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

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Contents

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http://github.com/sw1sh/paper

In order to establish an electronic structure of strongly correlated material, the most famous and effective way is to address the Dynamical mean-field theory. DMFT maps a lattice problem to a single site problem, with the only approximation of ignoring the spatial correlations between the sites. To go beyond DMFT to higher-order approximations, one can use an efficient diagrammatic method to describe those correlations - Dual fermion approach. It makes an exact transition to a dual set of variables and provides a way to treat vertices of an effective single-impurity problem as small parameters. We then compute some local properties of the one particular model, such as Green's functions within imaginary time representation and corresponding Matsubara space. Especially we need to know whether a two-particle vertex is enough to describe the system, and high-order momenta are therefore redundant. The only way to check this is to derive an expression for the sixth order vertex and compare them.

1 Introduction: Basic concepts

1.1 Second quantization for fermions

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

$$a_\alpha, a^\dagger_\beta = a_\alpha a^\dagger_\beta + a^\dagger_\beta a_\alpha = \delta_{\alpha,\beta} \tag{1.1}$$

$$a_\alpha, a_\beta = a^\dagger_\alpha, a^\dagger_\beta = 0 \tag{1.2}$$

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

$$\hat{A} = \sum_{\alpha\beta} \langle\alpha| A |\beta\rangle a^\dagger_\alpha a_\beta \tag{1.3}$$

$$\hat{B} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta| B |\alpha\beta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \tag{1.4}$$

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

$$\hat{H} = \hat{T} + \hat{V} = \sum_{\alpha\beta} \langle\alpha| T |\beta\rangle a^\dagger_\alpha a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta| V |\alpha\beta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \tag{1.5}$$

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

$$i\frac{\partial}{\partial t} |\psi_I(t)\rangle = V_I(t) |\psi_I(t)\rangle \tag{1.6}$$

$$-i\frac{\partial O_I(t)}{\partial t} = [H_0, O_I(t)] \tag{1.7}$$

with states and operators defined as

$$|\psi_I\rangle = e^{iH_0 t} |\psi_S(t)\rangle \tag{1.8}$$

$$O_I(t) = e^{iH_0 t} O_S e^{-iH_0 t} \tag{1.9}$$

The evolution of the wave function is thus

$$|\psi_I(t)\rangle = U(t) |\psi_I(0)\rangle \tag{1.10}$$

so that

$$i\frac{\partial U(t)}{\partial t} = V(t)U(t) \tag{1.11}$$

using T-operator we obtain time-ordered exponential

$$U(t) = T\left[exp\left\{-i\int_0^t V(t')dt'\right\}\right] \tag{1.12}$$

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.

$$\hat{\rho} \propto e^{-\beta\hat{H}} = U(-i\hbar\beta) \tag{1.13}$$

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 $t = -i\hbar\beta$,

$$Z = Tr\ e^{-\beta H} = Tr\ U(-i\hbar\beta) \tag{1.14}$$

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

$$< A >= \frac{Tr[U(-i\hbar\beta)A]}{Tr[U(-i\hbar\beta)]} \tag{1.15}$$

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

$$U(\tau) = T\left[exp\left\{-\int_0^\tau V(\tau')d\tau'\right\}\right] \tag{1.16}$$

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

$$Z = Tr\left[e^{-\beta H}\right] = Z_0 \left\langle U(\beta)\right\rangle_0 \tag{1.17}$$

where

$$Z_0 = Tr\left[e^{-\beta H_0}\right] \tag{1.18}$$

$$\langle A\rangle_0 = \frac{Tr\left[e^{-\beta H_0} A\right]}{Z_0} \tag{1.19}$$

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

$$S = \frac{Z}{Z_0} = \langle T\ exp\left[-\int_0^\beta V(\tau) d\tau \right] \rangle \tag{1.20}$$

1.4 Perturbation expansion

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

$$S = \frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta \dots \int_0^\beta d\tau_1 \dots d\tau_n \langle T V(\tau_1) \dots V(\tau_n) \rangle \tag{1.21}$$

