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Many-particle Green's functions of correlated electrons on lattices

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In order to establish an electronic structure of strongly correlated material, one can use a Dynamycal mean-field theory. DMFT maps a lattice problem to a single site problem, in our case we transform a celebrated Hubbard model to the Anderson impurity model, using so-called Dual-fermion approach. We then calculate the local properties of this model, such as Green and vertex functions within imaginary time representation and corresponding Matsubara space.

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http://github.com/sw1sh/paper

1 Introduction: Basic concepts

1.1 Second quantization for fermions

The fermion creation and annihilation operators obey the following fundamental anticommutation relations

$$a_\alpha, a^\dagger_\beta = a_\alpha a^\dagger_\beta + a^\dagger_\beta a_\alpha = \delta_{\alpha,\beta}$$

$$a_\alpha, a_\beta = a^\dagger_\alpha, a^\dagger_\beta = 0$$

One-body and two-body operators in Fock space have the following form respectively

$$\hat{A} = \sum_{\alpha\beta} \langle\alpha| A |\beta\rangle a^\dagger_\alpha a_\beta$$

$$\hat{B} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta| B |\alpha\beta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$

Using this Fock space formulation, the Hamiltonian of a many-particle system in second quantized form can be written as

$$\hat{H} = \hat{T} + \hat{V} = \sum_{\alpha\beta} \langle\alpha| T |\beta\rangle a^\dagger_\alpha a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta| V |\alpha\beta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$

where $\hat{T}$ and $\hat{V}$ are the kinetic energy and two-body interaction operators.

1.2 Interaction representation

Given the Hamiltonian $H = H_0 + V$ with H_0 and V as noninteracting and interacting part respectively, evolution of states and operators are described by following equations

$$i\frac{\partial}{\partial t} |\psi_I(t)\rangle = V_I(t) |\psi_I(t)\rangle$$

$$-i\frac{\partial O_I(t)}{\partial t} = [H_0, O_I(t)]$$

with states and operators defined as

$$|\psi_I\rangle = e^{iH_0 t} |\psi_S(t)\rangle$$

$$O_I(t) = e^{iH_0 t} O_S e^{-iH_0 t}$$

The evolution of the wave function is thus

$$|\psi_I(t)\rangle = U(t) |\psi_I(0)\rangle$$

so that

$$i\frac{\partial U(t)}{\partial t} = V(t)U(t)$$

using T-operator we obtain time-ordered exponential

$$U(t) = T\left[exp\left\{-i\int_0^t V(t')dt'\right\}\right]$$

1.3 Finite temperature

The essential step to finite temperature is possible due to the Japanese physicist Kubo, who noticed that the quantum-mechanical partition function can be regarded as a time-evolution operator in imaginary time.

$$\hat{\rho} \propto e^{-\beta \hat{H}} = U(-i\hbar\beta)$$

Later, Matsubara wrote down the first imaginary time formulation of finite temperature many body physics. In the imaginary time approach, the partition function of a quantum system is simply the trace of the time-evolution operator, evaluated at imaginary time $t = -i\hbar\beta$,

$$Z = Tr\ e^{-\beta H} = Tr\ U(-i\hbar\beta)$$

whilst the expectation value of a quantity A in thermal equilibrium is given by

$$< A >= \frac{Tr[U(-i\hbar\beta)A]}{Tr[U(-i\hbar\beta)]}$$

Switching from t to $i\tau$ with $\tau \in \{0, \beta = \frac{1}{k_B T}\}$ we obtain

$$U(\tau) = T\left[exp\left\{-\int_0^\tau V(\tau')d\tau'\right\}\right]$$

We can relate the partition function to the evolution operator as follows

$$Z = Tr\left[e^{-\beta H}\right] = Z_0 \left\langle U(\beta)\right\rangle_0$$

where

$$Z_0 = Tr\left[e^{-\beta H_0}\right]$$

$$\langle A\rangle_0 = \frac{Tr\left[e^{-\beta H_0} A\right]}{Z_0}$$

Now we can write the ratio of the interacting to the non-interacting partition function

$$S = \frac{Z}{Z_0} = \langle T\ exp\left[-\int_0^\beta V(\tau)d\tau\right]\rangle$$

