0, 0\}, \{0, 0\}\}$ ✓
$\Sigma[G]$ minus the skeletons of the perturbative Σ (section 5), $D_0 \rightarrow G$	0 ✓
the same for the electron gas, $G_0 \rightarrow G$	0 ✓
$\int_{x,y} \Sigma^{(m)}(x, y) G(y, x) = 2m \Phi^{(m)}, m = 1, 2, 3$ ($\Phi^{(m)}$ has $2m$ lines)	$\{0, 0, 0\}$ ✓

The derivative with respect to the interaction opens an interaction line: $\delta\Phi/\delta V(x, y)$ is $-\frac{1}{2}$ times the skeleton density correlation $\langle\rho(x)\rho(y)\rangle_c$ without its reducible part, the two ends of the line becoming density points:

$$\frac{\delta\Phi}{\delta V(x, y)} =$$

$$V^0 \quad -\frac{1}{2} \begin{array}{c} x \quad y \\ \text{---} \text{---} \end{array} + \frac{1}{2} \begin{array}{c} x \quad y \\ \text{---} \text{---} \end{array}$$

$$V \quad -\frac{1}{2} \begin{array}{c} x \quad y \\ \text{---} \text{---} \end{array} + \frac{1}{2} \begin{array}{c} x \quad y \\ \text{---} \text{---} \end{array}$$

The grand potential. At its stationary point Γ is $-\log Z$, and per unit of β times the volume $\mathcal{V}$ it is the grand potential $\Omega/\mathcal{V}$. EvaluateMatsubara (section 7) evaluates its traces too, with the dressed line given an energy like a free one (DressedGreenFunction $\rightarrow$ {"Fermion", xi} added to the rules). The logarithms are summed with the ordering of the operators at equal times (paragraph Three orderings): for the free electron gas, with $e^{i\omega_n 0^+}$ (normal order), $e^{-i\omega_n 0^+}$ (marked (-)) and the symmetric sum (marked sym),

$$\frac{\Omega_0}{\mathcal{V}} = 2 T \sum_p \log(1 - n_F(\xi_p)),$$

$$\frac{\Omega_0^{(-)}}{\mathcal{V}} = -2 \sum_p (-T \log(1 - n_F(\xi_p)) + \xi_p), \quad \frac{\Omega_0^{\text{sym}}}{\mathcal{V}} = -2 \sum_p \left(-T \log(1 - n_F(\xi_p)) + \frac{1}{2} \xi_p \right),$$

and $-T \ln(1 - n_F(\xi)) = T \ln(1 + e^{-\xi/T})$; for free bosons, $\langle\phi\phi\rangle_0 = 1/(\omega_k^2 + \nu_n^2)$, with the zero-point energy and every ordering, $\Omega_0/\mathcal{V} = \frac{1}{2} \sum_p (-2 T \log(1 + n_B(\omega_p)) + \omega_p)$. The Hartree-Fock approximation (the first order of Φ , at $G(k, i\omega) = 1/(i\omega - \epsilon_k)$) and the Hartree approximation of ϕ^4 theory ($G(k, i\omega) = 1/(M_k^2 + \nu^2)$):

$$\begin{aligned} \frac{\Omega_{\text{HF}}}{\mathcal{V}} &= 2 T \sum_{p_1} \log(1 - n_F(\epsilon_{p_1})) - \sum_{p_1, p_2} n_F(\epsilon_{p_1}) n_F(\epsilon_{p_2}) v_{p_1 - p_2} \\ &\quad - 2 \sum_{p_1} (\epsilon_{p_1} n_F(\epsilon_{p_1}) - n_F(\epsilon_{p_1}) \xi_{p_1}) + 2 v_0 \sum_{p_1, p_2} n_F(\epsilon_{p_1}) n_F(\epsilon_{p_2}) \\ \frac{\Omega_{\text{H}}}{\mathcal{V}} &= \frac{1}{2} \sum_{p_1} (-2 T \log(1 + n_B(M_{p_1})) + M_{p_1}) + \frac{1}{32} \lambda \sum_{p_1, p_2} \frac{(1 + 2 n_B(M_{p_1})) (1 + 2 n_B(M_{p_2}))}{M_{p_1} M_{p_2}} \\ &\quad + \frac{1}{2} \sum_{p_1} \left(-\frac{1}{2} M_{p_1} - n_B(M_{p_1}) M_{p_1} + \frac{\omega_{p_1}^2}{2 M_{p_1}} + \frac{n_B(M_{p_1}) \omega_{p_1}^2}{M_{p_1}} \right) \end{aligned}$$

9.5 The derivatives with respect to the means

The stationarity conditions of $\Gamma[\bar{\phi}, G]$ are the field equation and the Dyson equation with $\Sigma[\bar{\phi}, G] = -2 \delta\Gamma_2/\delta G$:

$$\frac{\delta\Gamma}{\delta\bar{\phi}(a)} - \int D_0^{-1}\bar{\phi} =$$

$$\lambda \quad -\frac{1}{2} a \text{---} \bigcirc \quad -\frac{1}{6} a \text{---} \text{---} \text{---}$$

$$\lambda^2 \quad -\frac{1}{6} a \text{---} \bigcirc \text{---}$$

$$\Sigma[\bar{\phi}, G] - \Sigma[0, G] = \frac{1}{2} a \text{---} \bigcirc \text{---} b$$

to second order (the first-order $\lambda\bar{\phi}^2/2$ is in $D^{-1}[\bar{\phi}]$). The bubble with two vertices $\lambda\bar{\phi}$ is a skeleton, but not 2PI as an open graph (cutting its two lines separates a from b): in the background the perturbative Σ is selected with `SkeletonDiagrams`.

At zero mean field and fixed G the derivatives with respect to the means are skeleton vertex functions. Differentiating twice opens the diagrams with two means into the skeleton self-energy from the second order on: for an interaction even in the field the second derivative is $D_0^{-1} - \Sigma[G]$ at any G ($\delta^2\Gamma/\delta\bar{\Psi}\delta\Psi = G_0^{-1} - \Sigma[G]$ for fermions), which is G^{-1} on the Dyson equation. The fourth derivative is the fully irreducible vertex, with which the parquet equations of section 12 begin.

$\Gamma[0, G] = \Gamma[G]$	0 ✓
$\Gamma_2[0, G] - \Gamma_2[G]$ to λ^3 ; $\delta^2\Gamma_2/\delta\bar{\phi}(a)\delta\bar{\phi}(b) _{\bar{\phi}=0} + \Sigma[G](a, b)$ at λ^2, λ^3	$\{0, \{0, 0\}\}$ ✓
$\delta^2\Gamma/\delta\bar{\phi}\delta\bar{\phi} _{\bar{\phi}=0, G} = D_0^{-1} - \Sigma[G]$, orders 0 to 3	$\{0, 0, 0, 0\}$ ✓
$\Gamma_2[0, 0, G] - \Phi[G]$; $\delta^2\Gamma_2/\delta\bar{\Psi}(x)\delta\Psi(y) _0 + \Sigma[G](x, y)$ at V^2, V^3	$\{0, \{0, 0\}\}$ ✓
$\delta^2\Gamma/\delta\bar{\Psi}\delta\Psi _{0, G} = G_0^{-1} - \Sigma[G]$ (first order)	0 ✓

9.6 The irreducible vertex and the Ward identity

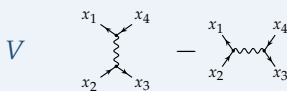
Differentiating once more gives the vertex irreducible in the particle–hole channel, the kernel of the Bethe–Salpeter equation (for the Hartree–Fock Φ , the antisymmetrized interaction):

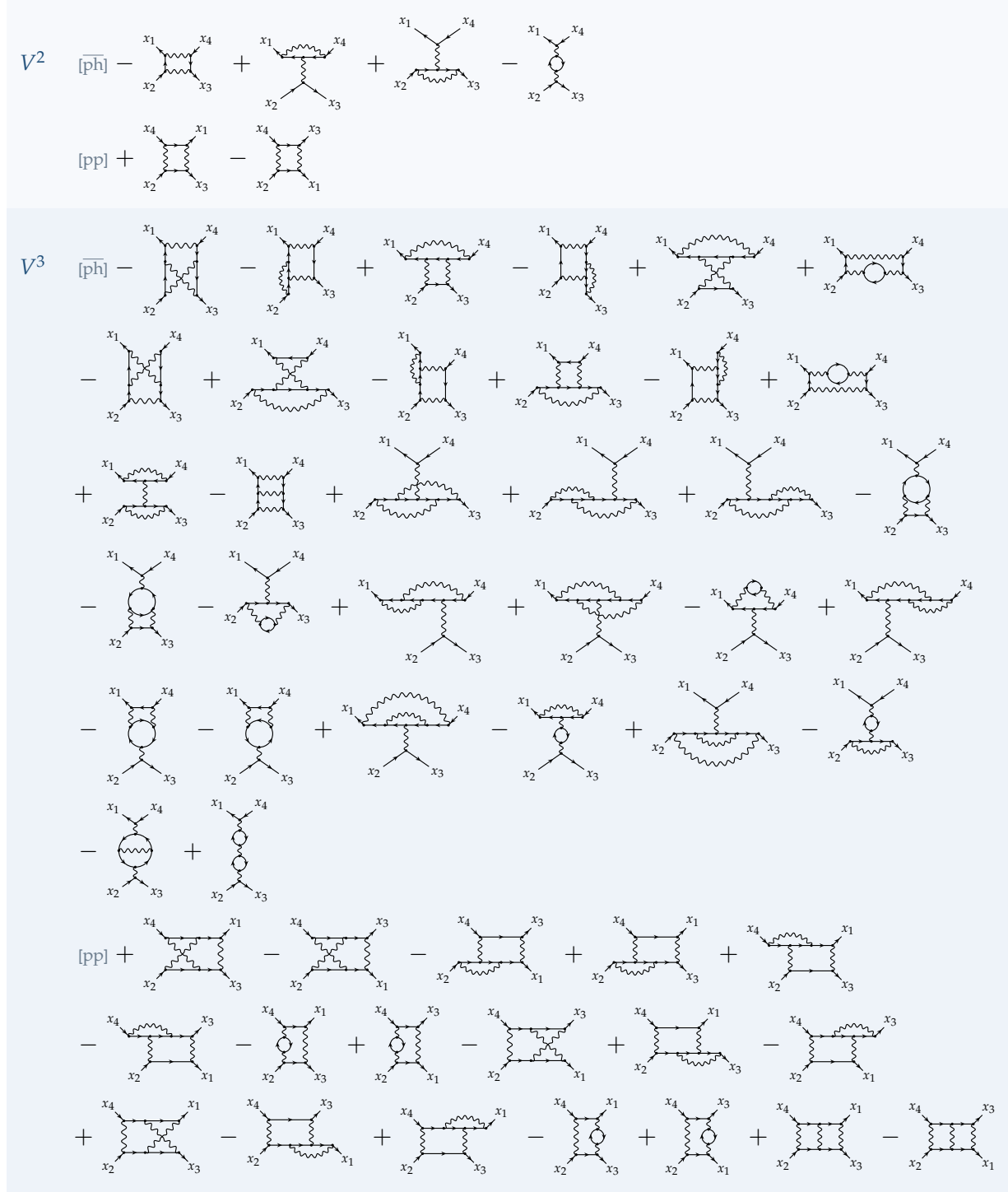
$$\Gamma^0(x_1, x_2; x_3, x_4) = \frac{\delta\Sigma(x_1, x_2)}{\delta G(x_4, x_3)} = \frac{\delta^2\Phi}{\delta G(x_2, x_1)\delta G(x_4, x_3)}.$$

The fermions leave at x_1, x_3 and enter at x_2, x_4 ; the legs are drawn counterclockwise from the top left, and points joined by delta functions are a single vertex. Up to third order every diagram of Γ^0 beyond first order is reducible either in the transverse particle–hole channel [ph] or in the particle–particle channel [pp]; the first fully irreducible diagrams beyond the bare vertex, of the envelope type (section 12), appear at fourth order. The [pp] diagrams are drawn with the incoming legs x_4, x_2 on the left, so that the two particles propagate from left to right (and, when a particle entering at x_2 leaves at x_1 , with x_1 and x_3 exchanged, so that the two lines stay parallel).

```
irreducibleVertex = FunctionalDerivative[luttingerWard,
  DressedGreenFunction[x4, x3], DressedGreenFunction[x2, x1]];
(* the same: IrreducibleVertex[luttingerWard, DressedGreenFunction, {x1, x2, x3, x4}]
*)
DiagramPlot[irreducibleVertex, {x1, x2, x3, x4}]
```

$$\Gamma^0 =$$





IrreducibleVertex minus $\delta^2\Phi/\delta G \delta G$ and $4\delta^2\Gamma_2/\delta G \delta G$; $-2\delta\Sigma/\delta G - \Gamma^0(\phi^4)$ residuals $\{0, 0, 0\}$ ✓
 symmetry $\Gamma_{12;34}^0 = \Gamma_{34;12}^0$ residual 0 ✓
 homogeneity $\int G_{43} \Gamma_{12;34}^{0(m)} = (2m-1) \Sigma_{12}^{(m)}$, $m = 1, 2, 3$ residuals $\{0, 0, 0\}$ ✓
 Ward identity $\int_{34} \Gamma_{12;34}^0 \delta G_{43} = i(\theta_1 - \theta_2) \Sigma_{12}$ for $\delta G_{43} = i(\theta_4 - \theta_3) G_{43}$ residual 0 ✓

The Ward identity of charge conservation holds diagram by diagram. Under the local phase rotation $G(x, y) \rightarrow e^{i\theta(x)} G(x, y) e^{-i\theta(y)}$ every diagram of Φ is invariant, because at each vertex one line enters and one leaves and V couples densities; hence $\Sigma[G]$ rotates like G , $\delta\Sigma_{12} = i(\theta_1 - \theta_2)\Sigma_{12}$, and the identity is the derivative of this covariance. It therefore holds for every truncation of Φ . An approximation is *conserving* when its propagator, and the response functions obtained from it with its own kernel $\Gamma^0 = \delta\Sigma/\delta G$ (the vertex equation of section 11), obey the conservation

laws of particle number, momentum and energy: the continuity equation and its analogues. This covariance, together with the invariance of Φ under translations in space and time, makes every Φ -derivable approximation — Σ and Γ^0 obtained from a truncated Φ , in field theory a truncation of the 2PI effective action — conserving [37, 38, 61], and the identity is the Ward–Takahashi identity of these approximations [62, 63].

Bosons. For real bosons $\Gamma_{ab;cd}^0 = -2\delta\Sigma_{ab}/\delta G_{cd}$ is irreducible in the channel s ($ab|cd$). In ϕ^4 theory, to third order, the bubbles of the channels t and u and their corrections:

```
4 FunctionalDerivative[gamma2, DressedPropagator[a, b], DressedPropagator[c, d]]
(* the same: IrreducibleVertex[gamma2, DressedPropagator, {a, b, c, d},
   "Statistics" -> "Boson"] *)
```

$\Gamma^0 =$

$$\lambda \quad - \quad \text{diagram: a four-point vertex with external lines } a, b, c, d \text{ and a central cross.}$$

$$\lambda^2 \quad - \frac{1}{2} \text{diagram: a bubble with external lines } a, b, c, d \text{ and a central cross.} \quad - \frac{1}{2} \text{diagram: a bubble with external lines } a, b, c, d \text{ and a central cross.}$$

$$\lambda^3 \quad - \frac{1}{2} \text{diagram: a bubble with a bubble inside, external lines } a, b, c, d. \quad - \frac{1}{2} \text{diagram: a bubble with a bubble inside, external lines } a, b, c, d. \quad - \frac{1}{2} \text{diagram: a bubble with a bubble inside, external lines } a, b, c, d. \quad - \frac{1}{2} \text{diagram: a bubble with a bubble inside, external lines } a, b, c, d. \quad - \frac{1}{4} \text{diagram: a bubble with a bubble inside, external lines } a, b, c, d. \quad - \frac{1}{4} \text{diagram: a bubble with a bubble inside, external lines } a, b, c, d.$$

symmetries $\Gamma_{ab;cd}^0 = \Gamma_{ba;cd}^0 = \Gamma_{cd;ab}^0$, homogeneity $\int G_{cd} \Gamma_{ab;cd}^{0(m)} = -2(2m-1) \Sigma_{ab}^{(m)}$, $m = 1, 2, 3$, $\Gamma^{(4)} - R_s - \Gamma^0$ (section 12) and the Bethe–Salpeter equation of the channel s (section 10): $\{0, 0, \{0, 0, 0\}, 0, 0\}$ ✓

10 Two particles: the Bethe–Salpeter equation

Expectation values as variations. A one-body source U in the bare inverse propagator of the 2PI action, "Source" $\rightarrow U$ ($G_0^{-1} \rightarrow G_0^{-1} - U$; $D_0^{-1} \rightarrow D_0^{-1} + U$ for real bosons), enters Γ only through the trace term. By stationarity only this explicit dependence counts:

$$\frac{\delta\Gamma}{\delta U(x, y)} = G(y, x), \quad \frac{\delta\Gamma}{\delta U(x, y)} \Big|_{\phi^4} = \frac{1}{2} G(x, y),$$

so that $N = -\partial\Omega/\partial\mu$ although Σ depends on μ , with $\Omega = T\Gamma$ the grand potential of section 9.4. The second variation is the response of the propagator.

The response of the propagator. The two-particle correlation function is the change of the propagator,

$$L(x_1, x_2; x_3, x_4) = \frac{\delta G(x_1, x_2)}{\delta U(x_4, x_3)},$$

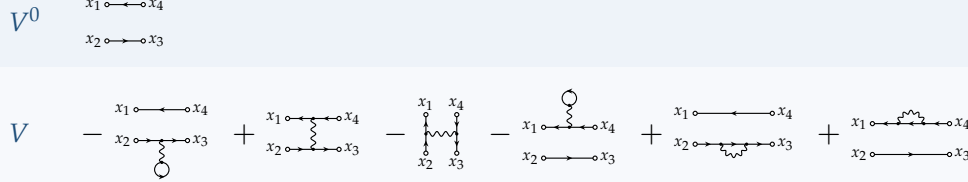
Schwinger's functional derivative with respect to a bilocal field [64], which the package computes as it stands. In perturbation theory G depends on U through its lines: $G_0^{-1} \rightarrow G_0^{-1} - U$ gives $\delta G_0(x_1, x_2)/\delta U(x_4, x_3) = G_0(x_1, x_4) G_0(x_3, x_2)$, a rule declared once (section 1), and FunctionalDerivative opens every line of every diagram of G :

```

DeclareSource[PotentialU];
DeclareFunctionalDerivative[BareGreenFunction[p_, q_], PotentialU[r_, s_],
  BareGreenFunction[p, r] BareGreenFunction[s, q]];
responseL = FunctionalDerivative[greenFunction /. {x -> x1, y -> x2},
  PotentialU[x4, x3]];

```

$$L(x_1, x_2; x_3, x_4) =$$



To zeroth order it is the pair of free lines, a particle and a hole that propagate independently; to first order the interaction acts between them, directly and by exchange, or dresses one of the two lines by its Hartree or Fock self-energy. It has 1, 6, 50 and 518 diagrams at orders V^0 to V^3 , and it is the pair of full propagators minus the connected four-point function of section 4, $L(1,2;3,4) = G(1,4)G(3,2) - \langle T\psi_1\bar{\psi}_2\psi_3\bar{\psi}_4 \rangle_c (\{0,0,0,0\})$ ✓.

The chain rule. Exactly, the propagator is the stationary point of the 2PI action with the source, $G^{-1} = G_0^{-1} - U - \Sigma[G]$, and the self-energy depends on U only through G . With $\delta G/\delta U = L$ declared for the dressed propagator, the derivative of $\Sigma[G]$ of section 9.4 is, by the chain rule, the irreducible vertex $\Gamma^0 = \delta\Sigma/\delta G$ of section 9.6 joined to L :

```

DeclareBlob[LBox, "L", "Shape" -> "Box", "Fill" -> "White"]; (* L, a box *)
DeclareFunctionalDerivative[DressedGreenFunction[p_, q_], PotentialU[r_, s_],
  LBox[p, q, s, r]];
FunctionalDerivative[selfEnergy /. {x -> x1, y -> x2}, PotentialU[x4, x3]]

```

$$\frac{\delta\Sigma^{(1)}(x_1, x_2)}{\delta U(x_4, x_3)} =$$

to first order, and to V^3 0 ✓ for $\delta\Sigma/\delta U - \Gamma^0 L$. Differentiating the Dyson equation, $\delta G^{-1}/\delta U = -1 - \Gamma^0 L$, so that $L = -G(\delta G^{-1}/\delta U)G$ is

$$L = L_0 + L_0\Gamma^0 L,$$

with L_0 the pair of full propagators: the response obeys an equation whose kernel is the second derivative of Φ .

The Bethe–Salpeter equation. The part of L with its four legs removed is the full vertex F of section 4, $L = L_0 + L_0FL_0$, and the equation for L becomes the Bethe–Salpeter equation [65] between F and Γ^0 , which resums the particle–hole channel: the diagrams of F that fall apart when a particle–hole pair of lines is cut are a Γ^0 , the pair of lines, and F again. The pair is a function of four points, a particle and a hole that propagate independently, each with the full propagator:

$$L_0(x_1, x_2; x_3, x_4) =$$

Four-point functions are multiplied in this channel by joining the right pair of labels of one to the left pair of the next, $(AB)(1, 2; 3, 4) = \int_{a,b} A(1, 2; a, b) B(b, a; 3, 4)$. In pictures, with Γ^0 cross-hatched, F hatched, every line a full propagator G (a plain line, as in all the exact equations from here on: section 5) and the legs x_1 (out), x_2 (in), x_3 (out), x_4 (in) counterclockwise from the top left of each square, the equation is

that is, $F = \Gamma^0 + \Gamma^0 L_0 F$, exact as the chain rule above. With the skeleton diagrams of $\delta^4 \Gamma / \delta \bar{\Psi} \delta \Psi \delta \bar{\Psi} \delta \Psi$ (section 8.4), F has 2, 10 and 82 diagrams of first, second and third order. The package checks the equation:

```
SimplifyDiagrams[fullVertex - irreducibleVertex -
  BetheSalpeterLadder[irreducibleVertex,
    fullVertex, {x1, x2, x3, x4}, "ParticleHole", DressedGreenFunction,
    "MaximumOrder" -> {InteractionPotential, 3}]]
```

residual of the Bethe–Salpeter equation up to V^3 : 0 ✓

`BetheSalpeterLadder[A, B, ...]` joins two vertices by the pair of propagators of a given channel, AL_0B in the particle–hole channel. Iterating the direct interaction alone gives the bubble chain of the random-phase approximation [35, 66], F_{chain} , whose interaction lines joined by bubbles, the pair closed on two points, $\chi_0(x, y) = L_0(x, x; y, y)$ (the polarization P of section 6 to lowest order; with bare lines, the Lindhard function of section 7), make up the screened interaction W between the two pairs of legs:

and the bare vertex iterated in the particle–particle channel gives the ladder of the T -matrix [67, 3] — the scattering amplitude of two particles in the medium, which governs a dilute gas with a short-range interaction — here its second-order term, $T^{(2)}$, drawn with the incoming particles on the left (option "ExternalOrder" -> {x4, x2, x3, x1}):

For real bosons the two lines of a pair are identical, and the pair carries the factor $-\frac{1}{2}$. With the full vertex $\Gamma^{(4)}$ drawn as a square, the equation of the channel s is

that is, $\Gamma^{(4)} = \Gamma^0 - \frac{1}{2} \Gamma^0 L_0 \Gamma^{(4)}$, with L_0 the pair of boson lines; with the Γ^0 of ϕ^4 theory (section 9.6) its residuals are $\{0, 0, 0, 0\}$ ✓. In its simplest approximation, $\Gamma^0 = \lambda$, the equation is solved by the bubble chain of the channel s :

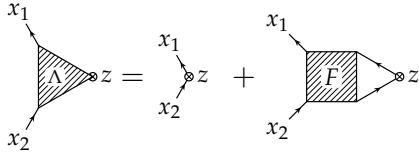
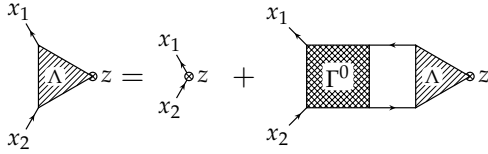
$$\Gamma_{\text{chain}}^{(4)} = - \begin{array}{c} a \\ \diagup \quad \diagdown \\ b \quad c \end{array} - \frac{1}{2} \begin{array}{c} a \quad d \\ \diagup \quad \diagdown \\ b \quad c \end{array} - \frac{1}{4} \begin{array}{c} a \quad d \\ \diagup \quad \diagdown \\ b \quad c \end{array} + \dots$$

11 Vertices and response functions

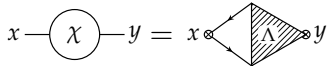
The vertex of a one-body operator. An external field U coupled to a one-body operator — the density $\rho = \bar{\psi}\psi$, a current, a spin density, any $\int \bar{\psi} \gamma \psi$ — changes the propagator, and the change defines a three-point vertex, drawn as a triangle with the two fermion legs on the left [1, 36]:

$$\Lambda = -\frac{\delta G^{-1}}{\delta U} = \gamma + \frac{\delta \Sigma}{\delta U}, \quad \delta G = L_0 \Lambda \delta U,$$

where γ is the bare vertex, for the density $\gamma(x_1, x_2; z) = \delta(x_1, z) \delta(x_2, z)$. The self-energy depends on U only through G , so that the chain rule of section 10 gives an exact equation for the vertex, the Bethe–Salpeter equation of section 10 closed on γ ; solved, it is the bare vertex corrected by the full vertex F :



that is, $\Lambda = \gamma + \Gamma^0 L_0 \Lambda = \gamma + F L_0 \gamma$ with the pair L_0 of section 10. The derivative of the density $\langle \rho(x) \rangle = G(x, x)$ is the density response $\chi = \delta \langle \rho \rangle / \delta U = -\langle \rho \rho \rangle_c$ (section 6), the pair closed on the point x and on the vertex, $\chi = \gamma L_0 \Lambda$:

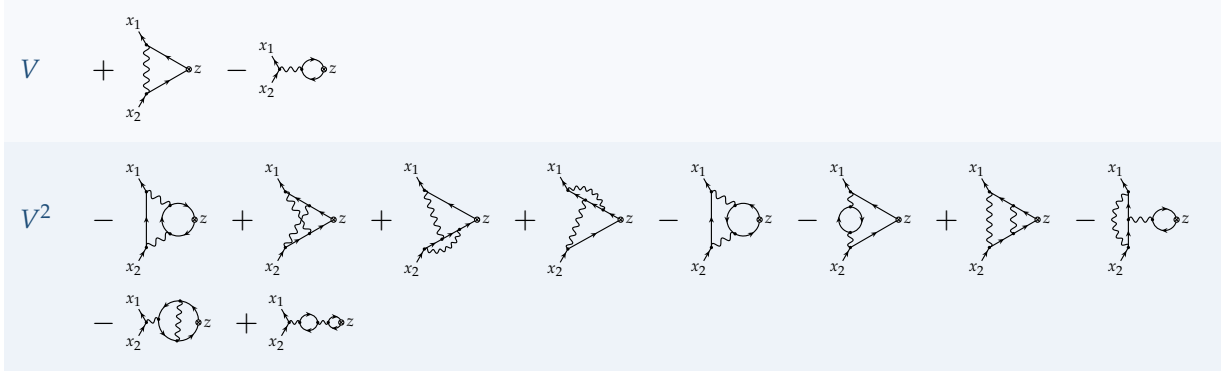


The package computes the vertex as the derivative that defines it, $\Lambda = \gamma + \delta \Sigma / \delta U$: the perturbative self-energy of section 5 depends on U through its bare lines, and the rule of section 6 inserts the potential into each of them; the skeleton diagrams of the result, with $G_0 \rightarrow G$, are $\Lambda[G]$, with 2, 10 and 82 diagrams at orders V , V^2 and V^3 . To second order, with the density at z ,

```
densityVertex = DeltaFunction[x1, z] DeltaFunction[x2, z] + (SkeletonDiagrams[
  FunctionalDerivative[selfEnergyPerturbative /. {x -> x1, y -> x2},
    LocalPotential[z]], {x1, x2, z}, {BareGreenFunction}] /.
  BareGreenFunction -> DressedGreenFunction);
(* the same: PerturbativeDensityVertex[FreeFermionGeneratingFunctional, CoulombVertex,
  3, {psi, psibar}, {x1, x2, z}, BareGreenFunction -> DressedGreenFunction] *)
```

$$\Lambda(x_1, x_2; z) =$$

$$V^0 \begin{array}{c} x_1 \\ \diagup \quad \diagdown \\ x_2 \quad z \end{array}$$



`PerturbativeDensityVertex` computes the same from the three-point function $\langle \psi \bar{\psi} \rho \rangle_c$ with its legs removed (0 ✓). The exact equations of the package (`ExactEquation`) take the full objects either as heads, to draw the equations as above, or as functions of their labels, to check them against the perturbative series order by order (`CheckEquation`):

```
objects = {"G" -> DressedGreenFunction, "Lambda" -> LabelFunction[densityVertex,
  {x1, x2, z}], "Gamma0" -> LabelFunction[irreducibleVertex, {x1, x2, x3, x4}],
  ...};
CheckEquation[ExactEquation["Vertex", objects, {x1, x2, z}], InteractionPotential, 3]
```

$\Lambda = \gamma + \Gamma^0 L_0 \Lambda$, $\Lambda = \gamma + F L_0 \gamma$, $\Sigma = \Sigma_H - V G \Lambda$ (below) to V^3 , and $\chi = \gamma L_0 \Lambda$ to V^2 : residuals $\{ \{0, 0, 0, 0\}, \{0, 0, 0, 0\}, \{0, 0, 0, 0\}, \{0, 0, 0\} \}$ ✓

For a real boson the operator is $\frac{1}{2}\phi^2$, a local mass term, with the bare vertex $\gamma(a, b; z) = \delta(a, z) \delta(b, z)$, and the pair of lines carries the factor $-\frac{1}{2}$ (section 10). In ϕ^4 theory the vertex equations are

$$\Lambda(a, b; z) = \gamma(a, b; z) - \frac{1}{2} \Gamma^0(a, b; z) \Lambda(a, b; z)$$

$$\Lambda(a, b; z) = \gamma(a, b; z) - \frac{1}{2} \Gamma^{(4)}(a, b; z)$$

that is, $\Lambda = \gamma - \frac{1}{2}\Gamma^0 L_0 \Lambda = \gamma - \frac{1}{2}\Gamma^{(4)} L_0 \gamma$. The vertex is again a derivative, $\Lambda = \delta G^{-1} / \delta U = \gamma - \delta \Sigma / \delta U$ with the source of $\frac{1}{2}\phi^2$ of section 6 (`PerturbativeDensityVertex` the same, 0 ✓); it has 1, 2 and 6 diagrams at orders λ , λ^2 and λ^3 ; to second order,

$$\Lambda(a, b; z) =$$

$$\lambda^0 \quad \gamma(a, b; z)$$

$$\lambda \quad + \frac{1}{2} \text{ (loop diagram) }$$

$$\lambda^2 \quad + \frac{1}{2} \text{ (triangle diagram) } + \frac{1}{4} \text{ (self-energy diagram) }$$

the vertex equations of ϕ^4 theory to λ^3 : residuals $\{\{0, 0, 0, 0\}, \{0, 0, 0, 0\}\}$ ✓

The self-energy from the vertex. The equation of motion of ψ expresses the self-energy through the vertex of the density: the Hartree term, and the vertex closed by a propagator and an interaction line,

$$\Sigma(x, y) = -x \text{---} \text{---} y + x \text{---} \text{---} \Lambda y$$

— the exchange–correlation part, $\Sigma_{xc} = \Sigma - \Sigma_H = -VG\Lambda$, is the interaction line closed on the vertex of the density.

11.1 Response functions from vertices

The vertices organize the diagrams of the response functions of section 6. A response function is the pair L_0 closed by the bare vertex γ_A of the observed operator at one end and by the vertex Λ_B of the perturbing one at the other, $\chi_{AB} = \gamma_A L_0 \Lambda_B$; for the density it is the picture above, $\chi = \gamma L_0 \Lambda$. With $\Lambda = \gamma + FL_0\gamma$ it is the bubble χ_0 of dressed lines, plus every interaction between the particle and the hole, collected in the full vertex F :

$$x \text{---} \chi \text{---} y = x \text{---} \text{---} y + x \text{---} \text{---} F y$$

Equivalently, $\chi_{AB} = \gamma_A L \gamma_B$, with the two-particle correlation function L of section 10, $L(1, 2; 3, 4) = \delta G(1, 2) / \delta U(4, 3)$, which is the pair plus F with its legs,

$$\begin{array}{c} x_1 \quad x_4 \\ \diagdown \quad \diagup \\ L \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} = \begin{array}{c} x_1 \text{---} x_4 \\ x_2 \text{---} x_3 \end{array} + \begin{array}{c} x_1 \quad x_4 \\ \diagdown \quad \diagup \\ F \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array}$$

With the Bethe–Salpeter equation of section 10 this is $L = L_0 + L_0 \Gamma^0 L$ (ExactEquation, "Response"; for ϕ^4 the pair carries $-\frac{1}{2}$), drawn as it stands (Γ^0 and L share two points):

$$\begin{array}{c} x_1 \quad x_4 \\ \diagdown \quad \diagup \\ L \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} = \begin{array}{c} x_1 \text{---} x_4 \\ x_2 \text{---} x_3 \end{array} + \begin{array}{c} x_1 \quad x_4 \\ \diagdown \quad \diagup \\ \Gamma^0 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array}$$

$$L|_{\phi^4} = \begin{array}{c} x_1 \text{---} x_4 \\ x_2 \text{---} x_3 \end{array} + \begin{array}{c} x_1 \quad x_4 \\ \diagdown \quad \diagup \\ \Gamma^0 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} - \frac{1}{2} \begin{array}{c} x_1 \quad x_4 \\ \diagdown \quad \diagup \\ \Gamma^0 \quad L \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array}$$

and iterated, the ladder of the kernel $\Gamma^0 = \delta \Sigma / \delta G$:

$$\begin{array}{c} x_1 \quad x_4 \\ \diagdown \quad \diagup \\ L \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} = \begin{array}{c} x_1 \text{---} x_4 \\ x_2 \text{---} x_3 \end{array} + \begin{array}{c} x_1 \quad x_4 \\ \diagdown \quad \diagup \\ \Gamma^0 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} + \begin{array}{c} x_1 \quad x_4 \\ \diagdown \quad \diagup \\ \Gamma^0 \quad \Gamma^0 \\ \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array} + \dots$$

$$L|_{\phi^4} = \begin{array}{c} x_1 \circ \text{---} x_4 \\ x_2 \circ \text{---} x_3 \end{array} + \begin{array}{c} x_1 \circ \text{---} x_3 \\ x_2 \circ \text{---} x_4 \end{array} - \begin{array}{c} x_1 \circ \text{---} x_4 \\ x_2 \circ \text{---} x_3 \end{array} \boxed{\Gamma^0} + \frac{1}{2} \begin{array}{c} x_1 \circ \text{---} x_4 \\ x_2 \circ \text{---} x_3 \end{array} \boxed{\Gamma^0} \text{---} \boxed{\Gamma^0} + \dots$$

A susceptibility is $\chi = \gamma L \gamma$ ("Susceptibility"):

$$\chi(z_1, z_2) = z_1 \text{---} \boxed{L} \text{---} z_2$$

$\chi = \chi_0 + \gamma L_0 F L_0 \gamma$ to V^2 , $L = L_0 + L_0 \Gamma^0 L$ to V^3 (with $L = L_0 + L_0 F L_0$, F and Γ^0 perturbative) and $\chi = P + P V \chi$ (section 6) to V^2 : residuals $\{\{0, 0, 0\}, \{0, 0, 0, 0\}, \{0, 0, 0\}\}$ ✓

The excitations of the system are the poles of L : particle-hole pairs, collective modes such as plasmons and spin waves, excitons. An approximation for the response is a choice of the kernel. Keeping only the Hartree part of Γ^0 , the direct interaction, gives the RPA chain of bubbles; the Hartree-Fock kernel, direct minus exchange, gives the ladders of time-dependent Hartree-Fock; the Hartree term plus the exchange of the screened interaction W gives the Bethe-Salpeter equation used after GW for the optical spectra and the excitons of solids [68, 69]. A choice is conserving when its kernel is $\delta\Sigma/\delta G$ of the self-energy in its propagators (see below): the RPA with Hartree propagators and time-dependent Hartree-Fock with Hartree-Fock ones are, the usual Bethe-Salpeter equation of GW, which drops $\delta W/\delta G$, is not exactly. Dropping the Hartree part of the kernel, $\Gamma^0 \rightarrow \Gamma_{xc}$, removes the chains joined by single interaction lines and leaves the proper response, the polarization P of section 6, which section 14 writes as $P = \gamma L_0 \tilde{\Lambda}$. The operator enters only through its bare vertex, and the kernels are the same for all operators: for the current γ is $(\mathbf{k} + \mathbf{q}/2)/m$ in momentum space, for the spin density a Pauli matrix.

11.2 Conserving approximations

The response is the second variation of the effective action: with the one-body source U of section 10, $\delta\Gamma/\delta U$ is the propagator, $\delta^2\Gamma/\delta U \delta U$ the response $L = \delta G/\delta U$, and its kernel is the $\Gamma^0 = \delta\Sigma/\delta G$ of the same Φ . For the Hartree-Fock Φ this is time-dependent Hartree-Fock (the RPA with exchange), order by order, with Hartree-Fock lines; the kernel is the derivative of the Hartree-Fock Φ , and the equation of the response is iterated:

```
phiHF = OrderPart[luttingerWard, InteractionPotential, 1];
gamma0HF = LabelFunction[FunctionalDerivative[phiHF, DressedGreenFunction[x4, x3],
  DressedGreenFunction[x2, x1]], {x1, x2, x3, x4}];
(* the same: IrreducibleVertex[phiHF, DressedGreenFunction, {x1, x2, x3, x4}] *)
nextL[l_] := ExactEquation["Response", {"L" -> LabelFunction[l, {x1, x2, x3, x4}],
  "Gamma0" -> gamma0HF, "G" -> DressedGreenFunction}, {x1, x2, x3, x4}][[2]];
lTDHF = Nest[nextL, DressedGreenFunction[x1, x4] DressedGreenFunction[x3, x2], 2];
chiTDHF = ExactEquation["Susceptibility", {"Chi" -> ChiBlob,
  "L" -> LabelFunction[lTDHF, {x1, x2, x3, x4}]}, {z1, z2}][[2]]
```

$$\chi_{\text{TDHF}} =$$

$$V^0 \quad z_1 \text{---} \text{---} z_2$$

$$V \quad + \quad z_1 \text{---} \text{---} z_2 \quad - \quad z_1 \text{---} \text{---} z_2$$

$$V^2 \quad - \quad z_1 \text{---} \text{---} z_2 \quad + \quad z_1 \text{---} \text{---} z_2 \quad - \quad z_1 \text{---} \text{---} z_2 \quad + \quad z_1 \text{---} \text{---} z_2$$

Static and dynamic limits. "Limit" $\rightarrow$ "Static" takes $q \rightarrow 0$ at zero frequency, the thermodynamic limit; "Dynamic" takes $q = 0$ first and the frequency to zero afterwards. For the bubble (the Lindhard function χ_0) and for time-dependent Hartree–Fock to first order:

$$\chi_0(q \rightarrow 0, 0) = 2 \sum_p n'_F(\xi_p),$$

$$\chi_{\text{TDHF}}(q \rightarrow 0, 0) = 2 \sum_{p_1} n'_F(\epsilon_{p_1}) - 2 \sum_{p_1, p_2} v_{p_1-p_2} n'_F(\epsilon_{p_1}) n'_F(\epsilon_{p_2}) + 4 v_0 \sum_{p_1, p_2} n'_F(\epsilon_{p_1}) n'_F(\epsilon_{p_2}).$$

In a Φ -derivable approximation the density is conserved, and its response vanishes at $q = 0$ and $\nu \neq 0$, order by order; the static limit is the thermodynamic derivative $\partial^2 \Omega / \partial \mu^2 = -\partial N / \partial \mu$ (the compressibility sum rule) when χ is the response of the Φ that gives Ω [37, 38]. The field ϕ^2 of ϕ^4 theory is not conserved, and the two limits of its Hartree response (chains of bubbles) differ:

$$\chi_H = -\frac{1}{2} z_1 \text{---} z_2 - \frac{1}{4} z_1 \text{---} z_2 - \frac{1}{8} z_1 \text{---} z_2$$

$$\chi_H^{(0)}(q \rightarrow 0, 0) = \frac{1}{8} \sum_{p_1} \frac{-1 - 2 n_B(M_{p_1}) + 2 M_{p_1} n'_B(M_{p_1})}{M_{p_1}^3},$$

$$\chi_H^{(0)}(0, \nu \rightarrow 0) = \frac{1}{8} \sum_{p_1} \frac{-1 - 2 n_B(M_{p_1})}{M_{p_1}^3}.$$

time-dependent Hartree–Fock, dynamic limit, orders 0 to 2	$\{0, 0, 0\}$ ✓
a ring of 8 sites, $\xi_k = -2 \cos k - \mu$, $v_q = 0.6 + 0.5 \cos q$, $T = \frac{1}{4}$, $\mu = 0.3$, self-consistent ϵ_k :	
$\partial \Omega_{\text{HF}} / \partial \mu + N$ with the three orderings	$\{0, 0, 0\}$ ✓
$\partial^2 \Omega_{\text{HF}} / \partial \mu^2 = -0.25704$, static TDHF response -0.25704	0 ✓
the bubble of Hartree–Fock lines alone, without the vertex corrections:	-0.3235

12 The parquet equations

The fully irreducible vertex. At zero mean field and fixed G the derivatives of the 2PI action with respect to the means are skeleton vertex functions (section 9.5): the second is $D_0^{-1} - \Sigma[G]$, and the fourth is the fully irreducible vertex,

$$\Gamma_{\text{irr}}(x_1, x_2, x_3, x_4) = \frac{\delta^4 \Gamma[\bar{\phi}, G]}{\delta \bar{\phi}(x_1) \delta \bar{\phi}(x_2) \delta \bar{\phi}(x_3) \delta \bar{\phi}(x_4)} \Big|_{\bar{\phi}=0, G}$$

($\delta^4 \Gamma / \delta \bar{\Psi} \delta \Psi \delta \bar{\Psi} \delta \Psi$ for fermions). Its diagrams are those of Γ_2 with four means, opened: a cut of two lines that separated the legs into two pairs would cut a vacuum diagram of Γ_2 in two, so that none of them is two-particle reducible in any channel. The parquet equations follow from the Legendre transform with respect to J and K [48, 52]. In ϕ^4 theory, to fourth order,

```
gammaPhiG4 = EffectiveAction2PI[FreeBosonGeneratingFunctional, Phi4Vertex, 4,
  FreePropagator -> DressedPropagator, "Statistics" -> "Boson",
  "MeanFields" -> {phi -> phiMean}, "MeanFieldDegree" -> {4}];
SetSourcesToZero[FunctionalDerivative[gammaPhiG4, phiMean[x1], phiMean[x2],
  phiMean[x3], phiMean[x4]]]
```

it is the point vertex up to third order, and at fourth order the envelope, whose four vertices, one on each leg, are joined pairwise by six lines — the sides and the diagonals of a square, like the back of an envelope:

$$\Gamma_{\text{irr}}(x_1, x_2, x_3, x_4)|_{\lambda^4} = - \begin{array}{c} x_1 \quad x_4 \\ \diagdown \quad \diagup \\ \quad \quad \diagup \quad \diagdown \\ x_2 \quad x_3 \end{array}$$

The diagrams of Γ_{irr} at fourth order: 1 for ϕ^4 , 64 for the electron gas; for the electron gas they are those that become this picture when every interaction line is shrunk to a point.

$\delta^4 \Gamma / \delta \bar{\phi}^4|_{\bar{\phi}=0, G} = \Gamma_{\text{irr}}$ of ParquetDecomposition (below), λ to λ^4 $\{0, 0, 0, 0\}$ ✓
 the same for the electron gas, $\delta^4 \Gamma / \delta \bar{\Psi} \delta \Psi \delta \bar{\Psi} \delta \Psi$, orders V and V^4 $\{0, 0\}$ ✓

The vertices of the channels. The vertex irreducible in one channel is a second derivative of the Luttinger–Ward functional with respect to the propagator: in the particle–hole channel $\Gamma_{\text{ph}} = \Gamma^0 = \delta^2 \Phi / \delta G \delta G$ (section 9.6). For real bosons the two lines of a pair are the same, and the kernels of the channels s ($ab|cd$), t ($ac|bd$) and u ($ad|bc$) of section 8.4 are one function, $\Gamma_s = \Gamma_{ab;cd}^0 = 4 \delta^2 \Gamma_2 / \delta G_{ab} \delta G_{cd}$, with b and c , or b and d , exchanged:

```
gammaS = 4 FunctionalDerivative[gamma2, DressedPropagator[a, b], DressedPropagator[c,
d]];
gammaT = gammaS /. {b -> c, c -> b}; gammaU = gammaS /. {b -> d, d -> b};
(* the same: IrreducibleVertex[gamma2, DressedPropagator, {a, b, c, d},
"Statistics" -> "Boson", "Channel" -> All] *)
```

the three derivatives minus IrreducibleVertex with "Channel" -> All: $\{0, 0, 0\}$ ✓

For fermions the particle–particle kernel, whose two lines run the same way, is not a derivative with respect to G : it is one with respect to the pairing propagators, and with the superfield of section 13 the kernels of all three channels are second derivatives of one functional.

The equations. The channels sort the diagrams of a four-point vertex: a diagram is reducible in a channel if cutting two propagator lines separates its legs into the two pairs of that channel, $(x_1 x_2 | x_3 x_4)$ for ph, $(x_1 x_4 | x_3 x_2)$ for $\overline{\text{ph}}$ and $(x_1 x_3 | x_2 x_4)$ for pp. These definitions do not depend on perturbation theory: the exact vertex F is the sum of the parts R_r reducible in each channel and of a fully (or totally) irreducible part Γ_{irr} (often written Λ), and since no diagram is reducible in two channels [70, 48, 71, 72, 58],

$$F = \Gamma_{\text{irr}} + R_{\text{ph}} + R_{\overline{\text{ph}}} + R_{\text{pp}}.$$

In each channel the vertex irreducible in that channel, $\Gamma_r = F - R_r$ (for ph the derivative above, for $\overline{\text{ph}}$ the same by crossing, for pp the derivative of section 13), generates the reducible part by a Bethe–Salpeter equation, Γ_r and F joined by the pair of lines of the channel: cutting the first pair of lines of a reducible diagram leaves an irreducible piece and the rest. In the particle–hole channel $\Gamma_{\text{ph}} = \Gamma^0$ and $R_{\text{ph}} = \Gamma^0 L_0 F$ (section 10); in $\overline{\text{ph}}$ the pair joins $(x_1 x_4)$ to $(x_3 x_2)$, and in pp its two lines run the same way, with the factor $\frac{1}{2}$ of two identical particles. In pictures, with Γ_{irr} grey and the Γ_r cross-hatched (the pp term turned as in the ladder of the T-matrix, the incoming x_4, x_2 on the left and the two lines parallel from left to right):

$$F = \Gamma_{\text{irr}} + \Gamma_{\text{ph}} + F - \frac{1}{2} \Gamma_{\text{pp}}$$

Given Γ_{irr} and G , these are closed equations for the three R_r . The Schwinger–Dyson (or Dyson–Schwinger) equation [17, 18], the first equation of motion of the Martin–Schwinger hierarchy [64], gives Σ in terms of F : the Hartree and Fock diagrams with the full G , and one diagram with F :

$$x \text{---} \Sigma \text{---} y = x \text{---} \text{Hartree} \text{---} y - x \text{---} \text{Fock} \text{---} y + x \text{---} F \text{---} y$$

With the Dyson equation, these equations determine G and F together. The parquet approximation replaces Γ_{irr} by the bare interaction — exact to third order, since the first fully irreducible diagrams, of the envelope type, appear at the fourth.

The check. The package also classifies the diagrams by cutting their lines, and checks every equation order by order:

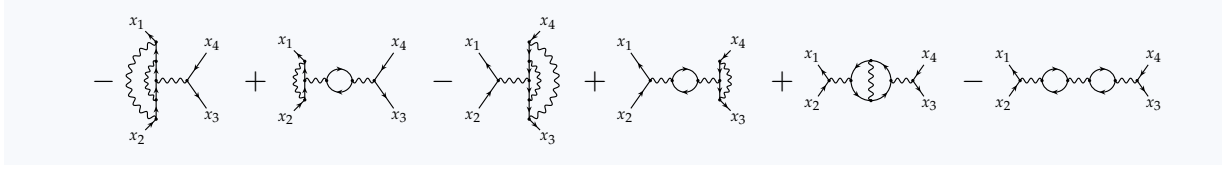
```
decomposition = ParquetDecomposition[fullVertex, {x1, x2, x3, x4},
  {DressedGreenFunction}];
```

The particle–hole irreducible part $F - R_{\text{ph}} = \Gamma_{\text{irr}} + R_{\text{ph}} + R_{\text{pp}}$ is the vertex Γ^0 of section 9.6, whose diagrams are grouped there by channel. The diagrams reducible in the particle–hole channel are

$$R_{\text{ph}} =$$

V^2

V^3



The vertex obtained by differentiating the Luttinger–Ward functional twice and the one obtained by cutting the perturbative diagrams are the same:

$$F - R_{\text{ph}} - \Gamma^0, \text{ to } V^3: 0 \checkmark$$

CheckParquetEquations verifies the Bethe–Salpeter equation of every channel, order by order:

```
CheckParquetEquations[fullVertex, {x1, x2, x3, x4}, DressedGreenFunction,
  InteractionPotential, 3]
```

The numbers of diagrams in each class, and the residuals of the three Bethe–Salpeter equations:

order	diagrams of F	Γ_{irr}	R_{ph}	$R_{\overline{\text{ph}}}$	R_{pp}	several channels	Bethe–Salpeter ph, $\overline{\text{ph}}$, pp
V	2	2	0	0	0	0	✓✓✓
V^2	10	0	4	4	2	0	✓✓✓
V^3	82	0	32	32	18	0	✓✓✓

The self-energy is in turn given by the full vertex: the Schwinger–Dyson equation drawn above closes the parquet equations; it is the reason why, beyond Hartree–Fock, $\Sigma[G]$ has as many diagrams at order V^{m+1} as F at order V^m ($m \geq 1$). The vertex is antisymmetric under the exchange of its two outgoing or of its two incoming legs (crossing), which maps the particle–hole channel onto the transverse one, hence their equal numbers of diagrams:

Schwinger–Dyson equation, V^2 and V^3 residuals $\{0, 0\}$ ✓
crossing $F_{12;34} = -F_{32;14} = -F_{14;32}$, $R_{\text{ph}}(1, 2; 3, 4) = -R_{\overline{\text{ph}}}(3, 2; 1, 4)$ residuals $\{0, 0, 0\}$ ✓

Bosons. The parquet equations hold for bosons too: with the option "Statistics" -> "Boson", ParquetDecomposition and CheckParquetEquations use the channels s ($ab|cd$), t ($ac|bd$) and u ($ad|bc$) of section 8.4. In ϕ^4 theory, up to third order, Γ_{irr} is the point vertex λ , and each channel has 1 and 3 diagrams at orders λ^2 and λ^3 ; those of the channel s are

```
ParquetDecomposition[vertexPhi4, {a, b, c, d}, {DressedPropagator},
  "Statistics" -> "Boson"]["s"]
CheckParquetEquations[vertexPhi4, {a, b, c, d}, DressedPropagator, lambda, 3,
  "Statistics" -> "Boson"]["Residuals"]
```

$R_s =$

$$\lambda^2 \quad -\frac{1}{2} \text{diagram}$$

$$\lambda^3 \quad -\frac{1}{2} \text{diagram} - \frac{1}{2} \text{diagram} - \frac{1}{4} \text{diagram}$$

At order λ^4 (three loops) $\Gamma^{(4)}$ has 37 skeleton diagrams, and ParquetDecomposition finds 1 fully irreducible diagram by cutting lines: the envelope, found above as $\delta^4 \Gamma / \delta \bar{\phi}^4$, the first correction

to the parquet approximation. Eckhardt, Kappl, Kauch and Held write the parquet equation of ϕ^4 theory for the four-point vertex, $\Gamma^{(4)} = \Gamma_{\text{irr}} - \frac{1}{2} \sum_r \Gamma^{(4)} L_0 \Gamma_r$, with the reducible parts as $\Gamma^{(4)} L_0 \Gamma_r$ instead of $\Gamma_r L_0 \Gamma^{(4)}$: the same, since the Bethe–Salpeter equation $\Gamma^{(4)} = \Gamma_r - \frac{1}{2} \Gamma_r L_0 \Gamma^{(4)}$ can be solved from either side.