Taking the logarithm of it yields

$$\ln S = \sum_{n=1}^{\infty} \frac{(S-1)^n}{n} = \sum_{n=1}^{\infty} \frac{(\sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \int_0^\beta \dots \int_0^\beta d\tau_1 \dots d\tau_k \langle T V(\tau_1) \dots V(\tau_k) \rangle)^n}{n} \tag{1.22}$$

1.5 Green functions

We define n-particle Green function as follows

$$\mathcal{G}(1 \dots n; 1' \dots n') = (-1)^n \langle T c(1) \dots c(n) c(1') \dots c(n') \rangle \tag{1.23}$$

Adding auxiliary source terms to our interaction

$$V(t) \mapsto V(t) + \sum_n \tilde{\alpha}(n) c(n) + c^\dagger(n) \alpha(n) \tag{1.24}$$

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

$$\mathcal{G}(1 \dots n; 1' \dots n') = \frac{1}{S} \frac{\partial^n S}{\partial \alpha(1) \partial \tilde{\alpha}(1') \dots \partial \alpha(n) \partial \tilde{\alpha}(n')} \bigg|_{\alpha, \tilde{\alpha}=0} \tag{1.25}$$

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.

$$\Gamma(1 \dots n; 1' \dots n') = \frac{\partial^n \ln S}{\partial \alpha(1) \partial \tilde{\alpha}(1') \dots \partial \alpha(n) \partial \tilde{\alpha}(n')} \bigg|_{\alpha, \tilde{\alpha}=0} \tag{1.26}$$

1.6 Matsubara representation

Green functions satisfy the relation

$$\mathcal{G}(\tau + \beta) = \pm \mathcal{G}(\tau) \tag{1.27}$$

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

$$\nu_n = 2\pi n k_B T \quad (Boson) \tag{1.28}$$

$$\omega_n = \pi(2n+1) k_B T \quad (Fermion) \tag{1.29}$$

Fourier expansion and its inverse then

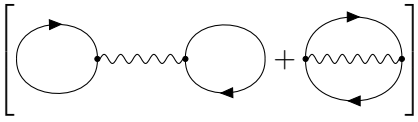
$$\mathcal{G}(\tau) = T \sum_n \mathcal{G}(i\alpha_n) e^{-i\alpha_n \tau} \tag{1.30}$$

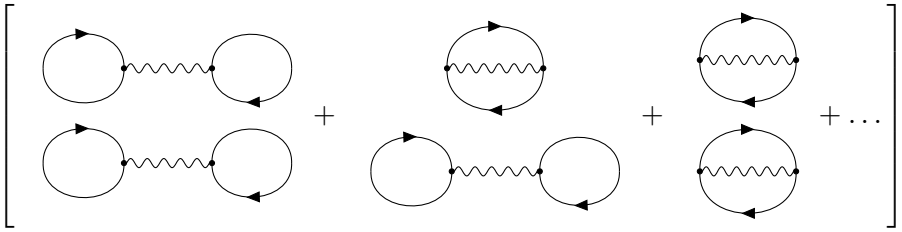
$$\mathcal{G}(i\alpha_n) = \int_0^\beta d\tau \mathcal{G}(\tau) e^{i\alpha_n \tau}, \quad \alpha_n = \nu_n, \omega_n \tag{1.31}$$

1.7 Feynman Diagrams

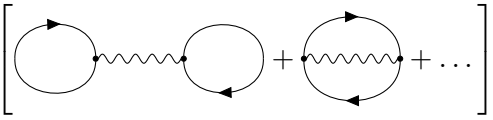
Feynman Diagram techniques help to visualize the structure and apply physical interpretation to the otherwise incomprehensible formulas. We show here some basic diagram expansions of many-body theory quantities. S-matrix consists of linked and unlinked cluster diagrams

$$S = \sum \{\text{Linked + Unlinked diagrams}\} \equiv \tag{1.32}$$

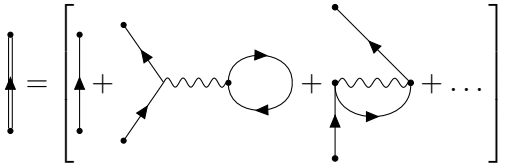
$1 +$  (1.33)

$+$  (1.34)

The Linked Cluster Theorem states that taking the logarithm of the S-matrix removes unlinked diagrams