1.4 Perturbation expansion

Expanding the time-ordered exponential, gives us a perturbation series for the S-matrix

$$S = \frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta \dots \int_0^\beta d\tau_1 \dots d\tau_n \langle TV(\tau_1)\dots V(\tau_n)\rangle$$

Taking the logarithm of it yields

$$\ln S = \sum_{n=1}^{\infty} \frac{(S-1)^n}{n} = \sum_{n=1}^{\infty} \frac{(\sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \int_0^\beta \dots \int_0^\beta d\tau_1 \dots d\tau_k \langle TV(\tau_1)\dots V(\tau_k)\rangle)^n}{n}$$

1.5 Green functions

We define n-particle Green function as follows

$$\mathcal{G}(1\dots n;1'\dots n') = (-1)^n\langle Tc(1)\dots c(n)c(1')\dots c(n')\rangle$$

Adding auxiliary source terms to our interaction

$$V(t) \mapsto V(t) + \sum_n \tilde{\alpha}(n)c(n) + c^\dagger(n)\alpha(n)$$

where $\alpha(t)$ and $\tilde{\alpha}(t)$ are the anti-commuting forces which "create" and "annihilate" particles respectively. We then obtain n-particle Green functions as follows

$$\mathcal{G}(1\dots n;1'\dots n') = \frac{1}{S}\frac{\partial^n S}{\partial\alpha(1)\partial\tilde{\alpha}(1')\dots\partial\alpha(n)\partial\tilde{\alpha}(n')}\bigg|_{\alpha,\tilde{\alpha}=0}$$

And the n-th order coefficient of α and $\tilde{\alpha}$ in the expansion of S-matrix is known as the irreducible n-point Green function $\mathcal{G}_{irr}$ or the n-point vertex function Γ.

$$\Gamma(1\dots n;1'\dots n') = \frac{\partial^n \ln S}{\partial\alpha(1)\partial\tilde{\alpha}(1')\dots\partial\alpha(n)\partial\tilde{\alpha}(n')}\bigg|_{\alpha,\tilde{\alpha}=0}$$

1.6 Matsubara Representation

Green functions satisfy the relation

$$\mathcal{G}(\tau+\beta) = \pm\mathcal{G}(\tau)$$

so that bosonic (fermionic) Green functions are periodic (antiperiodic), with period β.

The periodicity allow us to carry out a Fourier expansion of the Green functions in terms of discrete frequencies. Matsubara frequencies are defined as

$$\begin{aligned}\nu_n &= 2\pi n k_B T \quad (Boson)\\ \omega_n &= \pi(2n+1)k_B T \quad (Fermion)\end{aligned}$$

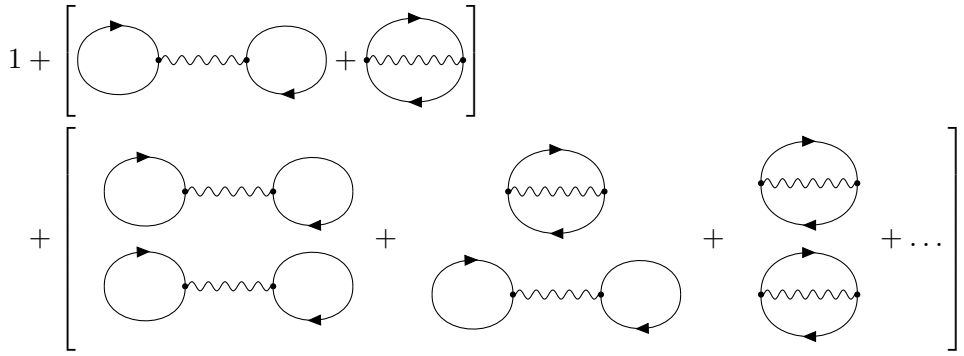
Fourier expansion and its inverse then

$$\begin{aligned}\mathcal{G}(\tau) &= T\sum_n \mathcal{G}(i\alpha_n)e^{-i\alpha_n\tau}\\ \mathcal{G}(i\alpha_n) &= \int_0^\beta d\tau\mathcal{G}(\tau)e^{i\alpha_n\tau}, \quad \alpha_n = \nu_n,\omega_n\end{aligned}$$

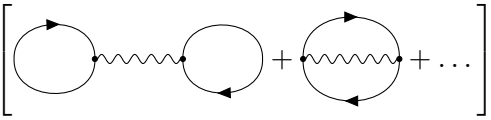
1.7 Feynman Diagrams

Feynman Diagram techniques help to visualize the structure and apply physical interpretation to the otherwise incomprehensible formulas.

