The crossing-symmetric pair approximation for many-body systems

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- The cumulant expansion is most prominent in statistical physics.

Introduction

- The theory of equilibrium and nonequilibrium GFs is a powerful tool in the field of many-particle physics.
- Diagrammatic decoupling schemas are applied to handle the exact but intractable basic theory.
- **Which systematic rearrangement of diagrammatic contributions justify a truncation at a given level?**
- The cumulant expansion is most prominent in statistical physics.
- There are problems with the crossing symmetry.

Thermodynamic GFs-Hamiltonian

Let us treat a system of Fermions with pair interaction:

$$H = \sum_s \int \mathrm{d}r \psi_s^\dagger(r,t) \left[-\frac{\hbar^2}{2m}\Delta_r + V(r) \right] \psi_s(r,t)$$
$$+ \frac{1}{2} \sum_{s,s'} \int \mathrm{d}r \mathrm{d}r' \psi_s^\dagger(r,t) \psi_{s'}^\dagger(r',t) v(r-r') \psi_{s'}(r',t) \psi_s(r,t)$$

Equations for the thermodynamic GFs

$$(i\hbar)^n G(1\ldots n, 1'\ldots n') = \langle T\{\psi(1)\ldots\psi(n)\psi^\dagger(n')\ldots\psi^\dagger(1')\}\rangle$$

are derived from the von Neumann equation

$$-i\hbar \frac{\partial}{\partial t}\psi_s(r,t) = [H, \psi_s(r,t)]_-$$

by taking into account the anticommutator relations.

Thermodynamic GFs-Eqs. of motion

The equation of motion is obtained from the generating functional:

$$G_{[c]}[\lambda,\eta] = 1 + \sum_{n=1}^{\infty} \frac{1}{(n!)^2} \int \mathrm{d}1 \ldots \mathrm{d}n \mathrm{d}1' \ldots \mathrm{d}n' \lambda(n) \ldots \lambda(1)$$
$$\times G_{[c]}(1 \ldots n, 1' \ldots n') \eta(1') \ldots \eta(n')$$

with $\eta(j)$, $\lambda(j)$ denoting anticommutating fields. The hierarchy is obtained from a functional differential Eq.:

$$\left\{ \frac{\hbar^2}{2m} \Delta_{r_1} - V(r_1) + i\hbar \frac{\partial}{\partial t_1} \right\} \frac{\delta}{\delta\lambda(1)} G[\lambda,\eta]$$
$$= \eta(1) G[\lambda,\eta] - i\hbar \int \mathrm{d}\bar{1} V(1-\bar{1}) \frac{\delta}{\delta\eta(\bar{1}^+)} \frac{\delta}{\delta\lambda(\bar{1})} \frac{\delta}{\delta\lambda(1)} G[\lambda,\eta]$$

where we used the abbreviation $V(1-2) = v(r_1 - r_2)\delta(t_1 - t_2)$.

Thermodynamic GFs-cumulant expansion

All the many-body physics can be exactly handled by the previous Eqs. However, approximations are necessary.
Should we, therefore, reorganize the whole chain of Eqs.?
What would be nice having a theory for:

$$G_c(12,1'2') = G(12,1'2') - [G(1,1')G(2,2') - G(1,2')G(2,1')]$$

A theory for these correlated GFs is easily derived from the generating functional given by:

$$\boxed{G[\lambda,\eta] = \exp\{G_c[\lambda,\eta]\}}$$

(A systematic n-particle approach is obtained by terminating at the $(n+1)$-particle level.)

Thermodynamic GFs-two-particle level

The first Eqs. of this infinite chain are given by:

$$G(1,1') = G_0(1,1') - i\hbar \int \mathrm{d}\bar{1}\mathrm{d}\bar{2}\, G_0(1,\bar{1}) V(\bar{1}-\bar{2}) G_c(\bar{2}\bar{1},\bar{2}^+1')$$

For the correlated two-particle GF:

$$\begin{aligned}
G_c(12,1'2') = i\hbar \int \mathrm{d}\bar{1}\mathrm{d}\bar{2}\, V(\bar{1}-\bar{2}) \Big\{ & -G_0(1,\bar{1}) {\color{red} G_c(\bar{2}\bar{1}2,\bar{2}^+1'2')} \\
& + \left[G_0(1,\bar{1})G(2,\bar{2})G(\bar{1},1')G(\bar{2},2') - G_0(1,\bar{1})G(2,\bar{2})G(\bar{1},2')G(\bar{2},1')\right] \\
& + \left[G_0(1,\bar{1})G(2,\bar{2})G_c(\bar{1}\bar{2},1'2')\right] \\
& + \left[G_0(1,\bar{1})G(\bar{2},1')G_c(\bar{1}2,\bar{2}^+2') + G_0(1,\bar{1})G(\bar{2},2')G_c(\bar{1}2,1'\bar{2}^+)\right] \\
& - \left[G_0(1,\bar{1})G(\bar{1},1')G_c(\bar{2}2,\bar{2}^+2') + G_0(1,\bar{1})G(\bar{1},2')G_c(\bar{2}2,1'\bar{2}^+)\right] \Big\}
\end{aligned}$$

G_0 denotes the Hartree-Fock GF.