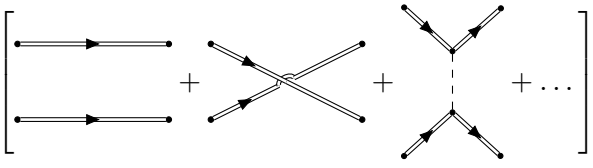
$$\ln S = \sum \{\text{Linked Cluster Diagrams}\} \equiv$$  (1.35)

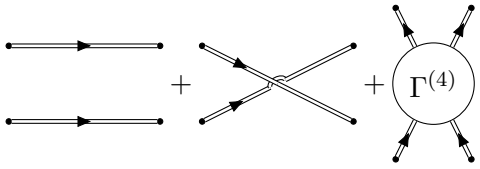
Two-leg diagrams describe one-particle Green function with external interaction V

$$\mathcal{G}(1,1') = \sum \{\text{Two-leg diagrams}\} \equiv$$  (1.36)

Vertex function contributes to the two-particle Green function and describes interaction between particles U

$$\mathcal{G}^{(4)}(1,2,1',2') = \sum \{\text{Four-leg diagrams}\} \tag{1.37}$$

$\equiv$  (1.38)

$=$  (1.39)

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 lattice problem into an effective single-site 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. In other words it is not static compared to the MFT method.

It is obvious that the impurity problem is much simpler than the origial lattice one. And an analytical solution can therefore be obtained. The only property of the impurity problem entering in the DMFT self-consistent equations is the Green's function $g_{\omega,\sigma}$ in Matsubara space. The DMFT approximation for the Green's function of the lattice problem with N sites, corresponds to the following expression

$$G^{DMFT}_{\omega,\sigma} = \frac{1}{N} \sum_k \frac{1}{g^{-1}_{\omega,\sigma} + \Delta_{\omega,\sigma} - \epsilon_k} \tag{2.6}$$

where the hybridization function Δ satisfies the self-consistency condition of DMFT

$$G^{DMFT}_{r=0,\omega,\sigma} = g_{\omega,\sigma} \tag{2.7}$$

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 of DMFT[5] 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

$$S[c,c^*] = \sum_i S_{imp}[c_i, c_i^*] - \sum_{\omega k\sigma} (\Delta_\omega - \epsilon_k) c^*_{\omega k\sigma} c_{\omega k\sigma} \tag{2.8}$$

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

$$e^{A^2 c^*_{\omega k\sigma} c_{\omega k\sigma}} = \left(\frac{A}{\alpha}\right)^2 \int e^{-\alpha(c^*_{\omega k\sigma} f_{\omega k\sigma} + f^*_{\omega k\sigma} c_{\omega k\sigma}) - \alpha^2 A^{-2} f^*_{\omega k\sigma} f_{\omega k\sigma}} df^*_{\omega k\sigma} df_{\omega k\sigma} \tag{2.9}$$

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

$$\begin{aligned} S[f,f^*] = &- \sum_{\omega k} \ln \alpha^{-2}_{\omega\sigma} (\Delta_\omega - \epsilon_k) - \sum_i \ln z_i^{imp} + \\ &+ \sum_{\omega k\sigma} \alpha_{\omega\sigma} ((\Delta_\omega - \epsilon_k)^{-1} + g_\omega) \alpha_{\omega\sigma} f^*_{\omega k\sigma} f_{\omega k\sigma} + \sum_i V_i \end{aligned} \tag{2.10}$$

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

$$\int e^{-S_{loc}[c_i^*, c_i, f_i^*, f_i]} \mathcal{D}c_i^* \mathcal{D}c_i = z_i^{imp} e^{\sum_{\omega\sigma} \alpha^2_{\omega\sigma} g_\omega f^*_{\omega i\sigma} f_{\omega i\sigma} - V[f_i^*, f_i]} \tag{2.11}$$

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 and the dual system as Appendix A of [5] describes. For example

$$G_{\omega,k} = (\Delta_\omega - \epsilon_k)^{-1} \alpha_{\omega\sigma} G^{dual}_{\omega,k} \alpha_{\omega\sigma} (\Delta_\omega - \epsilon_k)^{-1} + (\Delta_\omega - \epsilon_k)^{-1} \tag{2.12}$$

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

Even though the dual-fermion approach provides us with the convenient diagrammatic technique, every previous work in this field only included diagrams up to the second order. On the other hand there is some evidence exists, that already suggests the need of the third order []. This work tries to show whether or not the higher order is necessary by partially computing it.