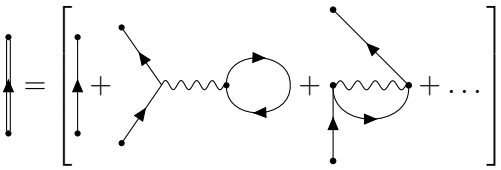
$S = \sum\{\text{Disconnected Feynman diagrams}\} \equiv$



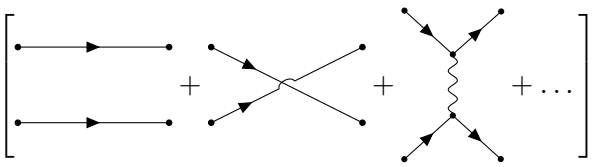
$\ln S = \sum\{\text{Linked Cluster Diagrams}\} \equiv$



$\mathcal{G}(1,1') = \sum\{\text{Two legged diagrams}\} \equiv$



$\mathcal{G}^{(4)}(1,2,1',2') = \sum\{\text{Four legged diagrams}\} \equiv$



2 Theory and Motivation

2.1 Strongly correlated systems

Strongly correlated system is a class of materials, where the behavior of their electrons can't be described effectively in terms of non-interacting entities. Therefore models of the electronic structure of strongly correlated system must include electronic correlation.

For example, semiconductors and most metals can be described as having non-interacting electrons. This simple approach is valid because the interaction (Coulomb) energy of electrons is much smaller than their kinetic energy. However there are important systems for which interactions between the particles are not weak, and these interactions play a major role in determining the properties of such systems. Some examples of such "strongly correlated systems" include:

- High-temperature superconductors. The transition temperature for these materials is surprisingly high. The origin of superconductivity is still unclear, but it is commonly believed that it comes mostly from the Coulomb interaction between the electrons, rather than the electron-ion interactions that are important for the conventional superconductors.

- Magnetic systems. Coulomb interaction between electrons may lead to a variety of spin ordering patterns, including ferromagnetism and antiferromagnetism.
- Quantum Hall systems. In the presence of a strong perpendicular magnetic field electrons confined in one or several two-dimensional layers form a new quantum liquid state, that may have some unusual properties.
- One dimensional electron systems. Electrons carry two important quantum numbers: charge and spin. When a single electron moves in a vacuum or in a conventional insulator we can observe charge and spin propagating together. By contrast in one dimensional systems interacting electrons disintegrate into charge and spin solitons that propagate at different velocities.

At this point we do not have a good general approach for understanding "strongly correlated systems". We only know certain aspects of several systems, and understand very poorly some other ones.

2.2 The Hubbard model

One of the models of a particular interest is the Hubbard model. The Hubbard model, named after John Hubbard, is the simplest model of interacting particles in a lattice, with only two terms in the Hamiltonian: a kinetic term allowing for tunneling ("hopping") of particles between sites of the lattice and a potential term consisting of an on-site interaction. So, having a lattice of atoms with electrons, that are almost localized at each site with possibility to hop only between nearest neighbors and approximation that electrons interact with each other only in a single orbit, the Hamiltonian for the Hubbard model can be thus be written as

$$H = -t \sum_{i,j,\sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma} \tag{2.1}$$

with the corresponding imaginary-time action

$$S = \int_0^\beta d\tau \left\{ -t \sum_{i,j,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_{i,\sigma} c^\dagger_{i\sigma} (\partial_\tau - \mu) c_{i\sigma} \right\} \tag{2.2}$$

and its Fourier transform

$$S[c, c^*] = \sum_{\omega k \sigma} (\epsilon_k - \mu - i\omega) c^*_{\omega k\sigma} c_{\omega k\sigma} + U \sum_i \int_0^\beta n_{i\uparrow\tau} n_{i\downarrow\tau} d\tau \tag{2.3}$$

here $\epsilon_k = -2t(\cos k_x + \cos k_y)$ - the bare dispersion law,
c, c^* - Grassmann numbers,
ω - Matsubara frequencies.