The Schwinger–Dyson equation of ϕ^4 theory gives the self-energy by the tadpole with the full propagator and one diagram with the full vertex $\Gamma^{(4)}$, the box of the Bethe–Salpeter equation (section 10), sitting on the line from a to b as F in the equation of the electron gas; every line is the full propagator G :

$$a \text{---} \textcircled{\Sigma} \text{---} b = \frac{1}{2} a \text{---} \textcircled{} \text{---} b - \frac{1}{6} a \text{---} \text{---} b$$

parquet residuals of ϕ^4 theory, orders λ to λ^3

$\Gamma^{(4)} - R_r - \Gamma_r$, the kernels Γ_r of s, t, u from $\Gamma_2[G]$, to λ^3

Schwinger–Dyson equation, λ^2 and λ^3

crossing $\Gamma_{abcd}^{(4)} = \Gamma_{bacd}^{(4)} = \Gamma_{acbd}^{(4)}$, $R_s(a, b, c, d) = R_t(a, c, b, d)$

$s: \{0, 0, 0\}, t: \{0, 0, 0\}, u: \{0, 0, 0\}$ ✓

$\{0, 0, 0\}$ ✓

residuals $\{0, 0\}$ ✓

residuals $\{0, 0, 0\}$ ✓

13 Pairing: the superfield of Nambu and Gor'kov

The superfield. The 2PI functional of fermions of section 9 has one variable, $G = -\langle T\psi\bar{\psi} \rangle$, and two shortcomings. Its second derivative joins a particle and a hole, so it gives the kernels of the channels ph and $\bar{p}\bar{h}$ but not that of pp, whose two lines run the same way (section 12); and at finite means it misses the anomalous propagator $-\langle T\psi\psi \rangle$, of order $V\Psi\Psi$ (section 9.3). The same propagator, at zero means, is the order parameter of a superconductor. Both are removed by one change of variable, that of Nambu and Gor'kov [73, 74]: ψ and $\bar{\psi}$ are the two components of one field, the superfield $\psi_a = (\psi, \bar{\psi})$, whose label $a = (x, s)$ is a point and a component. For the package it is an ordinary Grassmann field, with one source; its propagator

$$\mathcal{G}_{ab} = -\langle T\psi_a\psi_b \rangle_c = -\mathcal{G}_{ba}, \quad \mathcal{G}(x, y) = \begin{pmatrix} \mathcal{G}_{\psi\psi}(x, y) & G(x, y) \\ -G(y, x) & \mathcal{G}_{\bar{\psi}\bar{\psi}}(x, y) \end{pmatrix} = \begin{pmatrix} x \circ \longleftrightarrow y & x \circ \longleftrightarrow y \\ -x \circ \longrightarrow y & x \circ \longleftarrow y \end{pmatrix},$$

is antisymmetric, a Nambu matrix with the normal block $G = \mathcal{G}_{\psi\bar{\psi}}$ and the anomalous (pairing) blocks $\mathcal{G}_{\psi\psi}(x, y) = -\langle T\psi(x)\psi(y) \rangle$ and $\mathcal{G}_{\bar{\psi}\bar{\psi}}(x, y) = -\langle T\bar{\psi}(x)\bar{\psi}(y) \rangle$. An anomalous line has two arrowheads (line styles "DivergingArrows" and "ConvergingArrows"), which point to its two ψ ends and away from its two $\bar{\psi}$ ends, as the arrow of a normal line points to its ψ end: along a fermion line the arrows turn inside the anomalous lines. Since such a line shows no orientation, the weight of a picture reads it along its fermion line, a loop in either sense and an open line from its first external point.

The free functional and the interaction are written as for ϕ^4 theory, one source, one antisymmetric propagator and one totally antisymmetric vertex $\mathcal{V}$, a point in the pictures:

```
DeclareGrassmannSource[NambuSource]; DeclareField[NambuField, NambuSource];
DeclareAntisymmetric[BareNambuPropagator, NambuPropagator, NambuVertex];
DeclareLocalVertex[NambuVertex];
nambuZ0 = Exp[1/2 IntegralOver[BareNambuPropagator[a, b] NambuSource[a] **
  NambuSource[b], {a, b}]];
nambuInteraction = 1/24 IntegralOver[NambuVertex[a, b, c, d] NambuField[a] **
  NambuField[b] ** NambuField[c] ** NambuField[d], {a, b, c, d}];
```

that is, $Z_0[J] = e^{\frac{1}{2}J \cdot \mathcal{G}_0 \cdot J}$ with $\mathcal{G}_0$ the Nambu matrix of G_0 alone, and $S_{\text{int}} = \frac{1}{4!} \int \mathcal{V}_{abcd} \psi_a \psi_b \psi_c \psi_d$. For the electron gas the components of $\mathcal{V}$ are the derivatives of $\frac{1}{2} \int V \bar{\psi} \psi \psi \psi$, $\mathcal{V}(x_1 \bar{\psi}, x_2 \bar{\psi}, x_3 \psi, x_4 \psi) = V(x_1, x_2) (\delta_{14} \delta_{23} - \delta_{13} \delta_{24})$, and the others follow by antisymmetry or vanish: one vertex holds the normal interaction and, once the means are shifted, the anomalous vertices.

The functional. The two-point source is a Nambu matrix too, the action gaining $\frac{1}{2} \int \psi K \psi$: its normal block is the one-body source U coupled to $\bar{\psi} \psi$, and its anomalous blocks are the pairing sources, coupled to $\psi \psi$ and $\bar{\psi} \bar{\psi}$. The Legendre transform of $W[J, K]$ with respect to J and to the whole of K makes the whole Nambu propagator the variable; at zero means

$$\Gamma[\mathcal{G}] = \Phi[\mathcal{G}] - \frac{1}{2} \text{Tr} \left(-1 + \left(-K + \mathcal{G}_0^{-1} \right) \mathcal{G} \right) - \frac{1}{2} \text{Tr} \ln \left(-\mathcal{G}^{-1} \right),$$

an exact definition, like the transforms before it: stationary at the exact Nambu propagator, where its value is $-\log Z$, with $\Phi[\mathcal{G}]$ minus the 2PI vacuum diagrams in the expansion. The trace terms are half those of section 9.4, with the opposite sign to those of a real boson: the Gaussian integral over one Grassmann field is a Pfaffian, $\log \int e^{-\frac{1}{2} \psi A \psi} = \frac{1}{2} \log \det A$. In components the trace-log is

$$-\frac{1}{2} \text{Tr} \ln(-\mathcal{G}^{-1}) = -\text{Tr} \ln(-G^{-1}) + \frac{1}{2} \text{Tr} \ln(1 + G^{-T} \mathcal{G}_{\bar{\psi}\bar{\psi}} G^{-1} \mathcal{G}_{\psi\psi}),$$

so that at zero anomalous propagator and pairing source the trace terms are those of section 9.4, and $\Phi[\mathcal{G}]$ is $\Phi[G]$ (below): the functional of section 9 is this one at $\mathcal{G}_{\psi\psi} = \mathcal{G}_{\bar{\psi}\bar{\psi}} = 0$, and nothing found there changes.

Φ and its components. Expanded in the interaction, $\Phi[\mathcal{G}]$ has the pictures of $\Gamma_2[G]$ of ϕ^4 theory, one diagram at each order:

```
nambuPhi = LuttingerWardFunctional[nambuZ0, nambuInteraction, 3,
  BareNambuPropagator -> NambuPropagator];
```

$\Phi[\mathcal{G}] =$

$$\mathcal{V} - \frac{1}{8} \infty$$

$$\mathcal{V}^2 - \frac{1}{48} \ominus$$

$$\mathcal{V}^3 + \frac{1}{48} \bigcirc$$

Here lines and vertex are antisymmetric, so that a picture gives a term up to the order of its labels, which the formula fixes: to first order $\Phi = \frac{1}{8} \int_{z_1 z_2 z_3 z_4} \mathcal{G}(z_1, z_2) \mathcal{G}(z_3, z_4) \mathcal{V}(z_1, z_2, z_3, z_4)$. SuperfieldComponents writes such an expression in the components: the rules give the components of the superfield, the blocks of each propagator, and for the vertex the component interaction, whose derivatives are its components.

```
nambuRules = {NambuField -> {psi, psibar}, NambuPropagator -> {DressedGreenFunction,
  AnomalousGreenFunction, AnomalousGreenFunctionBar}, NambuVertex -> CoulombVertex};
SuperfieldComponents[nambuPhi, {}, nambuRules]
```

To first order,

$$\Phi[G, \mathcal{G}_{\psi\psi}, \mathcal{G}_{\bar{\psi}\bar{\psi}}] = -\frac{1}{2} \int_{z_1 z_2} \mathcal{G}_{\psi\psi}(z_1, z_2) \mathcal{G}_{\bar{\psi}\bar{\psi}}(z_1, z_2) V(z_1, z_2) \\ - \frac{1}{2} \int_{z_1 z_2} G(z_1, z_2) G(z_2, z_1) V(z_1, z_2) + \frac{1}{2} \int_{z_1 z_2} G(z_1, z_1) G(z_2, z_2) V(z_1, z_2),$$

the Hartree and Fock diagrams of $\Phi[G]$ and a pairing (Bogoliubov) term with the geometry of the Fock diagram; to V^3 the components have 3, 7, 52 diagrams, those of $\Phi[G]$ and those in which the fermion lines run through pairs of anomalous lines:

$$\Phi[G, \mathcal{G}_{\psi\psi}, \mathcal{G}_{\bar{\psi}\bar{\psi}}] =$$

$$V \quad -\frac{1}{2} \text{ (Hartree)} + \frac{1}{2} \text{ (Fock)} - \frac{1}{2} \text{ (pairing)}$$

$$V^2 \quad +\frac{1}{4} \text{ (Hartree)} - \frac{1}{2} \text{ (Hartree)} - \text{ (Fock)} + \frac{1}{4} \text{ (Fock)} - \frac{1}{4} \text{ (pairing)} + \frac{1}{2} \text{ (pairing)} - \frac{1}{4} \text{ (pairing)}$$

$$V^3 \quad +\frac{1}{2} \text{ (Hartree)} - \frac{1}{2} \text{ (Hartree)} - \text{ (Fock)} + \frac{1}{2} \text{ (Fock)} + \frac{1}{2} \text{ (Hartree)} - \text{ (Hartree)} + \text{ (Fock)} - \text{ (Fock)} \\ - \frac{1}{2} \text{ (Hartree)} + \frac{1}{6} \text{ (Fock)} + \text{ (Hartree)} - \text{ (Hartree)} + \frac{1}{2} \text{ (Hartree)} - \frac{1}{6} \text{ (Hartree)} + \text{ (Hartree)} - \text{ (Hartree)} \\ - \frac{1}{6} \text{ (Fock)} + \frac{1}{2} \text{ (pairing)} - \text{ (pairing)} - \text{ (Hartree)} + \text{ (Hartree)} + \text{ (Hartree)} - \frac{1}{6} \text{ (Hartree)} \\ + \text{ (pairing)} - \frac{1}{2} \text{ (pairing)} + \text{ (Hartree)} - \text{ (Hartree)} - \text{ (Hartree)} - \text{ (pairing)} - \frac{1}{2} \text{ (Hartree)} + \text{ (pairing)} \\ - \frac{1}{6} \text{ (pairing)} - \text{ (Hartree)} - \text{ (Hartree)} + \text{ (Hartree)} + \text{ (Hartree)} - \text{ (pairing)} + \text{ (pairing)} + \frac{1}{6} \text{ (pairing)} \\ + \frac{1}{2} \text{ (Hartree)} - \frac{1}{2} \text{ (pairing)} + \frac{1}{2} \text{ (pairing)} + \frac{1}{2} \text{ (Hartree)} - \frac{1}{2} \text{ (Hartree)} - \frac{1}{2} \text{ (Fock)} - \frac{1}{2} \text{ (Hartree)} \\ + \frac{1}{2} \text{ (Fock)} + \frac{1}{2} \text{ (Hartree)} + \frac{1}{2} \text{ (pairing)} - \frac{1}{2} \text{ (pairing)} + \frac{1}{2} \text{ (Fock)} - \frac{1}{2} \text{ (Hartree)}$$

the components of $\Phi[G]$ minus the Φ of a Z_0 with the pairing terms $\frac{1}{2}\bar{\eta} \mathcal{G}_{0,\psi\psi}\bar{\eta} + \frac{1}{2}\eta \mathcal{G}_{0,\bar{\psi}\bar{\psi}}\eta$, order by order; at zero anomalous propagators, minus $\Phi[G]$: $\{\{0, 0, 0\}, 0\}$ ✓

Self-energy, gap function, Gor'kov equations. The self-energy is the Nambu matrix $\Sigma = -2\delta\Phi/\delta\mathcal{G}$, the derivative with respect to an antisymmetric kernel being antisymmetrized ($\delta\mathcal{G}_{cd}/\delta\mathcal{G}_{ab} = \frac{1}{2}(\delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc})$, as for real bosons it is symmetrized), one diagram at each order:

```
nambuSigma = -2 FunctionalDerivative[nambuPhi, NambuPropagator[a, b]]
(* the same: SelfEnergy[nambuPhi, NambuPropagator, {a, b},
  "Statistics" -> "Superfield"] *)
```

$$\Sigma[\mathcal{G}](a, b) =$$

$$\mathcal{V} \quad \frac{1}{2} a \text{---} \bigcirc \text{---} b$$

$$\mathcal{V}^2 \quad + \frac{1}{6} a \text{---} \bigcirc \text{---} b$$

$$\mathcal{V}^3 \quad - \frac{1}{4} a \text{---} \bigcirc \text{---} b$$

The stationarity of Γ , with the source, is the Dyson equation in Nambu form; to first order

$$-2 \frac{\delta \Gamma}{\delta \mathcal{G}(a, b)} = -2 \left(\frac{1}{4} \int_{z_1 z_2} \mathcal{G}(z_1, z_2) \mathcal{V}(a, b, z_1, z_2) - \frac{1}{2} K(a, b) + \frac{1}{2} \mathcal{G}_0^{-1}(a, b) - \frac{1}{2} \mathcal{G}^{-1}(a, b) \right),$$

and in general $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - K - \Sigma[\mathcal{G}]$. As a matrix,

$$\Sigma = \mathcal{G}_0^{-1} - K - \mathcal{G}^{-1} = \begin{pmatrix} \bar{\Delta} & -\Sigma^T \\ \Sigma & \Delta \end{pmatrix},$$

with $\Sigma(x, y) = \Sigma_{x\bar{\psi}, y\psi}$ the self-energy of section 9.4 and the anomalous self-energies, the gap functions $\Delta(x, y) = \Sigma_{x\bar{\psi}, y\bar{\psi}}$ and $\bar{\Delta}(x, y) = \Sigma_{x\psi, y\bar{\psi}}$: at the stationary point the quadratic action is $-\bar{\psi}(G_0^{-1} - \Sigma)\psi + \frac{1}{2}\bar{\psi}\Delta\bar{\psi} + \frac{1}{2}\psi\bar{\Delta}\psi$. For a normal $\mathcal{G}_0$ the components of the Dyson equation are the Gor'kov equations; in these two pictures only, the double line is the full G , the single line G_0 , and the anomalous lines are full (the free propagator has none),

$$x \text{---} \bigcirc \text{---} y = x \text{---} \bigcirc \text{---} y + x \text{---} \bigcirc \text{---} \Delta \text{---} y + x \text{---} \bigcirc \text{---} \Sigma \text{---} y$$

$$x \text{---} \bigcirc \text{---} y = - x \text{---} \Delta \text{---} y + x \text{---} \Sigma \text{---} y$$

and the conjugate ones for G^T and $\mathcal{G}_{\bar{\psi}\bar{\psi}}$. To first order in Δ , $\mathcal{G}_{\psi\psi} = -G\Delta G^T$.

Hartree–Fock–Bogoliubov and BCS. To first order the self-energy is

$$\Sigma[\mathcal{G}](a, b) = -\frac{1}{2} \int_{z_1 z_2} \mathcal{G}(z_1, z_2) \mathcal{V}(a, b, z_1, z_2),$$

and its components are the Hartree and Fock potentials and the gap function (every line again the full propagator, drawn as a single line):

$$x_1 \text{---} \Sigma \text{---} x_2 = x_1 \text{---} \text{---} x_2 - x_1 \text{---} \text{---} x_2$$

$$x_1 \text{---} \Delta \text{---} x_2 = - x_1 \text{---} \text{---} x_2$$

that is, $\Delta(x_1, x_2) = V(x_1, x_2) \mathcal{G}_{\psi\psi}(x_1, x_2) = -V(x_1, x_2) \langle T\psi(x_1)\psi(x_2) \rangle$, and $\bar{\Delta} = V\mathcal{G}_{\bar{\psi}\bar{\psi}}$. With the Gor'kov equations these are the Hartree–Fock–Bogoliubov equations: the stationarity of Γ with Φ truncated at first order, a Φ -derivable approximation. Their pairing part is the gap equation of Bardeen, Cooper and Schrieffer [75, 73], the self-consistent decoupling of $\frac{1}{2}V\bar{\psi}\bar{\psi}\psi\psi$ in the pairs; with spin in the labels and an attraction, $\Delta_{\uparrow\downarrow}$ is the gap of the superconductor.

first order: $\Sigma - \Sigma_{\text{HF}}, \Delta - V\mathcal{G}_{\psi\psi}, \bar{\Delta} - V\mathcal{G}_{\bar{\psi}\bar{\psi}}$	$\{0, 0, 0\}$ ✓
the Dyson equation of $\mathcal{G}$ in components minus the Gor'kov equations	$\{0, 0\}$ ✓
$-2\delta\Gamma/\delta\mathcal{G} - (\Sigma[\mathcal{G}] + \mathcal{G}^{-1} - \mathcal{G}_0^{-1} + K)$, to $\mathcal{V}^3$	0 ✓

The kernels of the three channels. The kernel is $\Gamma_{abcd}^0 = -2\delta\Sigma_{ab}/\delta\mathcal{G}_{cd} = 4\delta^2\Phi/\delta\mathcal{G}_{ab}\delta\mathcal{G}_{cd}$, irreducible in the channel s ($ab|cd$) as for real bosons: the point vertex at first order, then 2 and 6 diagrams,

$$\Gamma^0(a, b, c, d) =$$

$$\mathcal{V} = - \begin{array}{c} a \quad d \\ \diagdown \quad \diagup \\ b \quad c \end{array}$$

$$\mathcal{V}^2 = + \frac{1}{2} \begin{array}{c} a \quad d \\ \diagdown \quad \diagup \\ \bigcirc \\ \diagup \quad \diagdown \\ b \quad c \end{array} - \frac{1}{2} \begin{array}{c} a \quad c \\ \diagdown \quad \diagup \\ \bigcirc \\ \diagup \quad \diagdown \\ b \quad d \end{array}$$

$$\mathcal{V}^3 = + \frac{1}{2} \begin{array}{c} a \quad c \quad d \\ \diagdown \quad \diagup \quad \diagup \\ \bigcirc \\ \diagup \quad \diagdown \quad \diagdown \\ b \quad d \end{array} + \frac{1}{2} \begin{array}{c} a \quad d \quad c \\ \diagdown \quad \diagup \quad \diagup \\ \bigcirc \\ \diagup \quad \diagdown \quad \diagdown \\ b \quad c \end{array} - \frac{1}{2} \begin{array}{c} a \quad c \quad d \\ \diagdown \quad \diagup \quad \diagdown \\ \bigcirc \\ \diagup \quad \diagdown \quad \diagup \\ b \quad d \end{array} - \frac{1}{2} \begin{array}{c} a \quad d \quad c \\ \diagdown \quad \diagup \quad \diagdown \\ \bigcirc \\ \diagup \quad \diagdown \quad \diagup \\ b \quad c \end{array} - \frac{1}{4} \begin{array}{c} a \quad d \quad c \\ \diagdown \quad \diagup \quad \diagup \\ \bigcirc \quad \bigcirc \\ \diagup \quad \diagdown \quad \diagdown \\ b \quad c \end{array} + \frac{1}{4} \begin{array}{c} a \quad c \quad d \\ \diagdown \quad \diagup \quad \diagup \\ \bigcirc \quad \bigcirc \\ \diagup \quad \diagdown \quad \diagdown \\ b \quad d \end{array}$$

With a single kind of line, the kernels of the other channels need no other derivative: those irreducible in t ($ac|bd$) and in u ($ad|bc$) are the same function with its labels exchanged, with the sign of the permutation of Grassmann labels,

$$\Gamma_s(a, b, c, d) = \Gamma^0(a, b, c, d), \quad \Gamma_t(a, b, c, d) = -\Gamma^0(a, c, b, d), \quad \Gamma_u(a, b, c, d) = \Gamma^0(a, d, b, c),$$

```
gammaS = 4 FunctionalDerivative[nambuPhi, NambuPropagator[a, b], NambuPropagator[c, d]];
gammaT = -4 FunctionalDerivative[nambuPhi, NambuPropagator[a, c], NambuPropagator[b, d]];
gammaU = 4 FunctionalDerivative[nambuPhi, NambuPropagator[a, d], NambuPropagator[b, c]];
(* the same: IrreducibleVertex[nambuPhi, NambuPropagator, {a, b, c, d},
  "Statistics" -> "Superfield", "Channel" -> All] *)
```

and each is $F - R_r$, the full vertex of the superfield minus its part reducible in that channel (section 12), whose Bethe–Salpeter equations have the ladders $+\frac{1}{2}, -\frac{1}{2}, +\frac{1}{2}$ with two lines $\mathcal{G}$ in s, t, u . With the legs $a = (x_1, \bar{\psi}), b = (x_2, \psi), c = (x_3, \bar{\psi}), d = (x_4, \psi)$ of $F(x_1, x_2; x_3, x_4)$ (fermions leaving at x_1, x_3 and entering at x_2, x_4) the channel s is ph , u is ph and t is pp , and at zero anomalous propagators

$$\Gamma_s \rightarrow \Gamma^0(x_1, x_2; x_3, x_4), \quad \Gamma_u \rightarrow -\Gamma^0(x_3, x_2; x_1, x_4),$$

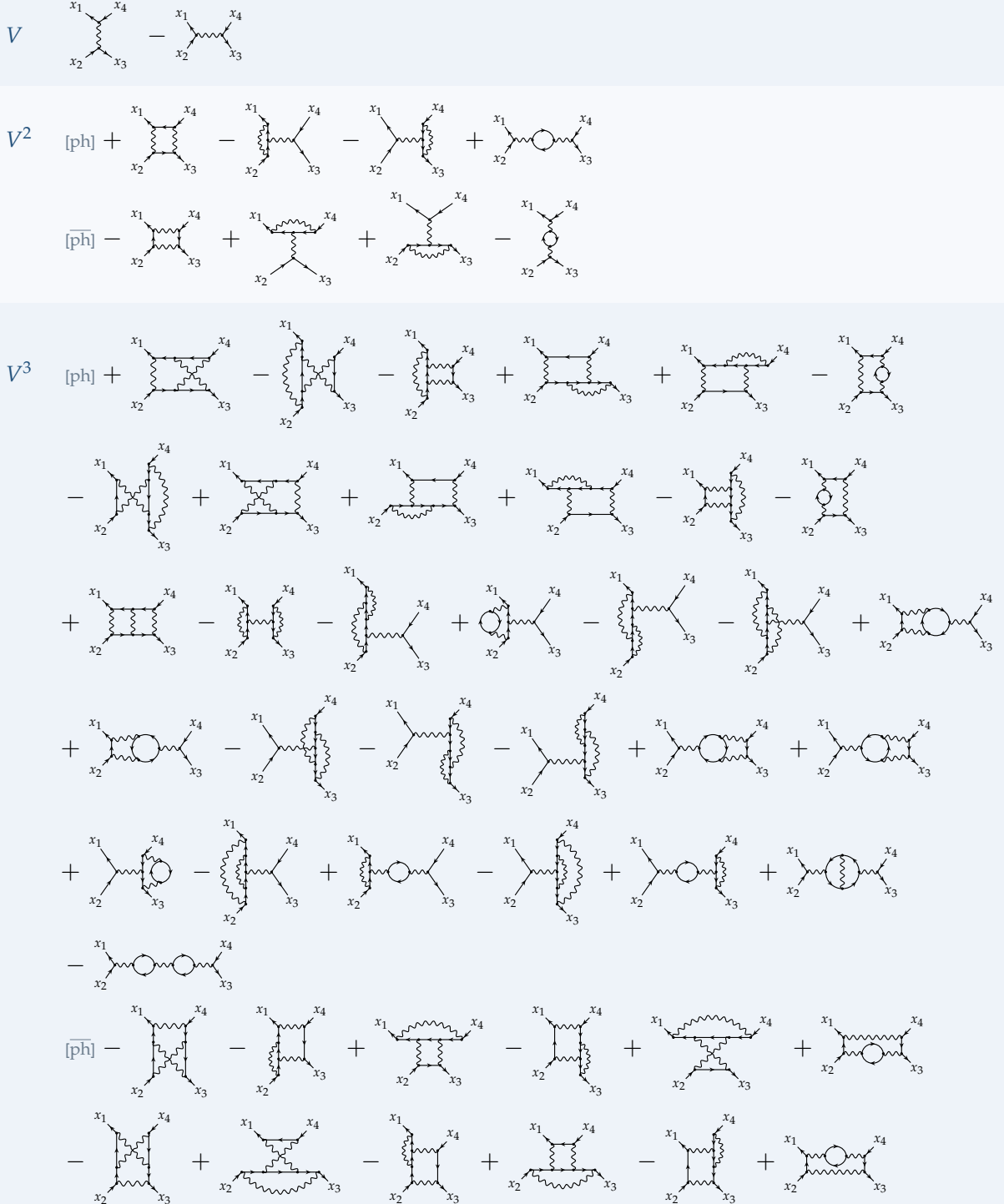
$$\Gamma_t \rightarrow \Gamma_{pp}(x_1, x_2; x_3, x_4) = -4 \frac{\delta^2\Phi}{\delta\mathcal{G}_{\bar{\psi}\bar{\psi}}(x_1, x_3)\delta\mathcal{G}_{\psi\psi}(x_2, x_4)} = 2 \frac{\delta\Delta(x_1, x_3)}{\delta\mathcal{G}_{\psi\psi}(x_2, x_4)} :$$