Thermodynamic GFs-crossing symmetry

The optimized pair approximation is obtained by neglecting the correlated three-particle GF. **However, the resulting Eq. is not crossing symmetric!** (which is a fundamental symmetry of particle statistics)

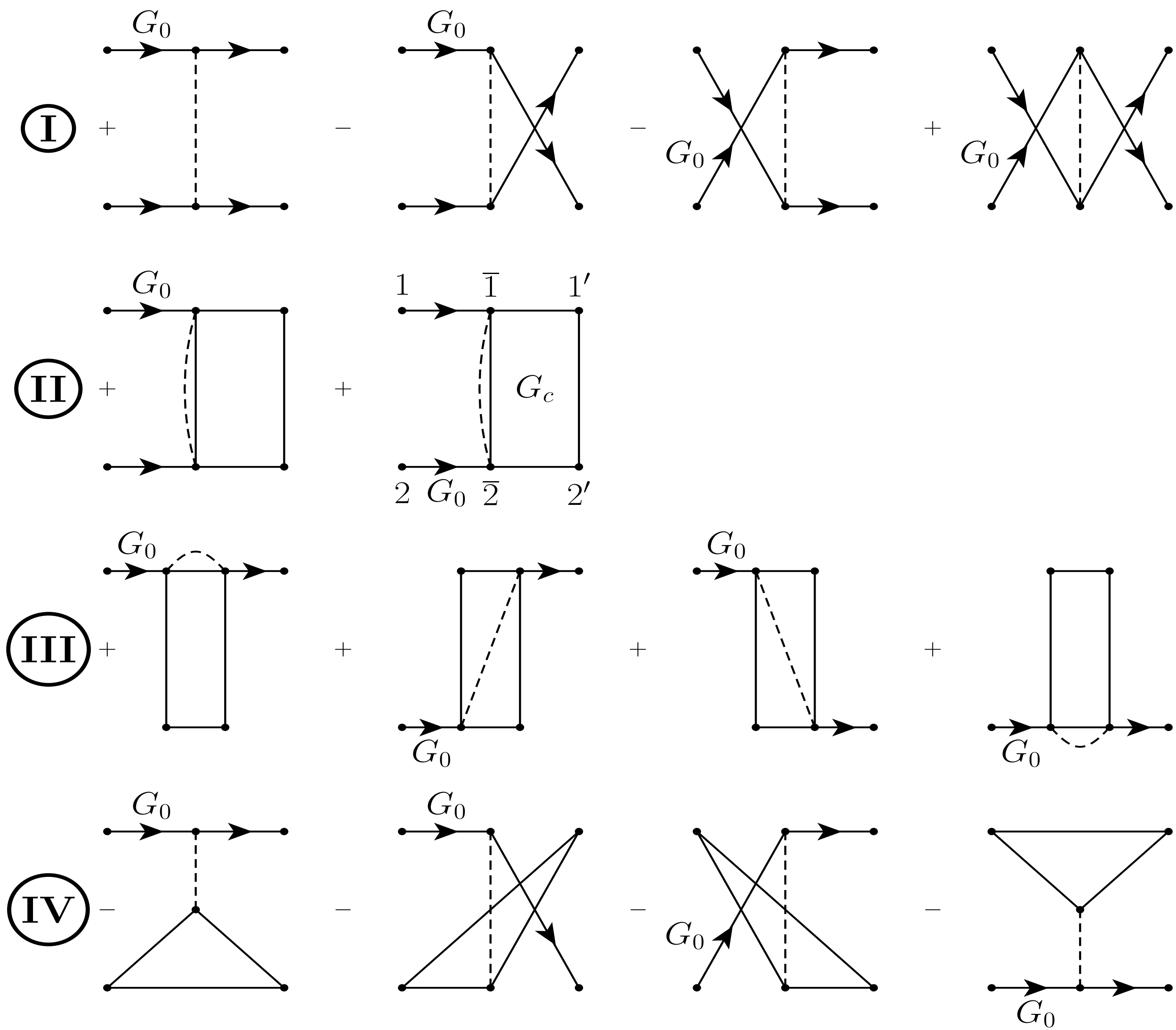
$$G(12,1'2') = -G(21,1'2') = -G(12,2'1') = G(21,2'1')$$

The crossing symmetry can be rescued by constructing the symmetric result with the help of the exact Eq.:

$$G_c(12,1'2') = \frac{1}{2}\{G_c(12,1'2') - G_c(21,1'2')\}$$

The diagrammatic representation is shown on the next slide.