2.3 Mean field theory

A many-body system with interactions is generally very difficult to solve exactly. The main idea of MFT is to replace all interactions to any one body with an average or effective interaction - the mean field. This reduces any many-body problem into an effective one-body problem. Mean field theory can be applied to a number of physical systems, for example Ising model.

In mean-field theory, the mean field appearing in the single-site problem is a time-independent quantity. However, this isn't always the case: in a variant of mean-field theory called Dynamical Mean Field Theory (DMFT), the mean-field becomes a time-dependent quantity. DMFT maps a lattice problem onto a single-site problem. In DMFT, the local observable is the local Green's function. Thus, the self-consistency condition for DMFT is for the impurity Green's function to reproduce the lattice local Green's function through an effective mean-field.

In our case DMFT maps Hubbard model onto the so-called Anderson impurity model. This model describes the interaction of one site (the impurity) with a "bath" of electronic levels through a hybridization function $\Delta(\tau)$. The corresponding Hamiltonian for the impurity is then

$$H_{imp} = \underbrace{\sum_{\nu,\sigma} \epsilon_\nu n^{bath}_{\nu,\sigma}}_{H_{bath}} + \underbrace{\sum_{\nu,\sigma} \left(V_\nu c^\dagger_\sigma a^{bath}_{\nu,\sigma} + h.c. \right)}_{H_{mix}} + \underbrace{U n_\uparrow n_\downarrow - \mu \left(n_\uparrow + n_\downarrow \right)}_{H_{loc}} \tag{2.4}$$

with the following action

$$S = \sum_{\omega\sigma} (\Delta_\omega - \mu - i\omega) c^*_{\omega\sigma} c_{\omega\sigma} + U \int_0^\beta n_{\uparrow\tau} n_{\downarrow\tau} d\tau \tag{2.5}$$

The hybridization function Δ_ω plays the role of a *dynamic* mean field.

2.4 Beyond DMFT

DMFT approach treats the local spin and orbital fluctuations of the correlated electrons in a correct self-consistent way, while spatial correlations between sites are ignored. The non-perturbed DMFT is successful, because a number of the most important correlation effects are indeed related to local fluctuations. For example, DMFT describes correctly such phenomena, as the local moment formation in itinerant magnets, some aspects of Kondo physics and the Mott insulator-to-metal transition on a lattice with a large connectivity in high-dimensional materials.

On the other hand, there are a lot of examples where non-locality of spatial correlations also plays an important role. DMFT has several extensions, extending the above formalism to multi-orbital, multi-site problems. It can be extended with multiple orbitals, so that electron-electron interaction term would include terms denoting different orbitals. Cluster approximations takes into account the short-range non-local fluctuations in real or k-space. In these methods, correlations are assumed to be localized within a cluster including several lattice sites.

2.5 Dual fermion approach

The dual fermion extension [4] of DMFT operates with a single-site impurity problem and treats spatial non-locality in a diagrammatic way. We start from the Hubbard model defined above (subsection 2.2). The goal is to derive the properties of the initial lattice problem via the quantities of the impurity problem. The lattice action can be represented in the following way

$$S[c, c^*] = \sum_i S_{imp}[c_i, c^*_i] - \sum_{\omega k\sigma} (\Delta_\omega - \epsilon_k) c^*_{\omega k\sigma} c_{\omega k\sigma} \tag{2.6}$$