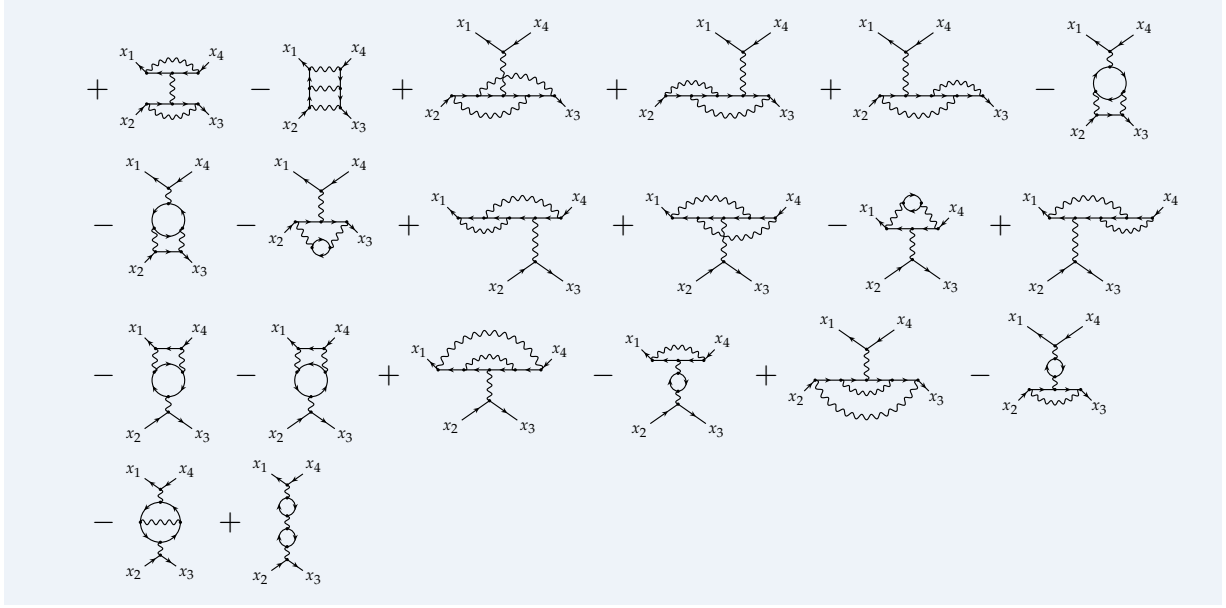
the first two the kernels of section 9.6, from G alone, and the third the particle–particle kernel, the derivative of the gap function with respect to the pair propagator (in a superconductor the blocks mix, and Γ^0 itself is the kernel). The package takes the derivative of the components of Φ with respect to the anomalous blocks; it has 2, 8, 64 diagrams at V, V^2, V^3 , grouped here by channel as Γ^0 in section 9.6:

```

phiComponents = SuperfieldComponents[nambuPhi, {}, nambuRules];
ppKernel = -4 FunctionalDerivative[phiComponents, AnomalousGreenFunction[x2, x4],
  AnomalousGreenFunctionBar[x1, x3]] /. {AnomalousGreenFunction[___] -> 0,
  AnomalousGreenFunctionBar[___] -> 0};
(* the same: the components of gammaT, SuperfieldComponents[gammaT, {a -> psibar[x1],
  b -> psi[x2], c -> psibar[x3], d -> psi[x4]}, {NambuField -> {psi, psibar},
  NambuPropagator -> {DressedGreenFunction, 0, 0}, NambuVertex -> CoulombVertex}] *)

```

 $\Gamma_{pp} =$




The superfield, to $\mathcal{V}^3$: the derivatives $\Sigma, \Gamma_s, \Gamma_t, \Gamma_u$ minus SelfEnergy and IrreducibleVertex with "Channel" $\rightarrow$ All, $\{0, 0, 0, 0\}$ ✓; $\Gamma_r = (F - R_r)$ in s, t, u , $\{0, 0, 0\}$ ✓; the Bethe-Salpeter equations of the three channels, order by order, s : $\{0, 0, 0\}$, t : $\{0, 0, 0\}$, u : $\{0, 0, 0\}$ ✓. The components, to V^3 : $\Gamma_s - \Gamma^0, \Gamma_{pp} - (F - R_{pp})$ and $\Gamma_u - (F - R_{ph})$ of the electron gas, $\{0, 0, 0\}$ ✓; the component of Γ_t minus $\Gamma_{pp} = -4\delta^2\Phi/\delta\mathcal{G}_{\bar{\psi}\psi}\delta\mathcal{G}_{\psi\psi}, 0$ ✓; the equation of the T -matrix, $F - \Gamma_{pp} - \Gamma_{pp} \circ_{pp} F$ ($\circ_{pp}$: the two vertices joined by the pair of lines of the pp channel, with the $\frac{1}{2}$ of identical particles, as in section 12), 0 ✓.

The Thouless criterion. Linear in the pairing, the gap equation is the homogeneous Bethe-Salpeter equation of the particle-particle channel: with $\mathcal{G}_{\psi\psi} = -G\Delta G^T$, $\Delta(x_1, x_3) = -2\delta\Phi/\delta\mathcal{G}_{\bar{\psi}\psi}(x_1, x_3)$ becomes, order by order (1, 4, 32 diagrams to V^3 ; every line the full propagator),

$$x_1 \rightarrow \Delta \rightarrow x_3 = -\frac{1}{2} \Delta \rightarrow \Gamma_{pp} \rightarrow x_3$$

with the two particles propagating from left to right, as in the pp term of the parquet equation (section 12). A solution $\Delta \neq 0$ appears where the ladder $F = \Gamma_{pp} + \Gamma_{pp} \circ_{pp} F$ has a pole, the instability of the normal state towards pairing: the criterion of Thouless for the critical temperature [76].

The gap equation linear in the pairing minus the homogeneous pp ladder, V to V^3 : $\{0, 0, 0\}$ ✓

At finite means. With the means $\Psi = \langle \psi \rangle = (\Psi, \bar{\Psi})$,

```
gammaNambu = EffectiveAction2PI[nambuZ0, nambuInteraction, 3,
  BareNambuPropagator -> NambuPropagator, "Statistics" -> "Superfield",
  "MeanFields" -> {NambuField -> NambuMean}];
```

is the form of section 9.2 with one field,

$$\Gamma[\Psi, \mathcal{G}] = -\frac{1}{2}\Psi\mathcal{G}_0^{-1}\Psi + S_{\text{int}}[\Psi] - \frac{1}{2}\text{Tr}\ln(-\mathcal{G}^{-1}) - \frac{1}{2}\text{Tr}(\mathcal{G}_0^{-1}\mathcal{G} - 1) + \langle S_{\text{int}}^{(2)}[\Psi] \rangle_{\mathcal{G}} + \Gamma_2[\Psi, \mathcal{G}],$$

in which $-\frac{1}{2}\Psi\mathcal{G}_0^{-1}\Psi$ is $-\bar{\Psi}G_0^{-1}\Psi$ and all the vertices of degree two, normal and anomalous, are

closed by $\mathcal{G}$: $V\Psi\Psi\bar{\psi}\bar{\psi}$ by $\mathcal{G}_{\bar{\psi}\bar{\psi}}$. To first order,

$$\begin{aligned}\Gamma[\Psi, \mathcal{G}] = & \frac{1}{24} \int_{z_1 z_2 z_3 z_4} \mathcal{V}(z_1, z_2, z_3, z_4) \Psi(z_1) \Psi(z_2) \Psi(z_3) \Psi(z_4) \\ & - \frac{1}{4} \int_{z_1 z_2 z_3 z_4} \mathcal{G}(z_3, z_4) \mathcal{V}(z_1, z_2, z_3, z_4) \Psi(z_1) \Psi(z_2) \\ & + \frac{1}{8} \int_{z_1 z_2 z_3 z_4} \mathcal{G}(z_1, z_2) \mathcal{G}(z_3, z_4) \mathcal{V}(z_1, z_2, z_3, z_4) \\ & - \frac{1}{2} \int_{z_1 z_2} \mathcal{G}_0^{-1}(z_1, z_2) \Psi(z_1) \Psi(z_2) - \frac{1}{2} \text{Tr} \left(-1 + \mathcal{G}_0^{-1} \mathcal{G} \right) - \frac{1}{2} \text{Tr} \ln \left(-\mathcal{G}^{-1} \right)\end{aligned}$$

Its stationary $\mathcal{G}[\Psi]$ has anomalous blocks of order $V\Psi\Psi$, and there the functional is the 1PI action $\Gamma[\Psi]$ (EffectiveAction1PI with "Statistics" -> "Superfield"), whose components are the $\Gamma[\bar{\Psi}, \Psi]$ of section 8.2, with all its 103 diagrams at V^3 , the 11 with an anomalous vertex included: the 2PI functional of fermions is exact at its stationary point at any means. At $\Psi = 0$ and fixed $\mathcal{G}$ its derivatives are those of section 9.5: $\mathcal{G}_0^{-1} - \Sigma[\mathcal{G}]$, and the fully irreducible vertex $\mathcal{V}$ to third order.

$\Gamma[\Psi, \mathcal{G}[\Psi]] - \Gamma[\Psi]$, orders 0 to 3	$\{0, 0, 0, 0\}$ ✓
components of $\Gamma[\Psi]$ minus $\Gamma[\bar{\Psi}, \Psi]$ of section 8.2, orders 0 to 3	$\{0, 0, 0, 0\}$ ✓
$\delta^2 \Gamma / \delta \Psi \delta \Psi _{0, \mathcal{G}} - \mathcal{G}_0^{-1} + \Sigma[\mathcal{G}]$ (orders 0 to 3); $\delta^4 \Gamma / \delta \Psi^4 _{0, \mathcal{G}} - \mathcal{V}$	$\{\{0, 0, 0, 0\}, 0\}$ ✓

On a single site the functional of the superfield can be computed exactly (section 16.1, paragraph *With pairing*).

14 Hedin's equations and the GW approximation

Hedin's equations. The vertex of section 11 contains the chains of bubbles joined by single interaction lines, which screen the interaction. Separating them — the *proper* vertex $\tilde{\Lambda}$ (Hedin's Γ ; for the current of QED the vertex function Γ^μ of section 20) has the diagrams that do not fall apart when an interaction line is cut, 1, 7 and 63 of them at orders V , V^2 , V^3 — gives the polarization P , the proper part of χ of section 6 (the irreducible polarizability, the proper polarization insertion Π^* of [3], the polarization operator of [2]; for photons the vacuum polarization), and the screened, or effective, interaction W , the interaction screened by the full response, $W = V + V\chi V$, drawn with each wavy line standing for $-V$ and the double one for $-W$ (the double wavy line marks W where V appears too, as the double arrow marks G in the Dyson equation):

$$x \text{~~~~~} y = x \text{~~~~~} y - x \text{~~~~~} \chi \text{~~~~~} y$$

The self-energy becomes a functional of G and W [77, 78, 7], and the kernel of the proper vertex is $\Gamma_{xc} = \delta \Sigma_{xc} / \delta G$, the irreducible vertex Γ^0 without its Hartree term.

As derivatives. These are Hedin's definitions [77], derivatives with respect to the total potential $U_{\text{tot}} = U + V\langle\rho\rangle$ of section 6, the external one plus the Hartree potential of the induced density: the proper vertex is $\tilde{\Lambda}(x_1, x_2; z) = -\delta G^{-1}(x_1, x_2) / \delta U_{\text{tot}}(z)$ (the vertex Λ of section 11 is the same derivative with respect to U), the polarization is $P = \delta\langle\rho\rangle / \delta U_{\text{tot}}$, and $W = (\delta U_{\text{tot}} / \delta U) V = \varepsilon^{-1} V$. Differentiating with respect to U_{tot} instead of U removes exactly the chains joined by single interaction lines; the package selects the same diagrams by cutting one interaction line (IrreducibleDiagrams), from the vertex $\Lambda = -\delta G^{-1} / \delta U$ and the density correlation, both derivatives, and section 15 obtains Σ and P as derivatives of a functional of G and W :

```

properVertex = IrreducibleDiagrams[densityVertex, {{x1, x2}, {z}}, 1,
  {InteractionPotential}]; (* densityVertex: Lambda = -dG^-1/dU *)
polarization = -IrreducibleDiagrams[densityCorrelationSkeleton, {{a}, {b}}, 1,
  {InteractionPotential}]; (* <rho rho>_c, skeletons with G0 -> G *)
hedin = ExactEquation["Hedin", {"G" -> DressedGreenFunction, "V" ->
  InteractionPotential,
  "Sigma" -> sigma, "W" -> w, "P" -> p, "Lambda" -> lambdaTilde,
  "GammaXC" -> gammaXC}, {x, y, z}]; (* the objects as LabelFunction *)
CheckEquation[#, InteractionPotential, 3] & /@ hedin

```

Hedin's equations are

$$\Sigma(x, y) = -x \text{---} \text{---} y + x \text{---} \text{---} \text{---} \text{---} \text{---} y$$

$$x \text{---} (P) \text{---} y = x \text{---} \text{---} \text{---} \text{---} y$$

$$x \text{---} \text{---} y = x \text{---} \text{---} y - x \text{---} (P) \text{---} y$$

$$x_1 \text{---} \text{---} z = x_1 \text{---} \text{---} z + x_1 \text{---} \text{---} \text{---} \text{---} z$$

that is, $\Sigma = \Sigma_H - GW\tilde{\Lambda}$, $P = \gamma L_0 \tilde{\Lambda}$, $W = V + VPW$ and $\tilde{\Lambda} = \gamma + \Gamma_{xc} L_0 \tilde{\Lambda}$. The package checks the four equations with the perturbative $\Sigma, \Gamma^0, \tilde{\Lambda}, P$ and W :

Hedin's equations for Σ, W and $\tilde{\Lambda}$ to V^3 , for P to V^2 ; residuals:
 $\{ \{0, 0, 0, 0\}, \{0, 0, 0\}, \{0, 0, 0, 0\}, \{0, 0, 0, 0\} \}$ ✓

The GW approximation. Replacing the proper vertex by the bare one, $\tilde{\Lambda} \rightarrow \gamma$, leaves the Hartree term and the exchange with the screened interaction, and the polarization of a pair of dressed propagators,

$$\Sigma_{GW}(x, y) = x \text{---} \text{---} y - x \text{---} \text{---} y$$

$$P_{GW}(x, y) = x \text{---} \text{---} y$$

which with $W = V + VPW$ and the Dyson equation are the self-consistent GW approximation; evaluated once with the propagator of a mean-field theory in place of G ($G_0 W_0$), it is the standard method for the quasiparticle band structures of solids [78]. The next section derives the self-consistent GW approximation from a 2PI functional of G and W .

15 Hubbard–Stratonovich: a functional of G and W

The auxiliary field. The interaction between densities is the exchange of a boson: for a Gaussian field ϕ with $\langle\phi\phi\rangle_0 = V$, $\langle e^{i\int\phi\rho}\rangle_\phi = e^{-\frac{1}{2}\int\rho V\rho}$, so that the electron gas is the same as fermions coupled to ϕ by $-i\int\phi\bar{\psi}\psi$ (Hubbard–Stratonovich transformation [79, 80, 4, 8]; ϕ is also called an auxiliary field). The package treats this as a theory of fermions and bosons like any other, and the two give the same Green function, order by order (two boson–fermion vertices for each V). Each vertex stands for $+i$, minus its coupling, so that a boson line with its two vertices is $i^2V = -V$, the interaction line: HubbardStratonovich declares the boson propagator with DeclareInteractionLine, and the pictures are those of the electron gas (the screened W below is declared in the same way). For any interaction of the form $\frac{1}{2}\int KOO$, given the operator O , HubbardStratonovich reads the kernel K off the interaction and returns the new free generating functional and the coupling; IntegrateOutField goes back, integrating out a Gaussian field coupled linearly:

```
hs = HubbardStratonovich[{FreeFermionGeneratingFunctional, CoulombVertex},
  psibar[#] ** psi[#] &, {hsField, Jhs}, HSPropagator];
(* hs["Interaction"] = -I IntegralOver[hsField[z] psibar[z] ** psi[z], {z}] *)
-PerturbativeCorrelationFunction[hs["FreeGeneratingFunctional"], {psi[x], psibar[y]},
  hs["Interaction"], 6]
IntegrateOutField[{hs["FreeGeneratingFunctional"], hs["Interaction"]}, hsField, Jhs]
```

G of the fermion–boson theory minus G of the electron gas, $\langle\phi\phi\rangle_0 = V$, orders V^0 to V^3 : $\{0, 0, 0, 0\}$ ✓
the coupling and the Gaussian of HubbardStratonovich, and the interaction given back by IntegrateOutField: $\{0, 0, 0\}$ ✓

The full propagator of the boson is the screened interaction, $\langle\phi\phi\rangle = V + V\chi V = W$ (section 14), and its self-energy is the polarization P : the boson line of section 14 has become a propagator in its own right.

The 2PI functional of G and W . A Legendre transform with respect to two-point sources of both fields makes G and W independent variables, and the functional $\Phi[G, W]$ is minus the sum of the vacuum diagrams that are two-particle irreducible in both kinds of lines [81, 59]: LuttingerWardFunctional with two replacement rules. Its derivatives are the self-energy $\Sigma = \delta\Phi/\delta G$ and the polarization $P = -2\delta\Phi/\delta W$, both functionals of G and W . In Φ and its derivatives every line is a full one, as in any skeleton expansion: the plain arrows are G and the wavy lines the screened interaction W , each standing for $-W$ (the double wavy line of section 14 is needed only where V and W appear together; here "Interactions" $\rightarrow$ {ScreenedW} draws W as an ordinary wavy line):

```
phiGW = LuttingerWardFunctional[hs["FreeGeneratingFunctional"], hs["Interaction"], 6,
  {BareGreenFunction -> DressedGreenFunction, HSPropagator -> ScreenedW}];
FunctionalDerivative[phiGW, DressedGreenFunction[y, x]]
-2 FunctionalDerivative[phiGW, ScreenedW[a, b]]
(* the same: SelfEnergy[phiGW, DressedGreenFunction, {x, y}],
  SelfEnergy[phiGW, ScreenedW, {a, b}, "Statistics" -> "Boson"] *)
```

$\Phi[G, W]$ has 1, 1 and 4 diagrams of orders W , W^2 , W^3 :

$$\Phi[G, W] =$$

$$W \quad \frac{1}{2} \text{ (bubble) }$$

$$W^2 \quad + \frac{1}{4} \text{ (two-bubble) }$$

$$W^3 \quad + \frac{1}{6} \text{ (three-bubble) } + \frac{1}{2} \text{ (triangle) } - \frac{1}{6} \text{ (triangle with bubble) } - \frac{1}{6} \text{ (triangle with bubble) }$$

and Σ has 1 diagrams at W^2 and P 1 at W :

$$\Sigma[G, W] =$$

$$W \quad x \text{ (tadpole) } y$$

$$W^2 \quad + \quad x \text{ (tadpole with bubble) } y$$

$$P[G, W] =$$

$$W^0 \quad a \text{ (loop) } b$$

$$W \quad + \quad a \text{ (tadpole) } b$$

The first diagram of Φ alone gives $\Sigma = -GW$ and the bubble, $P = \chi_0$: the GW approximation of section 14 is the lowest order of this functional, and therefore conserving; the next orders are its vertex corrections. The Hartree term is the mean field $\langle \phi \rangle$, a tadpole that is one-particle reducible in the boson line and not part of Φ . Eliminating W — writing it as the functional $W[G] = V + V\chi[G]V$ of the dressed G , with the skeleton diagrams of χ — brings back the skeleton expansion in G alone:

$\Sigma_H + \Sigma[G, W[G]] - \Sigma[G]$ (section 9.4), orders V^0 to V^3	residuals $\{0, 0, 0, 0\}$ ✓
$P[G, W[G]] - P[G]$ (section 14), orders V^0 to V^2	residuals $\{0, 0, 0\}$ ✓
the derivatives minus SelfEnergy of $\Phi[G, W]$, for Σ and P	residuals $\{0, 0\}$ ✓

These are the three levels of irreducibility of the same physics: skeletons in G and V (section 9.4), in G and W (here), and Hedin's equations, which close the second level by the vertex.

ϕ^4 theory. The quartic vertex is the exchange of a field σ coupled to $\frac{1}{2}\phi^2$: with $\langle \sigma \sigma \rangle_0 = \frac{\lambda}{3} \delta$ and the coupling $-\frac{i}{2} \int \sigma \phi^2$, the three pairings of the four legs give back $\frac{\lambda}{4!} \phi^4$, and the propagator of ϕ is the same as in section 3 to λ^3 :

```

DeclareSource[Jsigma]; DeclareField[sigmaField, Jsigma];
DeclareSymmetric[SigmaPropagator, FullSigmaPropagator];
(* <sigma sigma>_0 = SigmaPropagator, set to lambda/3 delta in the checks *)
FreeSigmaGeneratingFunctional = FreeBosonGeneratingFunctional
  Exp[1/2 IntegralOver[Jsigma[x] SigmaPropagator[x, y] Jsigma[y], {x, y}]];
SigmaVertex = -I/2 IntegralOver[sigmaField[w] phi[w]^2, {w}];
gamma2GD = LuttingerWardFunctional[FreeSigmaGeneratingFunctional, SigmaVertex, 6,
  {FreePropagator -> DressedPropagator, SigmaPropagator -> FullSigmaPropagator}];
sigmaGD = -2 FunctionalDerivative[gamma2GD, DressedPropagator[a, b]]

```

G of the theory with σ minus G of ϕ^4 theory, orders λ^0 to λ^3 : $\{0, 0, 0, 0\}$ ✓; σ integrated out (IntegrateOutField), minus $\frac{\lambda}{4!}\phi^4$: 0 ✓

(HubbardStratonovich with the operator $\text{phi}[\#]^2$ & reads the kernel $\frac{\lambda}{12}\delta$ off $\frac{\lambda}{4!}\phi^4 = \frac{1}{2} \cdot \frac{\lambda}{12}(\phi^2)^2$ and couples $-i \int \sigma \phi^2$, the same theory with σ rescaled by 2.) The 2PI functional of G and of the full propagator D_σ of σ (the wavy line: as for W , every line is a full one) has 1, 1 and 3 diagrams of orders D_σ , D_σ^2 , D_σ^3 , and its first diagram gives $\Sigma = -G D_\sigma$, the GW approximation of ϕ^4 theory:

$$\Gamma_2[G, D_\sigma] =$$

$$D_\sigma \quad - \frac{1}{4} \text{ (tadpole diagram) }$$

$$D_\sigma^2 \quad - \frac{1}{8} \text{ (tadpole with bubble) }$$

$$D_\sigma^3 \quad - \frac{1}{12} \text{ (tadpole with two bubbles) } - \frac{1}{4} \text{ (tadpole with triangle) } - \frac{1}{12} \text{ (tadpole with circle) }$$

$$\Sigma[G, D_\sigma] =$$

$$D_\sigma \quad a \text{---} \text{ (tadpole) } b$$

$$D_\sigma^2 \quad + a \text{---} \text{ (tadpole with bubble) } b$$

Here the mean field of σ gives one third of the tadpole, $-\frac{\lambda}{6}G_{aa}$, and the diagram $-GD_\sigma$ with $D_\sigma \rightarrow \frac{\lambda}{3}\delta$ the other two thirds:

$\frac{1}{3} \Sigma_{\text{tadpole}} + \Sigma[G, D_\sigma[G]] - \Sigma[G]$, with $D_\sigma[G] = \frac{\lambda}{3} - \frac{\lambda^2}{9} \langle \frac{1}{2} \phi^2 \frac{1}{2} \phi^2 \rangle_c$, orders λ^0 to λ^3 : residuals $\{0, 0, 0, 0\}$ ✓

16 Without the series: Potthoff's functionals and divergent vertices

The effective actions of sections 8 and 9 are exact: Legendre transforms of $W = \log Z$, defined without diagrams, stationary at the exact mean field and propagator, where their value is $-\log Z$. The skeleton series is one way of evaluating them, valid where it converges to the right functional. Two questions arise where it fails, in strongly correlated systems. Potthoff's self-energy functional is the same exact functional with the self-energy as the variable, one more Legendre transform: it turns the Luttinger–Ward functional into a variational principle for the self-energy, which can be evaluated with no series at all, on a reference system solved exactly. The divergences of the irreducible vertex mark where the map from G_0 to G stops being invertible, and the series in G can converge to the wrong branch of the exact functional. On a single site both can be followed exactly.

16.1 Potthoff's functionals

Potthoff's universal functional is the Legendre transform of Φ from G to the self-energy, $\mathcal{F}[\Sigma] = \Phi[G[\Sigma]] - \text{Tr}(\Sigma G[\Sigma])$, with $G[\Sigma]$ the propagator whose self-energy is Σ (LegendreTransform, LegendrePropagator); his self-energy functional is $\Omega_{G_0}[\Sigma] = \mathcal{F}[\Sigma] - \text{Tr} \ln(-(G_0^{-1} - \Sigma))$ [82] (he writes $\Omega_t[\Sigma]$, with t the one-body part):

```
omega = SelfEnergyFunctional[luttingerWard, BareGreenFunction -> TrialSelfEnergy,
  DressedGreenFunction];
FunctionalDerivative[omega, TrialSelfEnergy[x, y]]
```

$$\Omega_{G_0}[\Sigma] = \mathcal{F}[\Sigma] - \text{Tr} \ln (\Sigma - G_0^{-1}), \quad \frac{\delta \Omega_{G_0}}{\delta \Sigma(x, y)} = -G[\Sigma](y, x) + \left(-\Sigma + G_0^{-1} \right)^{-1}(y, x).$$

It is stationary where $G[\Sigma] = (G_0^{-1} - \Sigma)^{-1}$, the Dyson equation, with the value $-\log Z$. $\mathcal{F}$ is the same for every system with the same interaction, whatever its one-body part: the diagrams of Φ contain only G and the interaction, and exactly, since the two-point source K enters the action as G_0^{-1} does, $\log Z$ depends on the two only through one combination, and $\Gamma[G]$ depends on G_0 only through the term $\text{Tr}(G_0^{-1}G)$. It can be computed exactly on a simpler reference system (a cluster, an impurity), and the stationary point searched among its self-energies — the idea of the variational cluster approximation and of dynamical mean-field theory. Ω_{G_0} is a Legendre transform, not $\Gamma[(G_0^{-1} - \Sigma)^{-1}]$, which is stationary at the same point but has G_0 also inside Φ . Since $\mathcal{F}$ is stationary in G , its derivative with respect to the interaction is that of Φ at $G[\Sigma]$: $\delta \mathcal{F} / \delta V(x, y) = -\frac{1}{2} G[\Sigma](x, y) G[\Sigma](y, x) + \frac{1}{2} G[\Sigma](x, x) G[\Sigma](y, y)$ (first order).