Crossing-symmetric two-particle channels



Correlated GFs-BCS approach

From the Cooper channel, the BCS approach is easily obtained:

$$G_c(12,1'2') = i\hbar \int \mathrm{d}\bar{1}\mathrm{d}\bar{2} V(\bar{1}-\bar{2})$$
$$\times \frac{1}{2}\left[G_0(1,\bar{1})G(2,\bar{2}) + G(1,\bar{1})G_0(2,\bar{2})\right] G_c(\overline{12},1'2')$$

Crucial is the symmetry property of the four-point function:

$$G_c(x_1x_2,x_{1'}x_{2'}|z_\nu z_{\nu'}\omega_n) = -G_c^*(x_{1'}x_{2'},x_1x_2|z_{\nu'}^*,z_\nu^*\omega_n^*)$$

Besides the one-particle GF, we need the gap function defined by:

$$\Delta(x_1x_2,x_{1'}x_{2'}|\omega_n) = v(r_1-r_2)v(r_{1'}-r_{2'})\frac{1}{\beta^2}\sum_{\nu,\nu'} G_c(x_1x_2,x_{1'}x_{2'}|z_\nu z_{\nu'}\omega_n)$$

A coupled set of nonlinear integral Eqs. is derived fot the one- and two-particle GF.

Correlated GFs-BCS approach

The theory of BCS superconductivity is governed by the following Eqs.:

$$G(k,z_\nu) = G_0(k,z_\nu) - G_0(k,z_\nu)\frac{i}{\hbar\beta}\sum_{q,n} e^{\varepsilon\omega_n}\Delta(kk'q|\omega_n)$$
$$\times\frac{1}{2}\left[G_0(k,z_\nu)G(q-k,\omega_n - z_\nu) + G(k,z_\nu)G_0(q-k,\omega_n - z_\nu)\right]$$

and an Eq. for the gap function:

$$\Delta(kk'q|\omega_n) = \sum_{k_1} v(k-k_1)\Delta(k_1k'q|\omega_n)$$
$$\times\left\{-\frac{1}{2\beta}\sum_{\nu}\left[G_0(k_1,z_\nu)G(q-k_1,\omega_n - z_\nu) + G(k_1,z_\nu)G_0(q-k_1,\omega_n - z_\nu)\right]\right\}$$

Correlated GFs-BCS approach

Analytical results are obtained by adopting the simplifications:

1. $$G_0(k_1, z_\nu) = \frac{1}{\hbar z_\nu - \varepsilon(k)}$$

2. $$v(k - k') = -g\Theta(\omega_D - |\varepsilon(k - \mu|)\Theta(\omega_D - |\varepsilon(k' - \mu|)$$

3. $$\Delta(kk'q|\omega_n) = \frac{1}{2}\sum_{s_1,s_2} \Delta_{s_1 s_2, s_1 s_2}(kk'q|\omega_n) = -i\hbar\beta\delta_{n,0}\delta_{q,0}\Delta(k, k')$$

The final result is the gap Eq. for the transition temperature:

$$1 = \frac{g}{\beta}\sum_{k,\nu} \frac{1}{(\hbar z_\nu - \mu)^2 - E(k)^2}, \quad E(k) = \sqrt{(\varepsilon(k) - \mu)^2 + |\Delta(k)|^2}$$

Novel scattering channels

$$G_c(12,1'2') \sim i\hbar \int \mathrm{d}\bar{1}\mathrm{d}\bar{2} V(\bar{1}-\bar{2})$$
$$\times \frac{1}{2}\Big\{ G_0(1,\bar{1})G(\bar{2},1')G_c(\bar{1}2,\bar{2}^+2') + G_0(2,\bar{1})G(\bar{2},1')G_c(1\bar{1},\bar{2}^+2')$$
$$+ G_0(1,\bar{1})G(\bar{2},2')G_c(\bar{1}2,1'\bar{2}^+) + G_0(2,\bar{1})G(\bar{2},2')G_c(1\bar{1},1'\bar{2}^+) \Big\}$$

$$G_c(12,1'2') \sim -i\hbar \int \mathrm{d}\bar{1}\mathrm{d}\bar{2} V(\bar{1}-\bar{2})$$
$$\times \frac{1}{2}\Big\{ G_0(1,\bar{1})G(\bar{1},1')G_c(\bar{2}2,\bar{2}^+2') + G_0(1,\bar{1})G(\bar{1},2')G_c(\bar{2}2,1'\bar{2}^+)$$
$$+ G_0(2,\bar{1})G(\bar{1},1')G_c(1\bar{2},\bar{2}^+2') + G_0(2,\bar{1})G(\bar{1},2')G_c(1\bar{2},1'\bar{2}^+) \Big\}$$

Are there any interesting two-particle excitations in these less studied scattering channels?

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- **The theory of correlated GFs generates the Cooper channel, from which the BCS approach to superconductivity is easily obtained.**
- **Crossing symmetric linear parquet Eqs. were obtained for the correlated two-particle GF.**
- **There are two crossing symmetric pair contributions, which deserve further studies. Are there any interesting unexplored two-particle excitations?**

The end

Thank you for your attention