Performing a dual transformation to a set of new Grassmann variables f, f^*

$$e^{A^2 c^*_{\omega k\sigma} c_{\omega k\sigma}} = \left(\frac{A}{\alpha} \right)^2 \int e^{-\alpha(c^*_{\omega k\sigma} f_{\omega k\sigma} + f^*_{\omega k\sigma} c_{\omega k\sigma}) - \alpha^2 A^{-2} f^*_{\omega k\sigma} f_{\omega k\sigma}} df^*_{\omega k\sigma} df_{\omega k\sigma} \tag{2.7}$$

we can obtain an action depending on the new variables f, f^* only

$$S[f,f^*] = -\sum_{\omega k} \ln \alpha^{-2}_{\omega\sigma}(\Delta_\omega - \epsilon_k) - \sum_i \ln z_i^{imp} + \tag{2.8}$$

$$+ \sum_{\omega k\sigma} \alpha_{\omega\sigma}((\Delta_\omega - \epsilon_k)^{-1} + g_\omega)\alpha_{\omega\sigma} f^*_{\omega k\sigma} f_{\omega k\sigma} + \sum_i V_i \tag{2.9}$$

where $z_i^{imp} = \int e^{-S_{imp}[c_i^*, c_i]} \mathcal{D}c_i^* \mathcal{D}c_i$, and the dual potential $V_i \equiv V[f_i^*, f_i]$ is defined from the expression

$$\int e^{-S_{loc}[c_i^*, c_i, f_i^*, f_i]} \mathcal{D}c_i^* \mathcal{D}c_i = z_i^{imp} e^{\sum_{\omega\sigma} \alpha^2_{\omega\sigma} g_\omega f^*_{\omega i\sigma} f_{\omega i\sigma} - V[f_i^*, f_i]} \tag{2.10}$$

One can see that the $2n$-th coefficient from the Taylor series of $V[f_i^*, f_i]$ is proportional to vertex function $\gamma^{(2n)}$. Next we establish an exact relation between the Green's function and higher-order momenta of initial system and the dual system as Appendix A of [4] describes. For example

$$G_{\omega,k} = (\Delta_\omega - \epsilon_k)^{-1} \alpha_{\omega\sigma} G^{dual}_{\omega,k} \alpha_{\omega\sigma} (\Delta_\omega - \epsilon_k)^{-1} + (\Delta_\omega - \epsilon_k)^{-1} \tag{2.11}$$

The main idea of switching to the new variables is that, for a properly chosen δ, correlation properties of the f^*, f system are simpler than for the c^*, c original model. In other words, the magnitude of the nonlinear part in the dual action can be effectively decreased by the proper choice of Δ.

3 What was done

3.1 Preparations

Following the dual fermion approach we now consider only the local Hamiltonian of the impurity problem

$$H = -\frac{U}{2}(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow + \frac{U}{2} \tag{3.1}$$

with impurity states $|0\rangle, |\downarrow\rangle, |\uparrow\rangle, |\downarrow\uparrow\rangle$ and eigenenergies $\frac{U}{2}, 0, 0, \frac{U}{2}$ respectively.
The annihilation operator in this space then can be constructed as follows

$$c_\sigma = (|0\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow\uparrow|)\delta_{\sigma,\uparrow} + (|0\rangle\langle\downarrow| + |\downarrow\rangle\langle\downarrow\uparrow|)\delta_{\sigma,\downarrow} \tag{3.2}$$

Since we using an interaction representation, the operator also evolves with time

$$c_{\sigma,\tau} = e^{H\tau} c_\sigma e^{-H\tau} \tag{3.3}$$

We can now compute the quantum thermodynamic mean of any operator A as follow

$$\langle A \rangle = \frac{1}{Z_0} Tr[e^{-H\beta} A] \tag{3.4}$$

where $Z_0 = Tr[e^{-H\beta}] = 2(1 + e^{-\frac{U\beta}{2}})$.
Given this, it's now possible to compute $2n$-particle Green functions

$$G(1\ldots n; 1'\ldots n') = (-1)^n \langle c_1 \ldots c_n c^\dagger_{1'} \ldots c^\dagger_{n'} \rangle \tag{3.5}$$