$\mathcal{F}[\Sigma]$ does not contain G_0 (electron gas and ϕ^4) 0 ✓

Zero dimensions. For one level with spin $\frac{1}{2}$, $Z = a^2 - u$ and $G_0 = 1/a$, the integrals can be done: $G = a/(a^2 - u)$, $\Sigma = u/a$, and `ZeroDimensionalValue` gives every diagram its value. The skeleton series of the package,

$$\Sigma[g] = g u - g^3 u^2 + 2 g^5 u^3 - 5 g^7 u^4 + \dots,$$

has the Catalan numbers as coefficients: it is the expansion of $\Sigma_+(g) = (-1 + \sqrt{1 + 4ug^2})/(2g)$, one of the two solutions $\Sigma_{\pm}$ of $g\Sigma^2 + \Sigma - ug = 0$. The universal functional is $\mathcal{F}(\Sigma) = \ln(1 - \Sigma^2/u)$, independent of a , and $\Omega_a(\Sigma) = \mathcal{F}(\Sigma) - \ln(a - \Sigma)^2$ is stationary only at $\Sigma = u/a$, where it is $-\ln(a^2 - u)$.

the skeleton series = $\Sigma_+(g)$ to u^4	0 ✓
$\Gamma(g)$ at $g = a/(a^2 - u) = -\ln(a^2 - u)$ to u^4	0 ✓
Ω_a stationary at u/a ; its value; $\mathcal{F}$ from the package's $\Phi = \ln(1 - \Sigma^2/u)$ to u^4	$\{\{0, 0\}, 0\}$ ✓

With pairing. With spin $\frac{1}{2}$ on one site the superfield has four components $(\psi_{\uparrow}, \psi_{\downarrow}, \bar{\psi}_{\uparrow}, \bar{\psi}_{\downarrow})$, $G_0 = 1/a$, $S_{\text{int}} = u n_{\uparrow} n_{\downarrow}$, and with the pairing sources $k, \bar{k}$ the partition function is $Z = a^2 + k\bar{k} - u$. The Nambu matrix has g in the normal blocks and $\kappa = \mathcal{G}_{\psi_{\uparrow}\psi_{\downarrow}}$, $\bar{\kappa} = \mathcal{G}_{\bar{\psi}_{\uparrow}\bar{\psi}_{\downarrow}}$ in the anomalous ones, and `ZeroDimensionalValue` with array values (the labels running over the four states) gives $\Phi = s - 1 - \ln \frac{1+s}{2}$ with $s = \sqrt{1 + 4u(g^2 - \kappa\bar{\kappa})}$, the $\Phi(g)$ of the normal site above with $g^2 \rightarrow g^2 - \kappa\bar{\kappa}$, and the trace terms $\ln(g^2 - \kappa\bar{\kappa}) - 2(ag - 1)$ at zero source; with the source term $\bar{k}\kappa - k\bar{\kappa}$, Γ is stationary at the exact $g = a/Z$, $\kappa = -k/Z$, $\bar{\kappa} = \bar{k}/Z$, where it is $-\log Z$.

Φ of the package minus $s - 1 - \ln \frac{1+s}{2}$, to u^3	0 ✓
the trace terms minus $\ln(g^2 - \kappa\bar{\kappa}) - 2(ag - 1)$ (derivatives in $g, \kappa, \bar{\kappa}, a$)	$\{0, 0, 0, 0\}$ ✓
Γ stationary at the exact $g, \kappa, \bar{\kappa}$, to u^3	$\{0, 0, 0\}$ ✓
$\Gamma + \log Z$ there, to u^3 , at $a = 2, k = \frac{1}{3}, \bar{k} = \frac{1}{5}$	0 ✓

16.2 When the irreducible vertex diverges

The irreducible vertex $\Gamma^0 = \delta \Sigma / \delta G$ is the kernel of the response, $L = L_0 + L_0 \Gamma^0 L$, and therefore

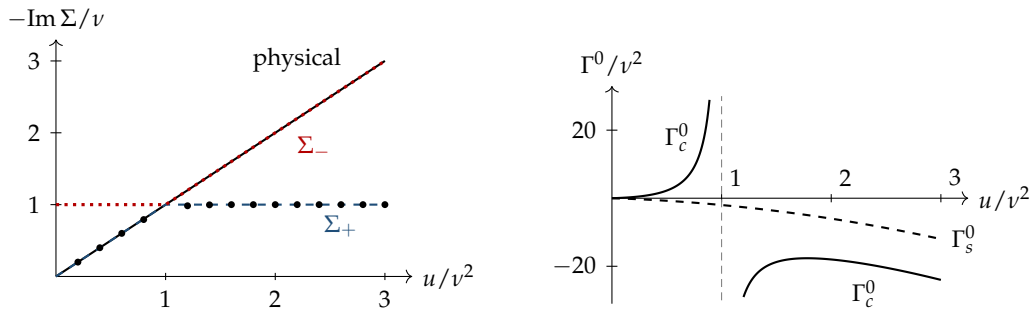
$$\Gamma^0 = L_0^{-1} - L^{-1}$$

in each channel, as matrices in the frequencies and momenta of the pair. Γ^0 diverges where the generalized susceptibility L has a vanishing eigenvalue, while the physical susceptibilities $\chi = \gamma L \gamma$, contractions of L with a bare vertex, stay finite. Since $\delta G / \delta G_0^{-1} = -L$ (the source U shifts G_0^{-1}), this is where the map $G_0 \mapsto G$ stops being invertible: two non-interacting propagators give the same G , $\Sigma[G]$ and the Luttinger–Ward functional have a branch point and become multivalued, and the skeleton series, a series in G , can converge to the wrong branch. These are the two-particle pathologies studied by Toschi, Sangiovanni, Rohringer, Schäfer and coworkers: the irreducible vertex of dynamical mean-field theory diverges in the charge channel well inside the metallic phase of the Hubbard model [83], and along infinitely many lines of its phase diagram around the Mott transition, in the charge and particle–particle channels [84]; the same divergences appear in the Anderson impurity model [85], and the Hubbard atom shows them in closed form [86]. The multivaluedness of the Luttinger–Ward functional and the misleading convergence of the skeleton series were found by Kozik, Ferrero and Georges [87] (see also [88, 89]), and the non-uniqueness of the map $G_0 \mapsto G$ was related to the divergences by Gunnarsson and coworkers [90].

One site, exactly. In zero dimensions with spin, $Z = a_\uparrow a_\downarrow - u$, $g_s = \partial \ln Z / \partial a_s$ and $\Sigma_s = a_s - 1/g_s = u/a_{-s}$. The response is $L = -\partial g / \partial a$, $L_0 = g^2$, and $\Gamma^0 = \partial \Sigma / \partial g$ is a 2×2 matrix in the spins, with a charge and a spin channel. For real a (attractive $u < 0$) Γ^0 diverges at $a^2 = -u$, where $\partial g / \partial a = 0$ and the two branches $\Sigma_\pm$ meet ($1 + 4ug^2 = 0$). With $a = iv$, a fermionic Matsubara frequency (then $g = 1/(iv - u/(iv))$) is the propagator of the Hubbard atom at half filling for $u = U^2/4$, the divergence moves to the repulsive side:

$$L_c = \frac{-v^2 + u}{(v^2 + u)^2}, \quad \Gamma_c^0 = \frac{u(v^2 + u)^2}{v^4 - v^2 u}, \quad \Gamma_s^0 = -\frac{u(v^2 + u)}{v^2}.$$

The charge vertex diverges at $u = v^2$, where $L_c = 0$; the spin vertex stays finite. There the two branches meet, $1 + 4ug^2 = ((v^2 - u)/(v^2 + u))^2$, and the physical self-energy $u/(iv)$ passes from the branch connected to $u = 0$, the one the skeleton series follows, to the other one. Beyond $u = v^2$ the skeleton series, evaluated at the exact G , converges to the wrong self-energy, and the self-consistent skeleton equation on its branch has no solution:



Left: $-\text{Im } \Sigma$ at the exact g : the physical self-energy (solid), the branches Σ_+ (dashed) and Σ_- (dotted), and the skeleton series summed to u^{61} (dots). Right: the charge (solid) and spin (dashed) irreducible vertices.

$\Gamma^0 = \partial \Sigma / \partial g = L_0^{-1} - L^{-1}$ (the 2×2 matrix)	$\{\{0, 0\}, \{0, 0\}\}$ ✓
$\Gamma_c^0 = \partial \Sigma / \partial g$ of the package's skeleton series at the exact g , to u^3	0 ✓
the branches meet at $u = v^2$	0 ✓
$u = 2v^2$: the series converges to Σ_+ , not to the physical $-2iv$	$\{0, 0\}$ ✓
$u = 2v^2$: solutions of $g(iv - \Sigma_+(g)) = 1$	0 ✓

In the Hubbard atom the same happens with the vertex a matrix in the fermionic frequencies: eigenvalues of the generalized susceptibility vanish one after the other as U grows, and at each of them Γ^0 diverges and the map $G_0 \mapsto G$ is not locally invertible [86, 90]. The package does not compute these frequency matrices; the zero-dimensional model shows the mechanism exactly.

17 Electrons and phonons

Electrons coupled to a phonon field, $g \int_z \varphi(z) \bar{\psi}(z) \psi(z)$ [91, 92, 5]: the free generating functional is the product of the fermionic and bosonic ones, and the phonon lines are dashed.

```

DeclareSource[Jphonon]; DeclareField[phonon, Jphonon];
DeclareSymmetric[PhononPropagator];
DeclareLineStyle[PhononPropagator, "Dashed"];
FreeElectronPhononGeneratingFunctional = FreeFermionGeneratingFunctional
  Exp[1/2 IntegralOver[Jphonon[x] PhononPropagator[x, y] Jphonon[y], {x, y}]];
ElectronPhononVertex = g IntegralOver[phonon[z] psibar[z] ** psi[z], {z}];
electronPhononGreen = -PerturbativeCorrelationFunction[
  FreeElectronPhononGeneratingFunctional, {psi[x], psibar[y]},
  ElectronPhononVertex, 2];

```

$G(x, y) =$

$$\begin{aligned}
 g^0 & \quad x \text{---} y \\
 g^2 & \quad - \text{ } x \text{---} \text{---} y + x \text{---} \text{---} y
 \end{aligned}$$

Here $D_0 = \langle \varphi \varphi \rangle_0$, without the minus sign of G_0 , and each vertex stands for $-g$ (the pictures are drawn with "Couplings" $\rightarrow \{g\}$). The electron Green function to order g^2 is that of the two-body interaction to first order with $V \rightarrow -g^2 D_0$: phonon exchange is an effective, retarded attraction, and its two vertices $(-g)^2$ and the dashed line D_0 give the wavy line $-V$. The phonon two-point function $D(x, y) = \langle \varphi(x) \varphi(y) \rangle$ (not connected) gets the polarization bubble and, since the phonon field acquires an expectation value at order g , the product of two tadpoles $\langle \varphi(x) \rangle \langle \varphi(y) \rangle$:

$D(x, y) =$

$$\begin{aligned}
 g^0 & \quad x \text{---} y \\
 g^2 & \quad - \text{ } x \text{---} \text{---} y + \text{ } x \text{---} \text{---} y
 \end{aligned}$$

The phonons integrated out. The phonon field enters linearly, so that it can be integrated out exactly: IntegrateOutField gives the retarded interaction between the densities that it carries,

```

IntegrateOutField[{FreeElectronPhononGeneratingFunctional, ElectronPhononVertex},
  phonon, Jphonon] ["Interaction"]

```

$$S_{\text{eff}} = \frac{1}{2} g^2 \int_{z_1 z_2} D_0(z_1, z_2) \psi(z_1) \psi(z_2) \bar{\psi}(z_1) \bar{\psi}(z_2),$$

an attractive interaction $-g^2 D_0$ between densities (the converse of the Hubbard–Stratonovich transformation of section 15); with it the electron gas gives the same G :

$S_{\text{eff}} + \frac{g^2}{2} \int \rho D_0 \rho$, and G of the electron–phonon theory minus G with S_{eff} to g^2 : $\{0, 0\}$ ✓

The functional of G and D . The phonon is a boson coupled to the density, like the field of the Hubbard–Stratonovich transformation (section 15). The Legendre transform with respect to two-point sources of both fields gives a functional $\Phi[G, D]$ of the full electron propagator and the connected phonon propagator, minus the vacuum diagrams two-particle irreducible in both kinds of lines, and the electron self-energy is its derivative, $\Sigma = \delta\Phi/\delta G$ (every line in these pictures a full propagator):

```
DeclareSymmetric[DressedPhononPropagator];
phiGD = LuttingerWardFunctional[FreeElectronPhononGeneratingFunctional,
  ElectronPhononVertex, 4, {BareGreenFunction -> DressedGreenFunction,
  PhononPropagator -> DressedPhononPropagator}];
FunctionalDerivative[phiGD, DressedGreenFunction[y, x]]
```

$\Phi[G, D] =$

$$g^2 \quad \frac{1}{2} \text{ (diagram: two vertices connected by a dashed line)}$$

$$g^4 \quad + \frac{1}{4} \text{ (diagram: two vertices connected by a dashed line with a loop on each vertex)}$$

$\Sigma[G, D](x, y) =$

$$g^2 \quad \text{(diagram: two vertices connected by a dashed line with external lines at } x \text{ and } y \text{)}$$

$$g^4 \quad + \text{ (diagram: two vertices connected by a dashed line with a loop on each vertex and external lines at } x \text{ and } y \text{)}$$

The first diagram gives the exchange of a full phonon, the GW approximation of section 15 with D in place of W ; the second its first vertex correction. By Migdal's theorem [91] the corrections to the electron–phonon vertex are smaller than the vertex by a factor of order Ω_D/E_F , the ratio of the phonon to the electron energy scale, which is of order $\sqrt{m/M}$ (electron and ion masses). The first diagram alone, a Φ -derivable approximation, is therefore accurate even at strong coupling — the Migdal–Eliashberg theory of metals and conventional superconductors [91, 92, 5].

The Migdal self-energy. The perturbative self-energy, the part of G that stays connected when any one electron line is cut, amputated, is at order g^2 the first derivative above with bare lines, and the tadpole, the phonon at zero momentum attached to the density: the mean field $\langle\varphi\rangle$, which is one-particle reducible in the phonon line and not part of Φ , like the Hartree term in section 15. The frequency sums of section 7 evaluate it, with each boson line given as a rational function of $z = iv_m$. For phonons of frequency Ω_q the field is $\varphi_q = b_q + b_{-q}^\dagger$ (the zero-point amplitude $(2M\Omega_q)^{-1/2}$ of the displacement is included in g), and for $0 < \tau < \beta$, $\langle T\varphi_q(\tau)\varphi_{-q}(0)\rangle_0 = (1 + n_B(\Omega_q))e^{-\Omega_q\tau} + n_B(\Omega_q)e^{\Omega_q\tau}$, the emission and the absorption of a phonon, whose Fourier transform is $D_0(q, iv_m) = 2\Omega_q/(\Omega_q^2 - (iv_m)^2)$, minus the phonon propagator $-\langle T\varphi\varphi\rangle_0 = 2\Omega_q/((iv_m)^2 - \Omega_q^2)$ of the textbooks [5]. For electrons of spin $\frac{1}{2}$, with "SpinDegeneracy" -> 2:

```

phononSelfEnergy = AmputateExternalLegs[ParticleIrreducibleDiagrams[
  OrderPart[electronPhononGreen, g, 2], 1, {x, y}, {BareGreenFunction}],
  {x, y}, {BareGreenFunction}];
phononRules = {BareGreenFunction -> {"Fermion", xi},
  PhononPropagator -> {"Boson", Function[{q, z}, 2 Om[q]/(Om[q]^2 - z^2)]}};
migdal = EvaluateMatsubara[phononSelfEnergy, twoPoint, phononRules,
  "SpinDegeneracy" -> 2, "LoopMomenta" -> {p}]
RetardedImaginaryPart[AnalyticContinuation[migdal, w -> omega], omega]

```

$$\Sigma_{\text{ph}}(x, y) = \text{diagram with two fermion lines and a dashed phonon line} - \text{diagram with two fermion lines and a tadpole phonon line}$$

$$\begin{aligned} \Sigma_{\text{ph}}(k, i\omega_n) &= g^2 \sum_p \left(\frac{1 + n_B(\Omega_{k-p}) - n_F(\xi_p)}{i\omega_n - \Omega_{k-p} - \xi_p} + \frac{n_B(\Omega_{k-p}) + n_F(\xi_p)}{i\omega_n + \Omega_{k-p} - \xi_p} \right) \\ &\quad - \frac{4g^2 \sum_p n_F(\xi_p)}{\Omega_0} \\ \text{Im } \Sigma_{\text{ph}}^R(k, \omega) &= -g^2 \pi \sum_p \left(\delta(\omega - \Omega_{k-p} - \xi_p) (1 + n_B(\Omega_{k-p}) - n_F(\xi_p)) \right. \\ &\quad \left. + \delta(\omega + \Omega_{k-p} - \xi_p) (n_B(\Omega_{k-p}) + n_F(\xi_p)) \right) \end{aligned}$$

The first term is the exchange of a phonon, the derivative of Φ , with the factors of the textbooks [91, 5]: $n_B + 1 - n_F$ for the emission of a phonon, $n_B + n_F$ for its absorption. The second is the tadpole, the phonon at zero momentum attached to the density $2 \sum_p n_F(\xi_p)$, whose factor 2 is the sum over spin of the closed loop: a constant, which shifts the chemical potential. The imaginary part is ≤ 0 , as it should be, and the cutting rules give the same; so does the brute-force sum of section 7, for $\Omega_q = 0.5 + 0.2q^2$ and $g = 0.7$:

the perturbative Σ at g^2 minus $\delta\Phi/\delta G$ with bare lines and the tadpole	0 ✓
the cutting rules minus the continued imaginary part	0 ✓
the brute-force frequency sums, error 2×10^{-9}	0 ✓

18 Disorder

Electrons in a metal scatter elastically off impurities at random positions. Their potential u is modelled as a static Gaussian random field, with $\overline{u(x)u(y)} = \Delta_{\text{imp}}(x, y)$ ($\Delta_{\text{imp}}(x, y) = n_i u_0^2 \delta(\mathbf{r}_x - \mathbf{r}_y)$) for impurities of density n_i and short range): just one more Gaussian field, so that the disorder average is given by Wick's theorem again [93, 2, 8], and the orders are those in Δ_{imp} ; the correlator is independent of the imaginary times, so that impurity lines transfer no frequency. The impurities do not move, and the average is *quenched*: what is averaged is $G[u]$, computed for each realization of u , not the numerator and $Z[u]$ separately, as for a field in equilibrium with the electrons (an *annealed* average). For non-interacting electrons $G[u] = (G_0^{-1} - u)^{-1}$ is a single open line with insertions of u , so the diagrams with closed fermion loops, which come from $Z[u]$, are dropped (DropClosedLoops); with n replicas of the electrons every closed loop carries a factor n , and the replica limit $n \rightarrow 0$ removes them in the same way. Impurity lines are dashed with a cross.

```

DeclareSource[Jimpurity]; DeclareField[impurityPotential, Jimpurity];
DeclareSymmetric[DisorderCorrelator];
DeclareLineStyle[DisorderCorrelator, "Impurity"];
FreeDisorderGeneratingFunctional = FreeFermionGeneratingFunctional
  Exp[1/2 IntegralOver[Jimpurity[x] DisorderCorrelator[x, y] Jimpurity[y], {x, y}]];
ImpurityVertex = IntegralOver[impurityPotential[z] psibar[z] ** psi[z], {z}];
disorderGreen = DropClosedLoops[-PerturbativeCorrelationFunction[
  FreeDisorderGeneratingFunctional, {psi[x], psibar[y]}, ImpurityVertex, 4],
  {BareGreenFunction}];

```

$$\overline{G}(x, y) =$$

$$\Delta_{\text{imp}}^0 \quad x \circ \longleftrightarrow y$$

$$\Delta_{\text{imp}} + x \circ \xrightarrow{\text{impurity}} y$$

$$\Delta_{\text{imp}}^2 + x \circ \xrightarrow{\text{rainbow}} y + x \circ \xrightarrow{\text{crossed}} y + x \circ \xrightarrow{\text{rainbow}} y$$

The self-energy Σ_{dis} contains the Born diagram and, at order Δ_{imp}^2 , the rainbow and the crossed diagram. The Born diagram, $\Sigma_{\text{dis}}^{(1)}(x, y) = \Delta_{\text{imp}}(x, y) G_0(x, y)$, gives the electrons a finite lifetime: at the Fermi level $\text{Im} \Sigma^R = -1/2\tau$, with the elastic scattering rate of Fermi's golden rule, $1/\tau = 2\pi\nu n_i u_0^2$ (ν the density of states per spin), and $\ell = v_F \tau$ is the mean free path.

The functional of the averaged propagator. As for the interaction, self-consistent approximations come from a functional of the averaged propagator $\overline{G}$: $\Phi[\overline{G}]$, minus the vacuum diagrams two-particle irreducible in the fermion and in the impurity lines, with the impurity line not dressed (its self-energy would be a closed loop), and $\Sigma = \delta\Phi/\delta\overline{G}$ without the diagrams with closed fermion loops (none to Δ_{imp}^2). The averaged propagator is a double line, as in the Dyson equation, since the check below compares it with the perturbative self-energy in G_0 :

```

DeclareSymmetric[FullDisorderCorrelator];
phiDisorder = LuttingerWardFunctional[FreeDisorderGeneratingFunctional,
  ImpurityVertex,
  4, {BareGreenFunction -> DressedGreenFunction, DisorderCorrelator ->
    FullDisorderCorrelator}] /. FullDisorderCorrelator -> DisorderCorrelator;
DropClosedLoops[FunctionalDerivative[phiDisorder, DressedGreenFunction[y, x]],
  {DressedGreenFunction}]

```

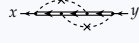
$$\Phi[\overline{G}] =$$

$$\Delta_{\text{imp}} \frac{1}{2} \text{impurity loop}$$

$$\Delta_{\text{imp}}^2 + \frac{1}{4} \text{impurity loop}$$

$$\Sigma[\overline{G}](x, y) =$$

$$\Delta_{\text{imp}} \quad x \xrightarrow{\text{impurity}} y$$

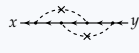
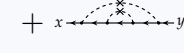
$$\Delta_{\text{imp}}^2 + \text{diagram}$$


The first diagram of Φ gives the self-consistent Born approximation (SCBA), the Born diagram with the averaged propagator, which keeps all the rainbows (the non-crossing diagrams): a Φ -derivable, and therefore conserving, approximation. The second adds the crossed diagram. The crossed diagrams are smaller by a factor $1/k_F \ell$, of the order of the Fermi wavelength over the mean free path, small in a weakly disordered metal [2, 8]. In the two-particle function, which gives the conductivity, the sum of the maximally crossed diagrams, the Cooperon, is instead singular at small total momentum: it describes the interference of an electron path with its time reverse, which lowers the conductivity (weak localization) [8, 6]; the same generating functional produces these diagrams.

The check. The perturbative self-energy, cut out of the diagrams of $\bar{G}$ above, is

$$\Sigma_{\text{dis}}(x, y) =$$

$$\Delta_{\text{imp}} + \text{diagram}$$


$$\Delta_{\text{imp}}^2 + \text{diagram} + \text{diagram}$$



$$\Sigma[\bar{G}] \text{ at } \bar{G} = G_0 + G_0 \Sigma_{\text{dis}}^{(1)} G_0 \text{ (the rainbow) minus } \Sigma_{\text{dis}}, \text{ to } \Delta_{\text{imp}}^2: 0 \checkmark$$

PART II Quantum field theory

19 ϕ^4 theory in dimensional regularization

At zero temperature the routing of momenta of section 7 turns the diagrams of ϕ^4 theory, with the action $\int (\frac{1}{2}(\partial\phi)^2 + \frac{1}{2}m^2\phi^2 + \frac{\lambda}{4!}\phi^4)$, into Euclidean loop integrals, in which a line is $1/(q^2 + m^2)$. The package evaluates them in $d = 4 - 2\varepsilon$ dimensions, where the ultraviolet divergences are poles in ε . The diagrams are those of the sections above, with their weights: the 1PI functions are the derivatives of the 1PI action at $\bar{\phi} = 0$ (section 8.3), the self-energy Σ , $\Sigma = D_0^{-1} - \delta^2\Gamma/\delta\bar{\phi}\delta\bar{\phi}$, the same diagrams as those cut out of the propagator in section 5, and the vertex $\Gamma^{(4)} = \delta^4\Gamma/\delta\bar{\phi}^4$, minus the amputated 1PI part of the connected four-point function of section 4.