3.1 Preparations

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

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

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 basis then can be constructed as follows

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

where $\delta_{\sigma_1,\sigma_2}$ - Kronecker's delta symbol.

Since we using an interaction representation, the operators also evolve 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 follows

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

where $Z_0 = Tr[e^{-H\beta}] = 2(1 + e^{-\frac{U\beta}{2}})$.

Given all the above definitions, it's now possible to compute $2n$-particle Green's functions and vertices of the system

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

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

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

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

where we use $1, 2\dots n; 1', 2'\dots n'$ as the shortcuts for the corresponding spin and time variables (σ_i, τ_i).

Fourier transform in Matsubara representation should take into account time ordering

$$\Gamma_{\omega}^{(2n)} = \sum_{P_i} \int_0^{\beta} \int_0^{\tau_{i_1}} \dots \int_0^{\tau_{i_{2n-1}}} \Gamma^{(2n)}(\tau_{i_1}, \dots, \tau_{i_{2n}}) e^{i(\omega_{i_1}\tau_{i_1} + \dots + \omega_{i_{2n}}\tau_{i_{2n}})} d\tau_{i_{2n}} \dots d\tau_{i_1} \tag{3.9}$$

where P_i are the permutations over time ordering $\tau_{i_1} > \tau_{i_2} > \ldots > \tau_{i_{2n}}$, so that integration is performed as time τ_i increases $\tau_{i_{2n}} < \tau_{2n-1} < \cdots < \tau_2 < \tau_1 < \beta$.

The $\gamma^{(2n)}$-functions used in diagrammatic technique of dual-fermion approach are defined as normalized vertex functions in Matsubara space

$$\gamma^{(2n)} = \frac{\Gamma_{\omega}^{(2n)}}{G(\omega_1) \dots G(\omega_{2n})} \tag{3.10}$$

where $G(\omega_i)$ will be derived later.

3.2 Calculations

Let's start with the detailed derivation of $G(1, 1')$ and its Fourier transform. Since $G(1, 1') \neq 0$ only when spins are parallel and depends only on time difference $\tau_1 - \tau_{1'}$, we only left with one case to consider

$$G^{\uparrow\downarrow} = G^{\downarrow\uparrow} = 0 \tag{3.11}$$

$$\begin{aligned} G^{\downarrow\downarrow}(\tau_1 - \tau_{1'} = \tau) = G^{\uparrow\uparrow}(\tau) &= (-1)^1 \left\langle e^{H\tau} c_{\uparrow} e^{-H\tau} c_{\uparrow}^{\dagger} \right\rangle \\ &= -\frac{1}{Z} \left[\langle 0 | \, e^{-H\beta} e^{H\tau} c_{\uparrow} e^{-H\tau} c_{\uparrow}^{\dagger} \, | 0 \rangle + \langle \downarrow | \, e^{-H\beta} e^{H\tau} c_{\uparrow} e^{-H\tau} c_{\uparrow}^{\dagger} \, | \downarrow \rangle \right] \\ &= -\frac{1}{2(1 + e^{-\frac{U\beta}{2}})} \left[\langle 0 | \, e^{-\frac{U}{2}\beta} e^{\frac{U}{2}\tau} e^{-0\times\tau} \, | 0 \rangle + \langle \downarrow | \, e^{-0\times\beta} e^{0\times\tau} (-1) e^{-\frac{U}{2}\tau} (-1) \, | \downarrow \rangle \right] \\ &= -\frac{1}{2(1 + e^{-\frac{U\beta}{2}})} \left[e^{-\frac{U}{2}\beta + \frac{U}{2}\tau} + e^{-\frac{U}{2}\tau} \right] = \frac{1}{2\cosh\frac{U\beta}{4}} \cosh\left(\frac{U}{2}(\frac{\beta}{2} + \tau)\right) \end{aligned} \tag{3.12}$$