Expressions for $\Gamma^{(2n)}$ are the n-th cumulants of the system

$$\Gamma^{(2)} = G(1,1') \tag{3.6}$$

$$\Gamma^{(4)} = G(1,2,1',2') + G(1,1')G(2,2') - G(1,2')G(2,1') \tag{3.7}$$

$$\begin{aligned}\Gamma^{(6)} = {} & G(1,2,3,1',2',3') \\ & - 2G(1,1')G(2,2')G(3,3') + 2G(1,1')G(2,3')G(3,2') - 2G(1,2')G(2,3')G(3,1') \\ & + 2G(1,2')G(2,1')G(3,3') - 2G(1,3')G(2,1')G(3,2') + 2G(1,3')G(2,2')G(3,1') \\ & - G(1,1')G(2,3,2',3') + G(1,2')G(2,3,1',3') - G(1,3')G(2,3,1',2') \\ & + G(2,1')G(1,3,2',3') - G(2,2')G(1,3,1',3') + G(2,3')G(1,3,1',2') \\ & - G(3,1')G(1,2,2',3') + G(3,2')G(1,2,1',3') - G(3,3')G(1,2,1',2')\end{aligned} \tag{3.8}$$

where variables $1,2\dots n;1',2'\dots n'$ are the shortcuts for corresponding spin and time (σ_i,τ_i) and also summation over time ordering ($(2n)!$ permutations $\beta > \tau_{i_1} > \tau_{i_2} > \dots > \tau_{i_{2n}}$) is implied.

The vertex functions $\gamma^{(2n)}$ are defined as follows

$$\gamma^{(2n)} = \frac{\Gamma^{(2n)}_\omega}{G(\omega_1)\dots G(\omega_{2n})} \tag{3.9}$$

with $\Gamma^{(2n)}_\omega$ being an imaginary time Fourier transform of $\Gamma^{(2n)}$ ($\Gamma^{(2n)}$ in Matsubara space)

$$\Gamma^{(2n)}_\omega(\omega_1,\dots,\omega_{2n}) = \int_0^\beta \int_0^{\tau_1} \dots \int_0^{\tau_{2n-1}} \Gamma^{(2n)}(\tau_1,\dots,\tau_{2n}) e^{i(\omega_1\tau_1+\dots+\omega_{2n}\tau_{2n})} d\tau_{2n}\dots d\tau_1 \tag{3.10}$$

where the integration is performed as time τ_i increases $\tau_{2n} < \tau_{2n-1} < \dots < \tau_2 < \tau_1 < \beta$.

3.2 Calculations

We require energy conservation law of the form $\omega_1 + \dots + \omega_{2n} = 0$.

$$G(\omega) = -\frac{i\omega}{\frac{U}{2}^2 + \omega^2}, \quad \omega_1 = -\omega_2 = \omega \tag{3.11}$$

$$\gamma^{\uparrow\uparrow\uparrow\uparrow} = \beta\frac{U^2}{4}\frac{\delta_{\omega_1,-\omega_3} - \delta_{\omega_2,-\omega_3}}{\omega_1^2\omega_2^2}(\omega_1^2 + \frac{U^2}{4})(\omega_2^2 + \frac{U^2}{4}) \tag{3.12}$$

$$\begin{aligned}\gamma^{\downarrow\uparrow\downarrow\uparrow} = {} & U - \frac{U^3}{8}\frac{\omega_1^2+\omega_2^2+\omega_3^2+\omega_4^2}{\omega_1\omega_2\omega_3\omega_4} - \frac{3U^5}{16\omega_1\omega_2\omega_3\omega_4} \\ & - \beta\frac{U^2}{4}\frac{1}{1+e^{\frac{U\beta}{2}}}\frac{2\delta_{\omega_1,-\omega_2}+\delta_{\omega_2,-\omega_3}}{\omega_1^2\omega_3^2}(\omega_1^2+\frac{U^2}{4})(\omega_3^2+\frac{U^2}{4}) \\ & + \beta\frac{U^2}{4}\frac{1}{1+e^{-\frac{U\beta}{2}}}\frac{2\delta_{\omega_1,-\omega_3}+\delta_{\omega_2,-\omega_3}}{\omega_1^2\omega_2^2}(\omega_1^2+\frac{U^2}{4})(\omega_2^2+\frac{U^2}{4})\end{aligned} \tag{3.13}$$

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