Divergences and dimensional regularization. At $T = 0$ the frequency sums become integrals, $T \sum_n \rightarrow \int dk_0/2\pi$, and $(k_0, \mathbf{k})$ is a Euclidean four-vector: imaginary time is already Euclidean, and no Wick rotation is needed. A loop with L lines behaves at large momentum as $\int d^4k/k^{2L}$: the tadpole of Σ ($L = 1$) diverges quadratically, the bubble of $\Gamma^{(4)}$ ($L = 2$) logarithmically. These ultraviolet divergences must be regularized, made finite, before renormalization removes them. A momentum cutoff would break the invariance under shifts of the loop momentum and, in gauge theories, gauge invariance; dimensional regularization [94, 95, 96] evaluates each integral in a dimension d in which it converges, as an analytic function of d , and continues it to $d = 4 - 2\varepsilon$. In spherical coordinates (the unit sphere in d dimensions has the area $2\pi^{d/2}/\Gamma(d/2)$) the radial integral is a Beta function, and

$$\int \frac{d^d k}{(2\pi)^d} \frac{1}{(k^2 + \Delta)^n} = \frac{\Gamma(n - d/2)}{(4\pi)^{d/2} \Gamma(n)} \Delta^{d/2 - n}$$

[11, section 7.5 and appendix A.4]: the divergences are the poles of $\Gamma(n - d/2)$, $\Gamma(\varepsilon) = 1/\varepsilon - \gamma_E + O(\varepsilon)$ for the bubble ($n = 2$) and $\Gamma(-1 + \varepsilon)$ for the tadpole ($n = 1$). The loop momentum can be shifted freely, and an integral without a scale vanishes, $\int d^d k (k^2)^{-a} = 0$, since nothing can give it its dimension $d - 2a$. This does not mean that it is finite: $\int d^d k/k^4$, for instance, diverges

logarithmically at large k and also at $k \rightarrow 0$, where a massless line of power 2 diverges as $\int d^4k/k^4$ (an infrared divergence), and its ultraviolet and infrared poles cancel, $1/\varepsilon_{\text{UV}} - 1/\varepsilon_{\text{IR}} = 0$.

The scale μ and the $\overline{\text{MS}}$ scheme. In d dimensions λ has the dimension of a mass to the power $4 - d = 2\varepsilon$; it is written $\lambda\mu^{2\varepsilon}$, with λ dimensionless and an arbitrary scale μ , so that every loop carries a factor $\mu^{2\varepsilon}$ and the logarithms come as $\log(p^2/\mu^2)$. A pole always comes with the same constants, $(4\pi)^\varepsilon \Gamma(\varepsilon) = 1/\varepsilon - \gamma_E + \log 4\pi + O(\varepsilon)$: minimal subtraction (MS) removes the $1/\varepsilon$ alone [97], the $\overline{\text{MS}}$ scheme the whole combination [98]. The package puts the factor $(e^{\gamma_E}/4\pi)^\varepsilon$ into the measure of every loop,

$$\int_k = \mu^{2\varepsilon} \left(\frac{e^{\gamma_E}}{4\pi} \right)^\varepsilon \int \frac{d^d k}{(2\pi)^d},$$

so that plain pole subtraction is the $\overline{\text{MS}}$ scheme, no γ_E or $\log 4\pi$ appears, and each loop is $\kappa = 1/(16\pi^2)$ times a function of ε and of $\log(p^2/\mu^2)$ [10, 11, 12, 53]; for instance $\int_k 1/(k^2 + m^2) = -\kappa m^2(1/\varepsilon + 1 - \log(m^2/\mu^2)) + O(\varepsilon)$.

How the package does the loop integrals. DiagramLoopIntegral routes the momenta as for the Matsubara sums (section 7). IntegrateLoops then integrates one loop momentum at a time, choosing one that runs through at most two different propagators (after a change of the loop momenta if needed), by one-loop formulas in d :

- a tadpole, $\int_k (k^2 + m^2)^{-a} = \kappa e^{\varepsilon\gamma_E} \mu^{2\varepsilon} \Gamma(a - 2 + \varepsilon) (m^2)^{2-\varepsilon-a} / \Gamma(a)$, which vanishes for $m = 0$;
- a massless bubble [99], for any powers a and b ,

$$\int_k \frac{1}{(k^2)^a ((k+p)^2)^b} = \kappa e^{\varepsilon\gamma_E} \mu^{2\varepsilon} G(a, b) (p^2)^{2-\varepsilon-a-b},$$

$$G(a, b) = \frac{\Gamma(a+b-2+\varepsilon) \Gamma(2-\varepsilon-a) \Gamma(2-\varepsilon-b)}{\Gamma(a) \Gamma(b) \Gamma(4-2\varepsilon-a-b)},$$

which leaves a massless line $1/(p^2)^{a+b-2+\varepsilon}$ of non-integer power: nested massless bubbles are products of G functions;

- a massive bubble at $p = 0$ by Gamma functions or partial fractions, and at $p \neq 0$ by one Feynman parameter [15], which combines the two denominators into one,

$$\frac{1}{A^a B^b} = \frac{\Gamma(a+b)}{\Gamma(a) \Gamma(b)} \int_0^1 dx \frac{x^{a-1} (1-x)^{b-1}}{(xA + (1-x)B)^{a+b}};$$

with $A = k^2 + m_1^2$ and $B = (k+p)^2 + m_2^2$, $xA + (1-x)B = (k + (1-x)p)^2 + \Delta$, the shifted momentum is integrated by the formula above, and

$$\int_k \frac{1}{(k^2 + m_1^2)^a ((k+p)^2 + m_2^2)^b} = \kappa e^{\varepsilon\gamma_E} \frac{\Gamma(a+b-2+\varepsilon)}{\Gamma(a) \Gamma(b)} \int_0^1 dx x^{a-1} (1-x)^{b-1} \Delta^{2-a-b} \left(\frac{\Delta}{\mu^2} \right)^{-\varepsilon},$$

$\Delta = x(1-x)p^2 + x m_1^2 + (1-x)m_2^2$, kept as an integral over x (BubbleIntegral) and expanded in ε under the integral sign; the single logarithm (the order needed at one loop) is integrated in closed form, higher powers stay as integrals over x and are evaluated by N; the bubble must not be nested inside another loop (its momentum p must be free of the other loop momenta);

- a numerator: q^2 is rewritten as a propagator minus m^2 , and $(q \cdot P)^{2j}$ is replaced by its angular average.

An integral without a scale is set to zero; a logarithmically divergent one, whose ultraviolet pole would be lost, and an infrared divergence give a message. EpsilonExpand expands in ε with Laurent series of its own, without Series: $\Gamma(x_0 + c\varepsilon) = \Gamma(x_0) \exp \sum_{k \geq 1} \psi^{(k-1)}(x_0) (c\varepsilon)^k / k!$, with the polygamma functions at integers given by γ_E and $\zeta(k)$ (hence the $\pi^2 = 6\zeta(2)$ of the results) and the poles by $\Gamma(x) = \Gamma(x+1)/x$, and every power $X^{c\varepsilon}$ written as $(X/\mu^2)^{c\varepsilon}$, which gives the logarithms. Feynman parameters are Schwinger's proper-time parameters, $1/A^a = \Gamma(a)^{-1} \int_0^\infty d\alpha \alpha^{a-1} e^{-\alpha A}$, normalized to $\sum_i \alpha_i = 1$, and the two representations give the same parametric integrals [100]; the package uses the Feynman form, only for the massive bubble and for the one-loop integrals of QED (section 20). Integration by parts and general massive two-loop integrals are not used.

One loop. The tadpole of Σ , with massive lines, and the massless bubble of $\Gamma^{(4)}$:

```
massive = {FreePropagator -> {"Scalar", m}};
massless = {FreePropagator -> {"Scalar", 0}};
tadpoleSigma = IntegrateLoops[DiagramLoopIntegral[
  OrderPart[sigma1PI, lambda, 1], {a -> p, b -> -p}, massive], eps];
bubble = IntegrateLoops[LoopIntegral[
  ScalarPropagator[k, 0] ScalarPropagator[k + p, 0], {k}], eps];
{EpsilonExpand[tadpoleSigma, eps, 0], EpsilonExpand[bubble, eps, 1]}
```

$$\begin{aligned}\Sigma^{(1)} &= -\frac{e^{\epsilon\gamma_E} \lambda (m^2)^{1-\epsilon} (\mu^2)^\epsilon \Gamma(-1+\epsilon)}{32 \pi^2} = \frac{\kappa \lambda m^2}{2} \left(1 + \frac{1}{\epsilon} - \log\left(\frac{m^2}{\mu^2}\right)\right) + O(\epsilon) \\ &\quad \int_k \frac{1}{k^2 (k+p)^2} = \frac{e^{\epsilon\gamma_E} (p^2)^{-\epsilon} (\mu^2)^\epsilon \Gamma(1-\epsilon)^2 \Gamma(\epsilon)}{16 \pi^2 \Gamma(2-2\epsilon)} \\ &= \kappa \left(2 + \frac{1}{\epsilon} - \log\left(\frac{p^2}{\mu^2}\right) + \epsilon \left(4 - \frac{1}{12} \pi^2 - 2 \log\left(\frac{p^2}{\mu^2}\right) + \frac{1}{2} \log\left(\frac{p^2}{\mu^2}\right)^2\right)\right) + O(\epsilon^2)\end{aligned}$$

the two expansions minus those of the textbooks: 0 ✓, 0 ✓

The quadratic divergence of the tadpole has become a pole proportional to m^2 , a shift of the mass that vanishes at $m = 0$. The pole of the bubble is the logarithmic divergence of the coupling; it comes as $1/\epsilon - \log(p^2/\mu^2)$, so its coefficient also fixes how the coupling depends on the scale (the beta function below).

The sunset. At two loops the massless sunset of Σ is a bubble inside a bubble: the inner one, $G(1,1)$, leaves a line $1/(q^2)^\epsilon$, and the outer one is the massless bubble $G(1,\epsilon)$. The other diagram of order λ^2 , the double tadpole, vanishes: its inner loop is a massless tadpole, an integral without a scale.

```
sunset = IntegrateLoops[DiagramLoopIntegral[OrderPart[sigma1PI, lambda, 2],
  {a -> p, b -> -p}, massless], eps];
EpsilonExpand[sunset, eps, 0]
```

$$\begin{aligned}\Sigma^{(2)} &= \frac{e^{2\epsilon\gamma_E} \lambda^2 (p^2)^{1-2\epsilon} (\mu^2)^{2\epsilon} \Gamma(1-\epsilon)^3 \Gamma(-1+2\epsilon)}{1536 \pi^4 \Gamma(3-3\epsilon)} \\ &= \frac{\kappa^2 \lambda^2 p^2}{6} \left(-\frac{13}{8} - \frac{1}{4\epsilon} + \frac{1}{2} \log\left(\frac{p^2}{\mu^2}\right)\right) + O(\epsilon)\end{aligned}$$

minus the expansion of the textbooks: 0 ✓

Its pole is proportional to p^2 , like the kinetic term $\frac{1}{2}(\partial\phi)^2$ of the action: it is removed by the renormalization of the field (Z_ϕ below), and it gives the field an anomalous dimension.

Renormalization. The poles mean that the parameters of the action, the bare field ϕ_B , mass m_B and coupling λ_B , are not the physical ones: they diverge as $\epsilon \rightarrow 0$, while the measurable quantities stay finite [11, sections 10.1–10.2]. They are written through renormalized ones,

$$\phi_B = Z_\phi^{1/2} \phi, \quad m_B^2 = Z_{m^2} m^2 / Z_\phi, \quad \lambda_B = \mu^{2\epsilon} (e^{\gamma_E}/4\pi)^\epsilon Z_\lambda \lambda,$$

with renormalization constants Z chosen to make the correlation functions of ϕ , as functions of m and λ , finite. Written with ϕ , the bare action is the renormalized one plus counterterms: the same three operators $\frac{1}{2}(\partial\phi)^2$, $\frac{1}{2}m^2\phi^2$ and $\lambda\phi^4/4!$ (with the factors of μ of λ_B), multiplied by $Z_\phi - 1$, $Z_{m^2} - 1$ and $Z_\phi^2 Z_\lambda - 1$, which are new vertices of perturbation theory. Three constants suffice: by power counting (each loop $\int d^4k$, each line $1/k^2$) a 1PI function with n legs has the superficial degree of divergence $4 - n$, so that only $\Gamma^{(2)}$, whose divergences are a constant times m^2 and one times p^2 , and $\Gamma^{(4)}$, a constant, diverge (the odd ones vanish by the symmetry $\phi \rightarrow -\phi$, and the vacuum energy does not enter the correlation functions): the theory is renormalizable [96, 12, 53]. In minimal subtraction the Z 's are pure poles in ϵ . From two loops on, a diagram contains divergent subdiagrams, and its poles include non-local terms, $\log(p^2/\mu^2)/\epsilon$, which no polynomial counterterm can remove; they cancel against the diagrams in which a subdiagram is replaced by its counterterm, and what is left is a polynomial in the momenta and in the masses. This is Bogoliubov's R -operation, and the content of the BPHZ theorem [11, section 10.4] [96].

Two loops: the infrared rearrangement. The vertex $\Gamma^{(4)}$ has 1, 3 and 12 diagrams at orders λ , λ^2 and λ^3 ; those of order λ^3 are

$$\Gamma_{\lambda^3}^{(4)} = -\frac{1}{2} \text{diagram}_1 - \frac{1}{2} \text{diagram}_2 - \frac{1}{2} \text{diagram}_3 - \frac{1}{2} \text{diagram}_4 - \frac{1}{2} \text{diagram}_5 - \frac{1}{2} \text{diagram}_6 - \frac{1}{4} \text{diagram}_7 - \frac{1}{4} \text{diagram}_8$$

$$- \frac{1}{4} \text{diagram}_9 - \frac{1}{2} \text{diagram}_{10} - \frac{1}{2} \text{diagram}_{11} - \frac{1}{2} \text{diagram}_{12}$$

Once the subdivergences are subtracted, the counterterm of $\Gamma^{(4)}$ is a constant, independent of the momenta and the masses: it can be computed at any momenta and masses that do not create infrared divergences, chosen to make the integrals simple (the infrared rearrangement [101, 102, 53]). In a massless theory zero momenta need care: an integral without any momentum is scaleless and vanishes, losing its ultraviolet pole together with an infrared one (above), and a massless line of power 2 or more diverges at small momentum. `InfraredRearrangedIntegral` lets one momentum p enter at one external leg and leave at another, the others at zero momentum, which turns the diagrams into nested massless bubbles, products of G functions; it tries the pairs of legs in order and takes, for each diagram, the first with which it reduces to nested one-loop integrals without infrared divergences or logarithmically divergent scaleless integrals. The vertex $\Gamma^{(4)}$ is the fourth derivative of the 1PI action, `gamma4` of section 8.3:

```
routed4 = InfraredRearrangedIntegral[OrderPart[gamma4, lambda, 3],
  {a, b, c, d}, p, massless, eps, "Routing" -> True];
```

The 6 diagrams with a bubble in a vertex (the first six above) are routed from the vertex with two external legs to a vertex with one, the 3 chains of two bubbles (the next three) through both bubbles, and the 3 bubbles with a tadpole on a line (the last three) vanish (the tadpole is massless). In units of $\lambda^3 \kappa^2$ their pole parts are

$$\text{bubble in a vertex: } \frac{1 + 5\epsilon - 2\epsilon \log\left(\frac{p^2}{\mu^2}\right)}{4\epsilon^2}, \quad \text{chain: } \frac{1 + 4\epsilon - 2\epsilon \log\left(\frac{p^2}{\mu^2}\right)}{4\epsilon^2}$$

the pole parts of the three topologies minus those of the textbooks: $\{0, 0, 0\}$ ✓

Their terms $\log(p^2/\mu^2)/\epsilon$ are not local: they cancel against the counterterms of the one-loop subdiagrams, and only what is left, the local counterterm of the two-loop diagram, is independent of the routing, while the pole parts of the single rearranged diagrams depend on it.

Counterterms and Z factors. With the Z's defined above, the functions $\Gamma_R^{(2)} = Z_\phi(p^2 - \Sigma)$, $\Gamma_R^{(4)} = Z_\phi^2 \Gamma^{(4)}$ and $\partial \Gamma_R^{(2)} / \partial m^2 = Z_{m^2}(1 - \partial \Sigma / \partial m^2)$ must be finite, with Σ and $\Gamma^{(4)}$ taken at λ_B : the substitution $\lambda \rightarrow Z_\lambda \lambda$ in the bare diagrams gives exactly the counterterm diagrams. In minimal subtraction the Z's do not depend on the masses (a mass-independent scheme [97]), so that Z_ϕ and Z_λ can be found in the massless theory, and Z_{m^2} from the first derivative with respect to m^2 at $m = 0$. That derivative is minus the insertion of $\phi^2/2$ in every line (MassInsertion), since $-\partial_{m^2}(k^2 + m^2)^{-1} = (k^2 + m^2)^{-2}$ is a line with an insertion; at $m = 0$ the momentum entering at the insertion u makes it infrared safe:

```
sigma21 = -MassInsertion[OrderPart[sigma1PI, lambda, {1, 2}],
  FreePropagator, u];
```

$$\frac{\partial \Sigma}{\partial m^2} = -\frac{1}{2} \text{diagram}_1 - \frac{1}{2} \text{diagram}_2 - \frac{1}{4} \text{diagram}_3 - \frac{1}{2} \text{diagram}_4$$

With unknown coefficients of the poles (in units of κ per loop), the poles of the three functions must vanish for every value of $\log(p^2/\mu^2)$, since a pole multiplied by a logarithm of the momentum would need a non-local counterterm; this gives equations for the coefficients, order by order (upTo[e, n] keeps the orders up to λ^n):

```
sigmaB = InfraredRearrangedIntegral[OrderPart[sigma1PI, lambda, {1, 2}],
  {a, b}, p, massless, eps];
gamma4B = InfraredRearrangedIntegral[gamma4, {a, b, c, d}, p, massless, eps];
sigma21B = InfraredRearrangedIntegral[sigma21, {a, b, u}, p, massless, eps];
z[c_] := 1 + c[1] lambda kappa/eps +
  lambda^2 kappa^2 (c[2]/eps^2 + c[3]/eps);
{zPhi, zLambda, zM2} = {z[zf], z[z1], z[zm]};
finite = {upTo[zPhi (p^2 - (sigmaB /. lambda -> lambda zLambda)), 2],
  upTo[zPhi^2 (gamma4B /. lambda -> lambda zLambda), 3],
  upTo[zM2 (1 - (sigma21B /. lambda -> lambda zLambda)), 2]};
equations = Flatten[CoefficientList[Expand[eps^4 PolePart[#, eps]] /.
  Log[p^2/RenormalizationScale^2] -> L, {lambda, eps, L, p}] & /@ finite];
solution = First[Solve[Thread[DeleteCases[equations, 0] == 0],
  Flatten[Table[c[i], {c, {zf, z1, zm}}, {i, 3}]]]];
{zPhi, zLambda, zM2} = {zPhi, zLambda, zM2} /. solution
```

With $Z_X = 1 + z_{X,1} \kappa \lambda / \epsilon + \kappa^2 \lambda^2 (z_{X,2} / \epsilon^2 + z_{X,3} / \epsilon)$ for $X = \phi, \lambda, m$ (the $c[i]$ of $zf, z1, zm$), the solution is

$$Z_\phi = 1 - \frac{\kappa^2 \lambda^2}{24 \epsilon}, \quad Z_{m^2} = 1 + \frac{\kappa \lambda}{2 \epsilon} + \frac{\kappa^2 \lambda^2}{2 \epsilon^2} - \frac{\kappa^2 \lambda^2}{4 \epsilon}$$

$$Z_\lambda = 1 + \frac{3 \kappa \lambda}{2 \epsilon} + \frac{9 \kappa^2 \lambda^2}{4 \epsilon^2} - \frac{17 \kappa^2 \lambda^2}{12 \epsilon}$$

poles left in $\Gamma_R^{(2)}, \Gamma_R^{(4)}, \partial \Gamma_R^{(2)} / \partial m^2$: $\{0, 0, 0\}$ ✓; $Z_\phi, Z_\lambda, Z_{m^2}$ minus those of the textbooks: $\{0, 0, 0\}$ ✓; the double poles minus those that the single ones fix, $z_{\lambda,2} - z_{\lambda,1}^2$ and $z_{m,2} - z_{m,1}(z_{m,1} + z_{\lambda,1})/2$: $\{0, 0\}$ ✓; the pole of $(Z_{m^2} - 1)m^2 - \Sigma^{(1)}$, with the massive tadpole: 0 ✓

The non-local poles cancel by themselves once the one-loop counterterms are in, and the double poles of the two-loop constants are fixed by the single poles of one loop, as the renormalization group requires [97] (below).

The renormalization-group functions. The scale μ is arbitrary, and the bare parameters do not depend on it: the renormalized coupling, field and mass must then change with μ , at the rates $\beta(\lambda) = \mu d\lambda/d\mu$, $\gamma_\phi = \frac{1}{2}\mu d\log Z_\phi/d\mu$ and $\gamma_{m^2} = \mu d\log m^2/d\mu$, taken at fixed bare parameters [11, sections 12.2–12.5]. Since $\Gamma_R^{(n)} = Z_\phi^{n/2}\Gamma^{(n)}$ and the bare $\Gamma^{(n)}$ does not depend on μ , the renormalized functions obey the renormalization-group (Callan–Symanzik) equation

$$\left(\mu \frac{\partial}{\partial \mu} + \beta \frac{\partial}{\partial \lambda} + \gamma_{m^2} m^2 \frac{\partial}{\partial m^2} - n\gamma_\phi\right) \Gamma_R^{(n)} = 0,$$

which trades a change of μ for a change of λ : with μ of the order of the momenta the logarithms $\log(p^2/\mu^2)$ are resummed into the running coupling $\lambda(\mu)$. From the definition of λ_B , $\mu d\lambda_B/d\mu = 0$ gives $2\epsilon\lambda Z_\lambda + \beta_\epsilon d(\lambda Z_\lambda)/d\lambda = 0$, the beta function in d dimensions,

$$\beta_\epsilon = -\frac{2\epsilon\lambda}{1 + \lambda \partial_\lambda \log Z_\lambda} = -2\epsilon\lambda + \beta(\lambda).$$

It is finite at $\epsilon \rightarrow 0$ only if the higher poles of $Z_\lambda = 1 + a_1(\lambda)/\epsilon + \dots$ are fixed by the simple one, and then $\beta = 2\lambda^2 a_1'(\lambda)$: at one loop $a_1 = \frac{3}{2}\kappa\lambda$ gives $\beta = 3\kappa\lambda^2$. The anomalous dimensions are $\gamma_\epsilon \partial_\lambda \log Z$ at $\epsilon = 0$:

```
beta = BetaFunctionFromZ[zLambda, lambda, eps, 3]
betaEps = -2 eps lambda + beta;
gammaPhi = 1/2 AnomalousDimensionFromZ[zPhi, lambda, eps, betaEps, 2]
gammaM2 = -AnomalousDimensionFromZ[zM2/zPhi, lambda, eps, betaEps, 2]
```

$$\beta = \mu \frac{d\lambda}{d\mu} = 3\kappa\lambda^2 - \frac{17}{3}\kappa^2\lambda^3$$

$$\gamma_\phi = \frac{1}{2}\mu \frac{d\log Z_\phi}{d\mu} = \frac{1}{12}\kappa^2\lambda^2, \quad \gamma_{m^2} = \mu \frac{d\log m^2}{d\mu} = \kappa\lambda - \frac{5}{6}\kappa^2\lambda^2$$

minus the values of the textbooks (the case $N = 1$ of the $O(N)$ model, a field of N components with the interaction $\frac{\lambda}{4!}(\phi \cdot \phi)^2$) [11, 12, 53]: $\{0, 0, 0\}$ ✓

Since $\beta > 0$, the coupling decreases at long distances and grows at short ones. The coefficients 3 and $-\frac{17}{3}$ of β and the coefficient of γ_ϕ are the same in every mass-independent scheme.

The Wilson–Fisher fixed point. Below four dimensions, in $d = 4 - \epsilon$ (the usual variable of the ϵ expansion, $\epsilon = 2\epsilon$, not to be confused with the ϵ of $d = 4 - 2\epsilon$), the beta function $-\epsilon\lambda + \beta(\lambda)$ has a second zero λ_* , a fixed point that is stable in the infrared [103]: at it the theory is scale invariant, and it describes the critical points of the Ising universality class — uniaxial magnets, the liquid–gas critical point. Near a critical point the correlation length diverges as $\xi \propto |T - T_c|^{-\nu}$ (here $m^2 \propto T - T_c$), at T_c the correlation function decays as a power, $G(p) \propto 1/p^{2-\eta}$, and the corrections to this scaling vanish as $\xi^{-\omega}$. At the fixed point the term with β drops out of the renormalization-group equation, whose solutions are then power laws, and the critical exponents are the anomalous dimensions there: $\eta = 2\gamma_\phi(\lambda_*)$, $1/\nu = 2 - \gamma_{m^2}(\lambda_*)$, and $\omega = \partial_\lambda(-\epsilon\lambda + \beta)$ at λ_* . Since λ_* is of order ϵ , the series in λ become series in ϵ , the ϵ expansion:

$$\kappa\lambda_* = \frac{1}{3}\epsilon + \frac{17}{81}\epsilon^2, \quad \eta = \frac{1}{54}\epsilon^2, \quad \nu = \frac{1}{2} + \frac{1}{12}\epsilon + \frac{7}{162}\epsilon^2, \quad \omega = \epsilon - \frac{17}{27}\epsilon^2$$

η, ν and ω minus the exponents of the Ising class to order ϵ^2 [12, 53]: $\{0, 0, 0\}$ ✓

At $\epsilon = 1$, in three dimensions, the series give $\eta, \nu, \omega = 0.019, 0.627, 0.37$; ν is already close to the three-dimensional value, about 0.630, which the resummed series of higher orders approach [12, 53]. The whole computation of this section, from the generating functional to the exponents, takes 0.8 s.

20 QED at one loop

The diagrams of a gauge theory carry spinor and Lorentz indices: in condensed notation a label stands for a point of space-time together with the spinor index of an electron or the Lorentz index of a photon (section 21 draws the vertices of QCD in the same way). For QED at one loop the package also evaluates the diagrams, in Minkowski space and in $d = 4 - 2\epsilon$ dimensions. QED is the theory of the electron field ψ and of the photon field A_μ , with the Lagrangian

$$\mathcal{L} = \bar{\psi} (i\gamma^\mu \partial_\mu - m) \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{1}{2\xi} (\partial_\mu A^\mu)^2 - e \bar{\psi} \gamma^\mu \psi A_\mu, \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu.$$

Without its third term it is invariant under the gauge transformations $\psi \rightarrow e^{i\alpha(x)}\psi$, $A_\mu \rightarrow A_\mu - \partial_\mu \alpha/e$, and the quadratic form of A_μ , which vanishes on the pure gauges $A_\mu = \partial_\mu \alpha$, has no inverse. The gauge-fixing term of the Faddeev–Popov procedure (whose ghosts do not couple to the photon in QED) makes it invertible, and its parameter ξ appears in the photon propagator [11, section 9.4] [10, 104]. Physical quantities — the S matrix, the pole mass of the electron, $g - 2$ — do not depend on ξ , while Green functions such as Σ do: the checks of the independence of ξ below test the computation. The conventions are those of Peskin and Schroeder [11], except for the sign of the charge: the metric $(+, -, -, -)$, $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$, $\text{tr } 1 = 4$, the electron line $i(\not{p} + m)/(p^2 - m^2)$, the photon $-i[g^{\mu\nu} - (1 - \xi)q^\mu q^\nu/q^2]/q^2$ in a general covariant gauge ($\xi = 1$ Feynman, $\xi = 0$ Landau), the vertex $+ie\gamma^\mu$ of $S_{\text{int}} = e \int \bar{\psi} \gamma^\mu \psi A_\mu$, the electron having the charge $-e$ with $e > 0$ (Peskin and Schroeder write $-e \int \bar{\psi} \gamma^\mu \psi A_\mu$ with $e < 0$), and $\alpha = e^2/4\pi$. Σ , Π , the form factors and $\beta(e)$ are the same in both conventions. Every loop has the measure of section 19, so that minimal subtraction is $\overline{\text{MS}}$: the $2/\epsilon - \gamma_E + \log 4\pi$ of Peskin and Schroeder, who write $d = 4 - \epsilon$, is $1/\epsilon$ here. The whole computation is the script `Tests/QEDOneLoop.wl`; its core is shown below.