Next follows a Fourier transform of $G(\tau)$ into Matsubara representation (subsection 1.6)

$$\begin{aligned} G(\omega) = \int_0^{\beta} G(\tau) e^{i\omega\tau} d\tau &= -\frac{1}{2(1 + e^{-\frac{U\beta}{2}})} \left[e^{-\frac{U}{2}\beta} \int_0^{\beta} e^{(i\omega + \frac{U}{2})\tau} d\tau + \int_0^{\beta} e^{(i\omega - \frac{U}{2})\tau} d\tau \right] \\ = -\frac{1}{2(1 + e^{-\frac{U\beta}{2}})} &\left[e^{-\frac{U}{2}\beta} \frac{e^{(i\omega + \frac{U}{2})\beta} - 1}{i\omega + \frac{U}{2}} + \frac{e^{(i\omega - \frac{U}{2})\beta} - 1}{i\omega - \frac{U}{2}} \right] \end{aligned} \tag{3.13}$$

We can now use the fact that $\omega = \frac{\pi}{\beta}(2n + 1)$, so that substitution of this definition into exponents, simplifies $e^{i\omega\beta}$ to just -1

$$\begin{aligned} G(\omega) &= -\frac{1}{2(1 + e^{-\frac{U\beta}{2}})} \left[e^{-\frac{U}{2}\beta} \frac{-e^{\frac{U}{2}\beta} - 1}{i\omega + \frac{U}{2}} + \frac{-e^{-\frac{U}{2}\beta} - 1}{i\omega - \frac{U}{2}} \right] \\ &= -\frac{1}{\cancel{2(1 + e^{-\frac{U\beta}{2}})}} \left[\frac{(i\omega - \frac{U}{2})\cancel{(1 + e^{-\frac{U}{2}\beta})} + (i\omega + \frac{U}{2})\cancel{(e^{-\frac{U}{2}\beta} + 1)}}{\omega^2 + \frac{U}{2}^2} \right] = -\frac{i\omega}{\omega^2 + \frac{U}{2}^2} \end{aligned} \tag{3.14}$$

We can also write full answer as

$$G^{\sigma_1\sigma_2}(\omega_1,\omega_2) = -\frac{i\omega_1}{\omega_1^2 + \frac{U}{2}^2}\delta_{\sigma_1,-\sigma_2}\delta_{\omega_1,-\omega_2} \tag{3.15}$$

Even though we have the explicit formulas for exact momenta derivation, it would be quite tedious to perform such derivation by hand of course. For example, in order to calculate $\gamma^{(4)}$ we need to permute three independent time variables $3! = 6$ times, and each time perform triple integration. And for $\gamma^{(6)}$ it's $5! = 120$ permutations and five integrations. For this purpose we bring heavy artillery to our aid of the form of the best known symbolical computation tools - Wolfram Mathematica. The code that does this, consists of the following basic parts:

- To represent operators it's either possible to deal directly with matrices or take advantage of Quantum package that provides convenient Bra-Ket notation and Quantum Algebra, which makes the code more concise. Therefore the latter was chosen.
- Assigning time-ordering attribute to imaginary time variables (τ_i) and the definition of time-ordering operator T that sorts provided operators accordingly, with appropriate fermionic permutation sign in front.
- To speed up the integration part, we define our own simplified version of integral function that can only deal with polynomials, exponentials and their product. Also it allows us to carry out Kronecker's delta symbols every time an exponential is integrated. In other words $\int e^{P(\omega)\tau}d\tau$ isn't just $\frac{e^{P(\omega)\tau}}{P(\omega)}$ but $\frac{e^{P(\omega)\tau}}{P(\omega)} + (\tau - \frac{e^{P(\omega)\tau}}{P(\omega)})\delta_{P(\omega)}$. Where $P(\omega)$ is some linear function of $\omega_1 \dots \omega_{2n}$ that together with energy conservation law $\omega_1 + \dots + \omega_{2n} = 0$ gives us a way to get the final result in just one run without substituting different frequency combinations each time or taking various limits in the end.