The theory. The free generating functional is that of a photon and an electron, with the propagators $\text{ElectronPropagator} = \langle T\psi\bar{\psi} \rangle_0$ and $\text{PhotonPropagator} = \langle TAA \rangle_0$; photons are wavy lines:

```
DeclareSource[Jphoton]; DeclareGrassmannSource[eta, etabar];
DeclareField[photon, Jphoton]; DeclareField[electron, etabar];
DeclareField[electronbar, eta, -1];
DeclareSymmetric[PhotonPropagator]; DeclareLocalVertex[QEDVertex];
DeclareLineStyle[PhotonPropagator, "Wavy"];
DeclareDirectedPropagator[ElectronPropagator];
qedZ0 = Exp[1/2 IntegralOver[Jphoton[x] PhotonPropagator[x, y] Jphoton[y], {x, y}] +
  IntegralOver[ElectronPropagator[x, y] etabar[x] ** eta[y], {x, y}]];
qedInteraction = e IntegralOver[QEDVertex[x, y, z] electronbar[x] ** electron[y]
  photon[z], {x, y, z}];
qedRules[xi_, lambda_: 0] := {ElectronPropagator -> {"Fermion", m},
  PhotonPropagator -> {"Photon", {xi, lambda}}, QEDVertex -> {"Vertex", -I}};
```

The package expands $e^{-S_{\text{int}}}$; in Minkowski space the weight is e^{iS} , so the interaction it is given is $-iS_{\text{int}} = e \int V \bar{\psi} \psi A$, with the local kernel $V(x, y, z) = -i\gamma_{a_x a_y}^{\mu_z} \delta(x - y) \delta(x - z)$: each vertex is then $(-1)e(-i\gamma^\mu) = ie\gamma^\mu$, and in the pictures, where a local vertex stands for minus its kernel, it is $ie\gamma^\mu$ with the factor e in the weight. The rules of `QEDIntegrand` give each line its form in momentum space ("Fermion" with mass m , "Photon" in the gauge ξ , with an optional photon mass λ as an infrared regulator, "Vertex" with the factor $-i$ of V). The 1PI functions are the derivatives of the 1PI action $\Gamma[\bar{\Psi}, \Psi, \bar{A}]$ at zero means $\bar{A} = \langle A \rangle$, $\Psi = \langle \psi \rangle$, $\bar{\Psi} = \langle \bar{\psi} \rangle$ (section 8): the self-energy from $\delta^2\Gamma/\delta\bar{\Psi}\delta\Psi$, the vacuum polarization from $\delta^2\Gamma/\delta\bar{A}_\mu\delta\bar{A}_\nu$ (each with its tree part, the inverse free propagator, removed) and the vertex from $\delta^3\Gamma/\delta\bar{\Psi}\delta\Psi\delta\bar{A}_\mu$. `EffectiveAction1PI` builds the action of one real boson or of one fermion field (several fields are not implemented yet); with both, the package takes the other side of the Legendre transform: the derivatives of W , the connected functions, are trees of the vertex functions (section 8.3), so that the vertex function of

order e^n is the one-particle-irreducible part of the connected function, with its legs removed; with the weight e^{iS} it is directly $-i\Sigma$, $i\Pi^{\mu\nu}$ or $ie\Gamma^\mu$:

```
qedLines = {PhotonPropagator, ElectronPropagator};
qedVertexFunction[fields_List, labels_List, n_Integer] := ParticleIrreducibleDiagrams[
  AmputateExternalLegs[ConnectedCorrelationFunction[qcdZ0, fields, qedInteraction,
    n, "CouplingOrder" -> {e, n}], labels, qedLines], 1, labels, qedLines];
treeVertex = qedVertexFunction[{electron[x1], electronbar[x2], photon[x3]},
  {x1, x2, x3}, 1];
DiracSimplify[QEDIntegrand[treeVertex, {x2 -> p1, x3 -> p2 - p1, x1 -> -p2},
  qedRules[1], "Indices" -> {x3 -> mu}]]
```

The tree vertex is $-e V(x_1, x_2, x_3)$, and in momentum space $ie\gamma^\mu$, with the momentum p_1 entering at x_2 , $p_2 - p_1$ at the photon leg and $-p_2$ at x_1 (minus $ie\gamma^\mu$: 0 ✓). The 1PI functions dress the propagators and the vertex [11, sections 7.1 and 7.5]: the full electron propagator is $i/(\not{p} - m_0 - \Sigma(p))$, with m_0 the bare mass; with $\Pi^{\mu\nu} = (q^2 g^{\mu\nu} - q^\mu q^\nu) \Pi(q^2)$ the full photon propagator is $-ig_{\mu\nu}/(q^2(1 - \Pi(q^2)))$ in the Feynman gauge, up to terms proportional to $q_\mu q_\nu$, which do not contribute to physical amplitudes; and the full vertex is $ie\Gamma^\mu$, with $\Gamma^\mu = \gamma^\mu + \delta\Gamma^\mu$.

The diagrams. At one loop the electron self-energy, the vacuum polarization and the vertex correction are

```
sigmaDiagrams = qedVertexFunction[{electron[x], electronbar[y]}, {x, y}, 2];
piDiagrams = qedVertexFunction[{photon[x], photon[y]}, {x, y}, 2];
vertexDiagrams = qedVertexFunction[{electron[x1], electronbar[x2], photon[x3]},
  {x1, x2, x3}, 3];
```

$$-i\Sigma_2 = e^2 \text{ (tadpole diagram)} \quad i\Pi_2^{\mu\nu} = -e^2 \text{ (vacuum polarization loop)} \quad ie\delta\Gamma^\mu = e^3 \text{ (vertex correction diagram)}$$

The closed electron loop carries the factor -1 of a Grassmann loop. The tadpoles are one-particle reducible; of the 6 diagrams of the amputated connected vertex of order e^3 the 1PI part keeps 1, the others are corrections of its legs.

From diagrams to integrals. QEDIntegrand routes the momenta as for the Matsubara sums (section 7) and follows the spinor indices along the fermion lines: an open line becomes a product of Dirac matrices, from its ψ end to its $\bar{\psi}$ end (DiracProduct), a closed loop a trace (DiracTrace), whose minus sign is the one in the weight of the package:

```
sigmaInt = QEDIntegrand[sigmaDiagrams, {y -> p, x -> -p}, qedRules[xi],
  "LoopMomentum" -> k];
piInt = QEDIntegrand[piDiagrams, {y -> q, x -> -q}, qedRules[xi],
  "Indices" -> {x -> mu, y -> nu}, "LoopMomentum" -> k];
vertexInt = QEDIntegrand[vertexDiagrams, {x2 -> p1, x3 -> p2 - p1, x1 -> -p2},
  qedRules[xi], "Indices" -> {x3 -> mu}, "LoopMomentum" -> k];
```

The contracted indices of the photon line are called ρ and σ here (all indices are written upper; a repeated index is contracted), and the vertex is shown in the Feynman gauge:

$$\begin{aligned}
-i\Sigma_2(p) &= -ie^2 \int_k \frac{(-i\gamma^\rho) i(m + \not{p} - \not{k}) (-i\gamma^\sigma) \left(g^{\rho\sigma} - \frac{(1-\xi)k^\rho k^\sigma}{k^2}\right)}{((p-k)^2 - m^2) k^2} \\
i\Pi_2^{\mu\nu}(q) &= -e^2 \int_k \frac{\text{tr}[i(m + \not{k} + \not{q}) (-i\gamma^\nu) i(m + \not{k}) (-i\gamma^\mu)]}{(k^2 - m^2) ((k+q)^2 - m^2)} \\
ie\delta\Gamma^\mu(p_2, p_1) &= ie^3 \int_k \frac{(-i\gamma^\rho) i(m + \not{p}_2 - \not{k}) (-i\gamma^\mu) i(m + \not{p}_1 - \not{k}) (-i\gamma^\sigma) g^{\rho\sigma}}{((p_1-k)^2 - m^2) ((p_2-k)^2 - m^2) k^2}
\end{aligned}$$

In the Feynman gauge these are the integrals of the textbooks [11, sections 7.1, 7.5 and 6.3]. IntegrateOneLoop evaluates them exactly in d , with Feynman parameters as in the textbooks, DiracSimplify does the Dirac algebra, and ExpandParameterIntegrals expands the result in ε :

How the package does the one-loop integrals.

- (1) The n denominators $D_i = (k + r_i)^2 - m_i^2 + i0$, of integer powers a_i ($n = 2$ for Σ and Π , 3 for the vertex), are combined with Feynman parameters [15], as two were in section 19, with $A = \sum_i a_i$:

$$\prod_i \frac{1}{D_i^{a_i}} = \frac{\Gamma(A)}{\prod_i \Gamma(a_i)} \int_0^1 dx_1 \cdots dx_n \delta\left(1 - \sum_i x_i\right) \frac{\prod_i x_i^{a_i-1}}{(\sum_i x_i D_i)^A}.$$

- (2) $\sum_i x_i D_i = (k + r)^2 - \Delta + i0$, with $r = \sum_i x_i r_i$ and $\Delta = r^2 - \sum_i x_i (r_i^2 - m_i^2)$: the loop momentum is shifted, $l = k + r$, in the numerator too (Dirac products, traces, scalar products).
- (3) Tensor reduction in d dimensions: odd powers of l vanish, $l^\mu l^\nu \rightarrow g^{\mu\nu} l^2/d$, $l^\mu l^\nu l^\rho l^\sigma \rightarrow (g^{\mu\nu} g^{\rho\sigma} + g^{\mu\rho} g^{\nu\sigma} + g^{\mu\sigma} g^{\nu\rho}) (l^2)^2/(d(d+2))$, and so on, with $l = \gamma_\mu l^\mu$.
- (4) The integral over l^0 is rotated to the imaginary axis, $l^0 = il_E^0$, which the $+i0$ allows without crossing a pole, and the Euclidean integral of section 19 gives [11, appendix A.4]

$$\int \frac{d^d l}{(2\pi)^d} \frac{(l^2)^s}{(l^2 - \Delta + i0)^A} = \frac{i(-1)^{A+s}}{(4\pi)^{d/2}} \frac{\Gamma(s + d/2) \Gamma(A - s - d/2)}{\Gamma(d/2) \Gamma(A)} (\Delta - i0)^{d/2+s-A},$$

times the factor $\mu^{2\varepsilon} (e^{\gamma_E}/4\pi)^\varepsilon$ of the measure; the package applies this formula directly.

- (5) DiracSimplify brings the result to a sum of Dirac and tensor structures, each multiplied by an integral over the Feynman parameters, ParameterIntegral (two lines, $x_2 = 1 - x_1$) or SimplexIntegral (three lines).
- (6) ExpandParameterIntegrals gives these integrals exactly in d , as Beta functions, $\int_0^1 dx x^a (1-x)^b = \Gamma(a+1)\Gamma(b+1)/\Gamma(a+b+2)$, where Δ is a product of powers of the parameters (on shell, at $q^2 = 0$); otherwise it expands $\Delta^{-\varepsilon} = 1 - \varepsilon \log \Delta + \cdots$ under the integral sign. An integrand that is not integrable at $\varepsilon = 0$ near a face of the parameter region (an infrared divergence: in the vertex at $q^2 = 0$, where the parameters of the two electron lines vanish) is first split: its Taylor terms at the face are integrated exactly in d , as Beta functions, which gives the infrared pole, and the remainder is expanded. N integrates the parameter integrals numerically, with $\log \Delta \rightarrow \log |\Delta| - i\pi$ where $\Delta < 0$, above the thresholds.

The tensor integrals are not reduced to scalar ones (Passarino–Veltman), and γ_5 is not implemented (below).

Since $g^\mu{}_\mu = d$, the Dirac algebra changes in d dimensions: $\gamma^\mu \gamma_\mu = d$, $\gamma^\mu \not{a} \gamma_\mu = -(d-2) \not{a}$, $\gamma^\mu \not{a} \not{b} \gamma_\mu = 4a \cdot b - (4-d) \not{a} \not{b}$ [11, appendix A.4]. The terms of order ε multiply the poles and leave finite parts, so the algebra is done in d dimensions throughout: DiracSimplify contracts by $\gamma^\mu X \not{a} \gamma_\mu = 2 \not{a} X - (\gamma^\mu X \gamma_\mu) \not{a}$, takes traces by the recursion over the pairings, with $\text{tr } 1 = 4$, and in a chain between on-shell spinors moves $\not{p}_1$ to $u(p_1)$ and $\not{p}_2$ to $\bar{u}(p_2)$, where they become m . The γ_5 of four dimensions, which anticommutes with every γ^μ and has $\text{tr}(\gamma_5 \gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma) \neq 0$, cannot keep both properties in d dimensions [94, 105], and the package does not implement it.

Renormalization of QED. As in section 19, the bare fields and parameters are written through renormalized ones [11, section 10.3],

$$\psi_0 = Z_2^{1/2} \psi, \quad A_0^\mu = Z_3^{1/2} A^\mu, \quad m_0 = Z_m m, \quad e_0 = \mu^\varepsilon (e^{\gamma_E} / 4\pi)^{\varepsilon/2} \frac{Z_1}{Z_2 Z_3^{1/2}} e,$$

with the counterterms $\delta_i = Z_i - 1$ ($i = 1, 2, 3$) and $\delta_m = Z_m m_0 - m$; the renormalized self-energy, for instance, is $\Sigma_R = \Sigma - \not{p} \delta_2 + \delta_m$. The conservation of the charge gives the Ward–Takahashi identity [62, 63]

$$q_\mu \Gamma^\mu(p+q, p) = S^{-1}(p+q) - S^{-1}(p), \quad S^{-1}(p) = \not{p} - m_0 - \Sigma(p),$$

which ties the vertex to the self-energy. With a regulator that respects it, as dimensional regularization does, it gives $Z_1 = Z_2$ [11, section 7.4], so that $e_0 = \mu^\varepsilon (e^{\gamma_E} / 4\pi)^{\varepsilon/2} Z_3^{-1/2} e$: the charge is renormalized by the vacuum polarization alone, by the same factor for every charged particle. Two schemes are used below. In $\overline{\text{MS}}$ the Z 's are pure poles, and m is a mass that runs with μ . On shell, m is the physical mass, the pole of the full propagator, $m = m_0 + \Sigma(\not{p} = m)$; Z_2 is the residue there, so that $\delta Z_2 = d\Sigma/d\not{p}$ at $\not{p} = m$ to this order; and e is the charge measured at $q^2 \rightarrow 0$, where the renormalized $\hat{\Pi}(0) = 0$ and $\alpha = 1/137.036$ [11, sections 7.1 and 7.5] [106].

The self-energy. $\Sigma_2 = mA + \not{p} B$, in a general gauge (coefficientOf, a function of the script, takes the coefficient of a Dirac structure):

```
electronSelfEnergy = DiracSimplify[I IntegrateOneLoop[sigmaInt, eps]];
{a, b} = {coefficientOf[electronSelfEnergy, DiracProduct[]]/m,
coefficientOf[electronSelfEnergy, DiracProduct[SlashedMomentum[p]]]};
ExpandParameterIntegrals[{a, b}, eps, -1]
```

$$\Sigma_2 = \frac{\alpha (m (3 + \xi) - \xi \not{p})}{4 \pi \varepsilon} + O(\varepsilon^0), \quad \delta_2 = -\frac{\alpha \xi}{4 \pi \varepsilon}, \quad Z_m = 1 - \frac{3 \alpha}{4 \pi \varepsilon}$$

$$\frac{m - m_0}{m} = \frac{\Sigma_2(\not{p} = m)}{m} = -\delta Z_2 = -\frac{d\Sigma_2}{d\not{p}} \Big|_{\not{p}=m} = \frac{\alpha}{4\pi} \left(4 + \frac{3}{\varepsilon} + 3 \log \left(\frac{\mu^2}{m^2} \right) \right)$$

the pole minus that of the textbooks (for $\xi = 1$ [11, section 10.3], for any ξ [106, eqs. (3.64) and (3.104)]): $\{0, 0\}$ ✓; the $\overline{\text{MS}}$ counterterms δ_2 (with $\Sigma_R = \Sigma - \not{p} \delta_2 + \delta_m$) and Z_m ($m_0 = Z_m m$) minus those of [106, eqs. (3.64) and (3.104)]: $\{0, 0\}$ ✓; on shell, $(m - m_0)/m$ minus the value of [11, section 10.3] (gauge invariant, infrared finite) and $\delta Z_2 + (m - m_0)/m$: $\{0, 0\}$ ✓

The field renormalization δ_2 depends on the gauge, and vanishes in the Landau gauge; Z_m does not depend on it.

On shell a second kind of divergence appears. An on-shell electron can emit and reabsorb a photon of arbitrarily small momentum k at almost no cost in energy, and the integrals over these soft virtual photons diverge logarithmically at small k : an infrared divergence [11, sections 6.4–6.5]. It can be regulated by a photon mass λ , $1/(k^2 - \lambda^2)$ in the photon line (the line rule {"Photon", {xi, lambda}}), or dimensionally, since these integrals converge at small k for $d > 4$, that is $\varepsilon < 0$; with one ε for both kinds of divergence, a scaleless integral vanishes (section 19). In a cross section the infrared poles cancel against the emission of real soft photons, which no detector can resolve [107]. On shell, δZ_2 is infrared divergent: with the infrared regulated dimensionally as well, the part that depends on ξ is a scaleless integral, which vanishes, and $(m - m_0)/m = -\delta Z_2$ in every gauge.

The vacuum polarization. $\Pi^{\mu\nu} = g^{\mu\nu} A + q^\mu q^\nu B$ comes out transverse, $A + q^2 B = 0$, exactly in d (the integrand of $A + q^2 B$ is zero, by FullSimplify), as the conservation of the current requires:

$q_\mu \Pi^{\mu\nu} = 0$ is a Ward identity, and it keeps the photon massless. It does not depend on ξ , since there is no internal photon. With $\Pi^{\mu\nu} = (q^2 g^{\mu\nu} - q^\mu q^\nu) \Pi_2(q^2)$:

```
piMuNu = DiracSimplify[-I IntegrateOneLoop[piInt, eps]];
```

$$\begin{aligned}\Pi_2(q^2) &= -\frac{\alpha}{3\pi\epsilon} + \frac{2\alpha}{\pi} \int_0^1 dx_1 (1-x_1) x_1 \log\left(\frac{m^2 - (1-x_1) x_1 q^2}{\mu^2}\right) + O(\epsilon) \\ \delta_3 &= -\frac{\alpha}{3\pi\epsilon}, \quad \beta(e) = \mu \frac{de}{d\mu} = \frac{e^3}{12\pi^2} \\ \hat{\Pi}_2(q^2) &= \frac{\alpha \log\left(\frac{\mu^2}{m^2}\right)}{3\pi} + \frac{2\alpha}{\pi} \int_0^1 dx_1 (1-x_1) x_1 \log\left(\frac{m^2 - (1-x_1) x_1 q^2}{\mu^2}\right)\end{aligned}$$

Since $Z_1 = Z_2$ (above), the function `BetaFunctionFromZ` of section 19, given $Z_3^{-1/2}$, gives $\beta(e)$. The renormalized $\hat{\Pi}_2(q^2) = \Pi_2(q^2) - \Pi_2(0)$ is, as $\int_0^1 x(1-x) dx = \frac{1}{6}$, the expression of the textbooks,

$$\hat{\Pi}_2(q^2) = -\frac{2\alpha}{\pi} \int_0^1 dx x(1-x) \log \frac{m^2}{m^2 - x(1-x) q^2},$$

and at $q^2 = -3m^2$ both are $0.003921482651 e^2$. With it the photon propagator is that of an effective coupling $\alpha_{\text{eff}}(q^2) = \alpha / (1 - \hat{\Pi}_2(q^2))$, which at $-q^2 \gg m^2$ grows as $\alpha / (1 - \frac{\alpha}{3\pi} \log(-q^2/m^2))$: virtual electron-positron pairs screen the charge, which looks larger at short distances, as $\beta(e) > 0$ says; at small momenta the same $\hat{\Pi}_2$ gives the Uehling correction to the Coulomb potential [11, section 7.5]. For $q^2 > 4m^2$, $m^2 - x(1-x) q^2$ is negative on part of the interval, and $\hat{\Pi}_2$ has an imaginary part, the rate of creation of real pairs (the optical theorem of section 7), whose sign the prescription $\Delta - i0$ fixes.

transversality, $A + q^2 B$: 0 ✓; $\partial \Pi^{\mu\nu} / \partial \xi$: 0 ✓; δ_3 and $\beta(e)$ minus those of the textbooks: $\{0, 0\}$ ✓; $\hat{\Pi}_2(-3m^2)$ minus the integral of the textbooks: 0 ✓

The vertex and the magnetic moment. Between on-shell spinors the vertex has three form factors,

$$\bar{u}(p_2) \Gamma^\mu u(p_1) = \bar{u}(p_2) \left[\gamma^\mu F_1(q^2) + \frac{i\sigma^{\mu\nu} q_\nu}{2m} F_2(q^2) + q^\mu F_3(q^2) \right] u(p_1), \quad q = p_2 - p_1.$$

Lorentz covariance and parity allow these three structures, and the conservation of the current excludes the third: $q_\mu \bar{u}(p_2) \Gamma^\mu u(p_1)$ must vanish, and since q between on-shell spinors is zero, this leaves $q^2 F_3 = 0$. The Gordon identity [11, section 6.2],

$$\bar{u}(p_2) \gamma^\mu u(p_1) = \bar{u}(p_2) \left[\frac{(p_1 + p_2)^\mu}{2m} + \frac{i\sigma^{\mu\nu} q_\nu}{2m} \right] u(p_1), \quad \sigma^{\mu\nu} = \frac{i}{2} [\gamma^\mu, \gamma^\nu],$$

shows what the other two mean: $F_1(0) = 1$ is the charge, and in a weak static magnetic field the vertex gives the energy $-\boldsymbol{\mu} \cdot \mathbf{B}$ of a magnetic moment $\boldsymbol{\mu} = g (e/2m) \mathbf{S}$, with $g = 2 (F_1(0) + F_2(0))$: the value $g = 2$ of Dirac's theory comes from γ^μ , the anomalous part from F_2 . `DiracSimplify` moves p_1 to the right and p_2 to the left of the spinor chain and uses the Dirac equation, which leaves $A\gamma^\mu + B_1 p_1^\mu + B_2 p_2^\mu$; `VertexFormFactors` separates them by the Gordon identity, $F_1 = A + m(B_1 + B_2)$, $F_2 = -m(B_1 + B_2)$, $F_3 = (B_2 - B_1)/2$:

```
dGamma = I/e IntegrateOneLoop[vertexInt, eps];
chain = DiracSimplify[SpinorChain[{p2, m}, dGamma, {p1, m}]] /.
  ScalarProduct[p1, p2] -> m^2 - q2/2;
{f1, f2, f3} = VertexFormFactors[chain, mu, {p1, p2, m}];
ExpandParameterIntegrals[f2 /. q2 -> 0, eps, 0]
```

$$F_2(q^2) = \frac{\alpha}{\pi} \int_0^1 dx_1 dx_2 dx_3 \delta(1 - x_1 - x_2 - x_3) \frac{m^2 (1 - x_1) x_1}{m^2 (1 - x_1)^2 - q^2 x_2 x_3}$$

$$F_2(0) = \frac{\alpha}{2\pi}, \quad F_1|_{\text{UV pole}} = \frac{\alpha \zeta}{4\pi \varepsilon} = -\delta_2$$

$$F_1(0) - 1 = \frac{\alpha}{4\pi} \left(4 + \frac{3}{\varepsilon} + 3 \log \left(\frac{\mu^2}{m^2} \right) \right) = -\delta Z_2$$

$F_2(q^2)$ is shown in the Feynman gauge, with x_1 the parameter of the photon line, and is finite; the pole of F_1 is taken with a photon mass, which separates it from the infrared divergence, and $F_1(0)$ with the infrared regulated dimensionally, as δZ_2 above. With $\varepsilon_{\text{UV}} = \varepsilon_{\text{IR}}$ the pole $3\alpha/4\pi\varepsilon$ of $F_1(0) - 1$ (and of $-\delta Z_2$) is the ultraviolet one, $\zeta\alpha/4\pi\varepsilon$, plus an infrared one, $(3 - \zeta)\alpha/4\pi\varepsilon$; $F_1(0) - 1 + \delta Z_2$ is free of both.

$F_2(0) - \alpha/2\pi$, in a general gauge: 0 ✓; $F_2(-m^2)$, 0.01090238584 e^2 in the Feynman gauge, minus the integral of the textbooks [11, section 6.3]: 0 ✓, and $\partial F_2/\partial \zeta$ there (photon mass $m/10$, exactly in d at $\varepsilon = -\frac{3}{10}$): 0 ✓; the ultraviolet pole of F_1 minus $\zeta\alpha/4\pi\varepsilon$, and plus δ_2 ($Z_1 = Z_2$): $\{0, 0\}$ ✓; $F_1(0) - 1 + \delta Z_2$: 0 ✓; F_3 at $q^2 = 0$ and its integrand, odd under $x_2 \leftrightarrow x_3$, symmetrized: $\{0, 0\}$ ✓

Once the legs are renormalized (a factor $Z_2 = 1 + \delta Z_2$), $F_1(0) - 1 + \delta Z_2 = 0$ above says that $F_1(0) = 1$: the Ward–Takahashi identity [62, 63] appears twice, as $Z_1 = Z_2$ in $\overline{\text{MS}}$ and on shell as $F_1(0) = 1$. The magnetic moment of the electron is then given by $g = 2(F_1(0) + F_2(0)) = 2 + \alpha/\pi$: the anomalous moment $a = (g - 2)/2 = F_2(0) = \alpha/2\pi$ is Schwinger’s result [108], the same in every gauge. With $\alpha = 1/137.036$ it is $a = 0.0011614$; the measured value, 0.00115965218 [109], agrees with the higher orders (with α measured independently), now known to the tenth order in e [110]. The section is computed in 4.7s.

Limits. The evaluation is limited to one loop (one loop momentum: QEDIntegrand and IntegrateOneLoop refuse more), to at most one open fermion line (no four-fermion amplitudes such as Møller or Bhabha scattering), and to the Dirac algebra without γ_5 (GammaMatrix[5] is refused: no anomalies, no chiral couplings). The momentum-space form of the lines is given by the rules, not derived; closed forms are obtained only where the Feynman-parameter integrals are products of Gamma functions, and the others are evaluated numerically (with $\Delta - i0$ above thresholds). An infrared divergence is subtracted when it sits at one face of the Feynman-parameter region (as in the one-loop vertex), otherwise ExpandParameterIntegrals gives a message; the closed forms with symbolic coefficients hold below thresholds.

21 Gauge theories: the vertices of QCD

QCD is the gauge theory of the colour group $\text{SU}(3)$: a quark field q has three colour components, and there are eight gluon fields A_μ^a . Its gauge-invariant Lagrangian $\bar{q} (i\gamma^\mu D_\mu - m) q - \frac{1}{4} F_{\mu\nu}^a F^{a\mu\nu}$, with $D_\mu = \partial_\mu - igA_\mu^a t^a$ and $F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + gf^{abc} A_\mu^b A_\nu^c$, has the form of that of QED, but the generators t^a do not commute, $[t^a, t^b] = if^{abc} t^c$: the gluons carry colour themselves, and F^2 contains vertices of three and four gluons [11, chapters 15 and 16]. As in QED (section 20), a label stands for a point of space-time together with its Lorentz and spinor indices, and here also a colour index; the interaction of QCD is the sum of four vertices,

$$S_{\text{int}} = g \int V_{\bar{q}qA} \bar{q} q A + \frac{g}{3!} \int V_3 AAA + \frac{g^2}{4!} \int V_4 AAAA + g \int V_{\bar{c}cA} \bar{c} c A,$$

whose kernels contain the colour factors, the Dirac matrices and the derivatives of the Feynman rules; V_3 and V_4 are totally symmetric [11, 111]. The ghosts $c, \bar{c}$ are Grassmann fields with a propagator of their own [104]: in a covariant gauge the Faddeev–Popov determinant, which in

QED does not depend on the field, here depends on the gluons, and is written as an integral over these scalar Grassmann fields, coupled to the gluons through f^{abc} ; in loops they cancel the contributions of the unphysical, timelike and longitudinal, gluon polarizations [11, sections 16.2 and 16.3]. The package does not do the colour algebra: the colour factors stay in the kernels, to be evaluated with $t^a t^a = C_F \mathbf{1}$, $f^{acd} f^{bcd} = C_A \delta^{ab}$ and $\text{tr } t^a t^b = T_F \delta^{ab}$, where $C_F = \frac{4}{3}$, $C_A = 3$ and $T_F = \frac{1}{2}$. The propagators are $D_0 = \langle AA \rangle_0$, $S_0 = \langle q\bar{q} \rangle_0$ and $\langle c\bar{c} \rangle_0$; `DeclareLocalVertex` draws the kernels as points, gluons are coils ("Curly") and ghosts dotted lines with an arrow ("DottedArrow"):

```

DeclareSource[Jgluon]; DeclareGrassmannSource[chi, chibar, sigma, sigmabar];
DeclareField[gluon, Jgluon]; DeclareField[quark, chibar];
DeclareField[quarkbar, chi, -1]; DeclareField[ghost, sigmabar];
DeclareField[ghostbar, sigma, -1];
DeclareSymmetric[GluonPropagator, ThreeGluonVertex, FourGluonVertex];
DeclareLocalVertex[QuarkGluonVertex, ThreeGluonVertex, FourGluonVertex,
  GhostGluonVertex];
DeclareLineStyle[GluonPropagator, "Curly"]; DeclareLineStyle[GhostPropagator,
  "DottedArrow"];
DeclareDirectedPropagator[QuarkPropagator];
FreeQCDGeneratingFunctional = Exp[
  1/2 IntegralOver[Jgluon[x] GluonPropagator[x, y] Jgluon[y], {x, y}] +
  IntegralOver[QuarkPropagator[x, y] chibar[x] ** chi[y], {x, y}] +
  IntegralOver[GhostPropagator[x, y] sigmabar[x] ** sigma[y], {x, y}]];
QCDVertices =
g IntegralOver[QuarkGluonVertex[x, y, z] quarkbar[x] ** quark[y] gluon[z],
  {x, y, z}] +
g/6 IntegralOver[ThreeGluonVertex[x, y, z] gluon[x] gluon[y] gluon[z],
  {x, y, z}] +
g^2/24 IntegralOver[FourGluonVertex[w, x, y, z] gluon[w] gluon[x] gluon[y]
  gluon[z], {w, x, y, z}] +
g IntegralOver[GhostGluonVertex[x, y, z] ghostbar[x] ** ghost[y] gluon[z],
  {x, y, z}];

```

A vertex function, a derivative of the 1PI action $\Gamma[\bar{A}, \bar{C}, C, \Psi, \bar{\Psi}]$ at zero means (of the gluon, ghost and quark fields), is computed as in QED, from the derivatives of W : the one-particle-irreducible part of a connected function, with its legs removed; at one loop the gluon self-energy, with $\langle AA \rangle = D + D \Pi D + \dots$, is

```

lines = {GluonPropagator, QuarkPropagator, GhostPropagator};
gluonSelfEnergy = ParticleIrreducibleDiagrams[AmputateExternalLegs[OrderPart[
  ConnectedCorrelationFunction[FreeQCDGeneratingFunctional, {gluon[x], gluon[y]},
    QCDVertices, 2], g, 2], {x, y}, lines], 1, {x, y}, lines]

```

$$\Pi(x, y) = \frac{1}{2} g^2 x \text{---} \text{gluon loop} \text{---} y - g^2 x \text{---} \text{ghost loop} \text{---} y - g^2 x \text{---} \text{quark loop} \text{---} y + \frac{1}{2} g^2 x \text{---} \text{tadpole} \text{---} y$$

The quark and the ghost loops carry the factor -1 of a closed Grassmann loop, the gluon loop and the tadpole their symmetry factor $\frac{1}{2}$; each vertex stands for minus its kernel, the sign of e^{-S} , with the powers of g in the weight. The self-energies of the quark and of the ghost, and the two corrections of the quark–gluon vertex: the abelian one, a gluon exchanged across the vertex as in QED, with the colour factor $t^b t^a t^b = (C_F - \frac{1}{2} C_A) t^a$, and the non-abelian one, through the three-gluon vertex, with $f^{abc} t^b t^c = \frac{i}{2} C_A t^a$:

$$\Sigma_q(x, y) = g^2 x \text{---} \text{---} y$$

$$\Sigma_c(x, y) = g^2 x \text{---} \text{---} y$$

$$\Gamma_{q\bar{q}A}(x_1, x_2, x_3) = g^3 \text{---} + g^3 \text{---}$$

The three-gluon vertex at one loop: three diagrams with a four-gluon vertex, the gluon triangle, and the ghost and the quark triangles, each with both orientations of its loop:

$$\Gamma_{AAA}(x_1, x_2, x_3) = \frac{1}{2} g^3 \text{---} + \frac{1}{2} g^3 \text{---} + \frac{1}{2} g^3 \text{---} - g^3 \text{---} - g^3 \text{---} - g^3 \text{---} + g^3 \text{---}$$

At two loops the quark self-energy has 7 diagrams: the rainbow, the crossed diagram, the non-abelian vertex correction and the four insertions of the gluon self-energy (the two-loop gluon self-energy takes a few minutes):

$$\Sigma_q^{(2)}(x, y) = \frac{1}{2} g^4 x \text{---} y - g^4 x \text{---} y + g^4 x \text{---} y + g^4 x \text{---} y - g^4 x \text{---} y + g^4 x \text{---} y + \frac{1}{2} g^4 x \text{---} y$$

symmetry of the gluon self-energy, $\Pi(x, y) - \Pi(y, x) = 0$ ✓

PART III Tools

22 Pictures and formulas for papers

DiagramPlot shows the diagrams of an expression in Mathematica; DiagramToTikZ writes the same pictures as TikZ code, with their weights, ready for a $\text{\LaTeX}$ document — every picture in this document was made this way. The code needs only the TikZ library `decorations.pathmorphing`. For instance, the first-order self-energy of section 9.4, with the external labels written x_1 and x_2 ,

```
DiagramToTikZ[OrderPart[selfEnergy, InteractionPotential, 1], {x, y},
  "Labels" -> {x -> "x_1", y -> "x_2"}]
```

gives a string with one tikzpicture per diagram, each with its weight in front; the first one is

```

\begin{tikzpicture}[x=0.700cm, y=0.700cm, line width=0.700pt, baseline={([yshift=-0.6ex]0,0)}]
\draw (0.500,0.000) -- (-0.500,0.000);
\fill (-0.097,0.000) -- (0.097,-0.083) -- (0.034,0.000) -- (0.097,0.083) -- cycle;
\draw plot[smooth, tension=0.7] coordinates {(-0.500,0.000) (-0.537,0.035) (-0.548,0.069) (-0.524,0.095)
→ (-0.476,0.110) (-0.427,0.121) (-0.401,0.138) (-0.405,0.168) (-0.427,0.213) (-0.445,0.260)
→ (-0.441,0.296) (-0.407,0.308) (-0.357,0.301) (-0.308,0.290) (-0.278,0.293) (-0.268,0.322)
→ (-0.269,0.372) (-0.265,0.423) (-0.245,0.453) (-0.209,0.450) (-0.167,0.422) (-0.128,0.390)
→ (-0.099,0.380) (-0.078,0.402) (-0.057,0.447) (-0.031,0.491) (0.000,0.509) (0.031,0.491) (0.057,0.447)
→ (0.078,0.402) (0.099,0.380) (0.128,0.390) (0.167,0.422) (0.209,0.450) (0.245,0.453) (0.265,0.423)
→ (0.269,0.372) (0.268,0.322) (0.278,0.293) (0.308,0.290) (0.357,0.301) (0.407,0.308) (0.441,0.296)
→ (0.445,0.260) (0.427,0.213) (0.405,0.168) (0.401,0.138) (0.427,0.121) (0.476,0.110) (0.524,0.095)
→ (0.548,0.069) (0.537,0.035) (0.500,0.000)};
\draw (-0.500,0.000) -- (-1.100,0.000);
\fill (-0.927,0.000) -- (-0.733,-0.083) -- (-0.796,0.000) -- (-0.733,0.083) -- cycle;
\draw (0.500,0.000) -- (1.100,0.000);
\fill (0.673,0.000) -- (0.867,-0.083) -- (0.804,0.000) -- (0.867,0.083) -- cycle;
\fill (-0.500,0.000) circle (0.064);
\fill (0.500,0.000) circle (0.064);
\node[font=\small, inner sep=0pt, anchor=0] at (-1.190,0.000) {$x_1$};
\node[font=\small, inner sep=0pt, anchor=180] at (1.190,0.000) {$x_2$};
\end{tikzpicture}

```

and the whole string typesets as

$$\Sigma^{(1)}(x_1, x_2) = x_1 \text{---} \text{---} \text{---} x_2 - x_1 \text{---} \text{---} \text{---} x_2$$

at the default size. The pictures in the rest of this document are smaller: they were made with the options "Scale" -> 0.34, "LineWidth" -> 0.42, "LabelFont" -> "\tiny". ExpressionToLaTeX does the same for formulas, as in section 1.

Line styles. DeclareLineStyle[head, style] sets how the lines of a function are drawn: propagators, interaction lines, gluons, ghosts, correlators of random potentials. The short forms DeclareDirectedPropagator and DeclareInteractionLine stand for "Arrow" and "Wavy"; lines without a declared style are plain; the last two are the anomalous propagators $-\langle T\psi\psi \rangle$ and $-\langle T\bar{\psi}\bar{\psi} \rangle$ of section 13. A kernel declared with DeclareLocalVertex is drawn as one point, a vertex of QCD for instance, not as a blob.

 "Plain"	 "Arrow"	 "DoubleArrow"
 "DottedArrow"	 "Double"	 "Wavy"
 "DoubleWavy"	 "Curly"	 "Dashed"
 "Dotted"	 "Zigzag"	 "Impurity"
 "DivergingArrows"	 "ConvergingArrows"	

Options. DiagramPlot, DrawDiagram and DiagramToTikZ take the same options:

"VertexLabels" -> All	labels of the integration points $z_1, z_2, \dots$ too (Automatic: only the external points; None: no labels)
"Labels" -> {x -> "x_1", ...}	the $\text{\LaTeX}$ of the labels
"ExternalOrder" -> {x4, x2, x3, x1}	the order of the external points, counterclockwise from the top left
"LegDirections" -> "Alternating"	arrows on the external legs of fermionic vertex functions (or a list of "Out", "In", None)
"AmputatedLegs" -> True	external points drawn with legs, as in amputated functions, or (False) as open circles
"InteractionStyle" -> "Dashed"	all the interaction lines in one style
"Scale" -> 0.7	TikZ: centimetres per unit of the drawing
"LineWidth" -> 0.7	the width of the lines in pt (arrow heads, dashes and double lines follow)
"LabelFont" -> "\\small"	TikZ: the font of the labels
"Output" -> "List"	TikZ: the list of the pairs {weight, picture} instead of one string
"Columns", "Weights", ImageSize	Mathematica: the layout of DiagramPlot

How the diagrams are drawn. No picture is drawn by hand and no coordinate is stored: the layout is computed from the diagram, by a few rules chosen to reproduce the way diagrams are drawn in textbooks.

- In a theory of fermions with density-type couplings every vertex lies on one fermion line, open or closed. The open lines are straight: the horizontal axis of a two-point function, two parallel rails — horizontal or vertical, according to which external points they join — for a four-point function, whose legs point to the corners of a rectangle. The closed lines are circles (bubbles when they have two vertices).
- The interaction lines between the rails are perpendicular to them where possible, so that ladders are ladders; two that cross make a symmetric cross. Arcs between vertices of one line go to the side where they cross nothing, as in the Fock-like and crossed diagrams of sections 3, 5 and 18; of two arcs that would cross, one goes to each side.
- Loops hang from the lines and from each other, pointing away from what they hang from; a loop joined to several vertices of a line sits above them, its lines perpendicular to the line when the vertices are close and leaning inwards when they are far apart; the vertices are spaced so that nothing overlaps. Vacuum diagrams made of several loops are trees, chains or rings of circles.
- Among the layouts of equal quality, the symmetric one is taken, so that symmetric diagrams are drawn symmetric.
- A bubble joined to two points of a line further apart than its width hangs below them, and its two interaction lines are bent into one round arc with it (a dressed interaction line). Three diameters of a fermion loop would meet at its centre: one is drawn outside, over the top, and the other two cross at the centre; four or more have their vertices moved alternately apart, so that they cross in pairs. Two bubbles side by side are joined at the sides facing each other, so that the lines leave the circles at a wide angle. Where two wavy lines cross, their waves are flattened, so that they read as a crossing.
- Trees of vertex functions (section 8.3) have their central vertex, or their two central vertices, in the middle; chains of vertices are straight, the legs at the ends of a chain fanned outwards and those along it perpendicular to it.
- Points joined by delta functions are drawn as one vertex; source insertions are crossed circles, vertex functions grey blobs. Other diagrams (bosons, ϕ^4 theory) are drawn with the external points on a circle and the rest placed by a barycentric embedding.

23 Under the hood

Differentiation. Every expression is kept as a sum of terms, each made of a coefficient, an integral over dummy labels and an ordered product of Grassmann factors. The derivative applies the product and chain rules, the declared rules for implicit dependence and the Grassmann signs; derivatives of sources give delta functions, which are integrated at once.

Canonical form. Two terms are the same diagram if one is obtained from the other by renaming the integration variables. A canonical renaming is computed by colour refinement — each variable is characterized by the factors it appears in, iteratively — followed by individualization of the remaining ties, as in graph-isomorphism algorithms [112]. Transpositions that leave a term unchanged are pruned; a term that changes sign under one of them vanishes.

Wick's theorem. Pairings are enumerated recursively. When the partner of a field lies on an interaction vertex not yet touched, only the first such vertex of each kind, and one field per orbit of the vertex symmetries, are tried, with their multiplicity; identical commuting fields are interchangeable; components that close without external points are discarded on the fly.

Cuts. Irreducibility, skeletons, channels and loops are decided on the graph whose nodes are the points glued by vertices and interaction lines, and whose edges are the propagators, by trying the cuts of one and two lines.

Frequency sums. Momenta and frequencies are routed along a spanning tree of the diagram, chosen with the interaction and boson lines first, so that every loop runs along fermion lines. The poles of a summand are read from the linear factors of its denominators (a boson propagator is split into two), and its residues, of any order, are Laurent coefficients computed by differentiation, without Residue, Limit or Apart. After each sum the statistical factors are freed of the other frequencies by periodicity; at the end the terms are put over common denominators, in partial fractions in the external frequency, and the occupation factors are written as a sum over processes. The cutting rules are derived independently, in imaginary time, from the product of the propagators of each chain of lines between the external time vertices.

Dimensional regularization. The lines become propagators $1/(q^2 + m^2)$, routed as for the Matsubara sums, and the loops are integrated one at a time: tadpoles and massless bubbles, which leave a line of non-integer power, in closed form in d , a massive bubble at non-zero momentum as an integral over one Feynman parameter, expanded in ε under the integral sign (the box in section 19). The scaleless and infrared-divergent integrals met on the way decide the routings of the infrared rearrangement. The expansion in ε uses Laurent series of its own.

QED. The spinor indices are followed along the fermion lines of a diagram, which become products of Dirac matrices or traces. The Dirac algebra is done in d dimensions (section 20): contractions, traces by the recursion over the pairings, spinor chains by anticommuting $\not{p}_1$ and $\not{p}_2$ to the spinors. The loop integrals are done with Feynman parameters, the shift of the loop momentum and the tensor reduction, exactly in d (the box in section 20); the parameter integrals that are products of Gamma functions are done in closed form, and an infrared divergence at a face of the simplex is subtracted, exactly in d , before the expansion under the integral sign.

Pictures. The fermion lines of a diagram are found by following its directed propagators; the open ones become the axis or the rails, the closed ones circles. The sides of the arcs and of the loops hanging from a line are chosen by trying all assignments and counting conflicts (crossings, a loop under an arc, nested parts); the positions along the lines follow from the room that what hangs from them needs, and are widened until nothing overlaps. Trees of vertex functions are laid out from their centre, the vertex (or the two vertices) of smallest eccentricity. In TikZ, wavy arcs are

curves through computed points and arrow heads small polygons, so that the code compiles at any scale.

Related software. Programs such as QGRAF [113] and FeynArts [114] generate Feynman diagrams from Feynman rules, FeynCalc [115] evaluates the amplitudes of particle physics, and DoFun [116, 117] derives Dyson–Schwinger and functional renormalization-group equations. FunctionalDiagrams derives the diagrams of many-body theory by differentiating generating functionals literally, with the Grassmann signs and the weights that this implies, and classifies them by their topology.

Performance. The script that computes and draws everything in this document, `make_figures.wl`, runs in 124.7 s in Mathematica (FunctionalDiagrams 2.4.0, Mathematica 15.0.1).

24 Function index

The public functions; the reference manual, `Documentation/FunctionalDiagrams_Manual.pdf`, describes each of them with its options and conventions, and `?Name` shows the same text in Mathematica.

Notation and declarations

IntegralOver, DeltaFunction, GrassmannProduct, DummyVariable DeclareSource, DeclareGrassmannSource, DeclareField DeclareSymmetric, DeclareAntisymmetric DeclareGrassmannOdd, DeclareGrassmannGraded DeclareFunctionalDerivative	integrals, delta functions, ordered Grassmann products, canonical integration variables sources and the fields they generate symmetries of functions Grassmann parity of other objects derivatives of objects that depend on the sources implicitly
DeclareDiscreteIndexValues DeclareLineStyle, DeclareDirectedPropagator, DeclareInteractionLine, DeclareLocalVertex, DeclareBlob DeclareCoupling	labels that are discrete values, such as spin projections how lines, vertices and blobs (full propagators and vertices) are drawn
DeclareDisplayName, ResetDeclarations	couplings: in the pictures each vertex stands for minus its coupling compact output; removing all declarations

Calculus and Wick's theorem

FunctionalDerivative	left derivatives with respect to bosonic and Grassmann sources
SimplifyDiagrams, DiagramTerms, SetSourcesToZero FieldDerivative, FieldExpectationValue	canonical form; list of terms with their weights; zero sources derivatives by fields; expectation values in any generating functional
GaussianExpectationValue	Wick's theorem (sum over pairings, or differentiation)

Perturbation theory

PerturbativeCorrelationFunction ConnectedCorrelationFunction, ConnectedVacuumDiagrams OrderPart	correlation functions without vacuum bubbles cumulants; $\log(Z/Z_0)$ the terms of a given order
--	--

Classes of diagrams

ConnectedDiagrams, DropVacuumBubbles ParticleIrreducibleQ, ParticleIrreducibleDiagrams, SkeletonDiagrams AmputateExternalLegs	connectivity n -particle-irreducible diagrams; skeletons vertex functions from correlation functions
ReducibleDiagrams, IrreducibleDiagrams, TwoParticleReducibleQ ClosedLoopCount, DropClosedLoops	cuts that separate groups of external points closed fermion loops

Many-body functionals and vertices

LuttingerWardFunctional, SelfEnergy, IrreducibleVertex	$\Phi[G], \Sigma = \delta\Phi/\delta G, \Gamma^0 = \delta^2\Phi/\delta G \delta G$
DysonSeries	chains of self-energy insertions
PerturbativeFullVertex	the full four-point vertex F
ParquetDecomposition, BetheSalpeterLadder, CheckParquetEquations	channels, ladders, parquet equations
ConnectedFunctionFromVertices	tree expansion (with FullPropagator, VertexFunction, MeanField, ExternalSource)
PerturbativeDensityVertex	the vertex Λ of the density
ExactEquation, CheckEquation, LabelFunction	exact equations, drawn or checked order by order
HubbardStratonovich, IntegrateOutField	auxiliary fields: introduced, integrated out

Effective actions and operator traces

EffectiveAction2PI, EffectiveAction1PI	$\Gamma[G]$ and $\Gamma[\bar{\phi}, G]; \Gamma[\bar{\phi}]$
SuperfieldComponents	a superfield expression in the components $\psi, \bar{\psi}$ (Nambu–Gor’kov)
LegendreTransform, LegendrePropagator, SelfEnergyFunctional	Potthoff’s $\mathcal{F}[\Sigma], G[\Sigma]$ and $\Omega[\Sigma]$
TraceLog, OperatorTrace, OperatorKernel, ExpandTrace	$\text{Tr} \ln A, \text{Tr} A, A(x, y)$; rings and Dyson series
ZeroDimensionalValue	the value of diagrams in zero dimensions

Momentum and Matsubara frequency

EvaluateMatsubara, DiagramIntegrand	diagrams in momentum and frequency, the frequencies summed; the integrand
MatsubaraSum, DeclareMatsubaraFrequency	frequency sums by residues; frequencies and their statistics
AnalyticContinuation, RetardedImaginaryPart, ZeroTemperatureLimit	real frequency, imaginary part, $T \rightarrow 0$
CuttingRuleImaginaryPart, CheckCuttingRules	the cutting rules at finite temperature
FermiFunction, BoseFunction, EnergyDelta, MomentumSum, LoopMomentum, LoopFrequency, Temperature	$n_F, n_B, \delta, \sum_p, p_i, \omega_i, T$

Dimensional regularization

DiagramLoopIntegral, LoopIntegral, ScalarPropagator, MomentumSquared, RenormalizationScale	diagrams as loop integrals in $d = 4 - 2\epsilon$; the lines $1/(q^2 + m^2)$, q^2 , the scale μ
IntegrateLoops, TadpoleIntegral, GFunction, BubbleIntegral	the loops one after the other; the one-loop integrals
EpsilonExpand, PolePart, FeynmanParameterIntegral, FeynmanParameter	Laurent expansion in ϵ ; the pole part; Feynman parameters
InfraredRearrangedIntegral, MassInsertion	counterterms by infrared rearrangement; $-\partial/\partial m^2$
BetaFunctionFromZ, AnomalousDimensionFromZ	β and anomalous dimensions from the Z factors

QED at one loop

GammaMatrix, SlashedMomentum, DiracProduct, DiracTrace, SpinorChain	$\gamma^\mu, \not{p}$, products, traces, $\bar{u}(p_2) \cdots u(p_1)$
LorentzMetric, FourVector, ScalarProduct, SpacetimeDimension	$g^{\mu\nu}, p^\mu, p \cdot q, d$
DiracSimplify, DiracOrder	the Dirac algebra in d dimensions; a canonical order
QEDIntegrand, FeynmanDenominator, MinkowskiLoopIntegral	diagrams as Minkowski loop integrals; $1/(q^2 - m^2)$
IntegrateOneLoop, ParameterIntegral, SimplexIntegral	one-loop integrals exactly in d ; Feynman-parameter integrals
ReduceParameterIntegrals, CombineParameterIntegrals, ExpandParameterIntegrals, DifferentiateUnderIntegral	closed forms; integrals with the same structure combined; Laurent expansion in ϵ ; derivatives under the integral (e.g. $\partial/\partial p^2, \partial/\partial \xi$)
VertexFormFactors	the form factors F_1, F_2, F_3

Pictures and formulas

DiagramPlot, DrawDiagram	Mathematica graphics
DiagramToTikZ	TikZ code for $\text{\LaTeX}$ documents
ExpressionToLaTeX	formulas for $\text{\LaTeX}$ documents

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