First we repeat the result of the Appendix B in [4] and compute $\gamma^{(4)}$. The following final formulas thus obtained

$$\gamma^{\uparrow\uparrow\uparrow\uparrow} = \beta\frac{U^2}{4}\frac{\delta_{\omega_1,-\omega_3} - \delta_{\omega_2,-\omega_3}}{\omega_1^2\omega_2^2}(\omega_1^2 + \frac{U^2}{4})(\omega_2^2 + \frac{U^2}{4}) \tag{3.16}$$

$$\begin{aligned}\gamma^{\downarrow\uparrow\downarrow\uparrow} = U &- \frac{U^3}{8}\frac{\omega_1^2+\omega_2^2+\omega_3^2+\omega_4^2}{\omega_1\omega_2\omega_3\omega_4} - \frac{3U^5}{16\omega_1\omega_2\omega_3\omega_4} \\ &- \beta\frac{U^2}{4}\frac{1}{1+e^{\frac{U\beta}{2}}}\frac{2\delta_{\omega_1,-\omega_2}+\delta_{\omega_2,-\omega_3}}{\omega_1^2\omega_3^2}(\omega_1^2+\frac{U^2}{4})(\omega_3^2+\frac{U^2}{4}) \\ &+ \beta\frac{U^2}{4}\frac{1}{1+e^{-\frac{U\beta}{2}}}\frac{2\delta_{\omega_1,-\omega_3}+\delta_{\omega_2,-\omega_3}}{\omega_1^2\omega_2^2}(\omega_1^2+\frac{U^2}{4})(\omega_2^2+\frac{U^2}{4})\end{aligned} \tag{3.17}$$

Note the similarities between vertices of 2nd and 3rd order

$$\Gamma^{\uparrow\uparrow\uparrow\uparrow}_{\tau_1>\tau_2>\tau_3} = -\frac{1}{4\cosh^2\frac{U\beta}{4}}\sinh(\frac{U}{2}(\tau_1-\tau_2))\sinh(\frac{U}{2}\tau_3) \tag{3.18}$$

$$\Gamma^{\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow}_{\tau_1>\tau_2>\tau_3>\tau_4>\tau_5} = -\frac{1}{4\cosh^3\frac{U\beta}{4}}\cosh(\frac{U}{8}(\frac{\beta}{2}-(\tau_1-\tau_4)))\sinh(\frac{U}{2}(\tau_2-\tau_3))\sinh(\frac{U}{2}\tau_5) \tag{3.19}$$

Similar expressions can easily be computed for the higher-order vertex functions with any spin configurations.

Then we conclude by computation that the $\Gamma^{(6)}$ vanishes when all spins are parallel

$$\Gamma^{\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow} = \Gamma^{\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow} = 0 \tag{3.20}$$

Even it is possible to compute $\gamma^{\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow}$, the result is quite huge, and it's impossible to represent it in any human readable form, even the first not vanishing term of Taylor expansion by U is very big. However we still can get some results by considering only the case $\tau_1 > \tau_2 > \ldots > \tau_{2n}$ and only pairwise equal frequencies. Also by taking into account only first two Taylor coefficient by U, we conclude that $\gamma^{\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow}(\omega_1 = -\omega_2, \omega_3 = -\omega_4, \omega_5 = -\omega_6) = O(U^2)$, i.e. has no terms up to the 4th order at least (because it should consist of only even terms), but $\gamma^{\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow}(\omega_1 = -\omega_4, \omega_2 = -\omega_3, \omega_5 = -\omega_6)$ has the 2nd order term and it's equal to

$$\begin{aligned}
&-\frac{U^2\left(U^2+4\omega_3^2\right)^2\left(U^2+4\omega_4^2\right)^2\left(U^2+4\omega_5^2\right)^2}{524288\omega_3^6\left(\omega_3-\omega_4\right)^2\omega_4^6\omega_5^5\left(\omega_4+\omega_5\right)^2\left(-\omega_3+\omega_4+\omega_5\right)^3}\Big(-\Big(\beta^2\omega_5\left(\beta\omega_5+2i\right)\omega_4^5 \\
&+2\left(\beta^3\omega_5^3+2\beta\omega_5+16i\right)\omega_4^4+\omega_5\left(\beta^3\omega_5^3-6i\beta^2\omega_5^2-16\beta\omega_5+24i\right)\omega_4^3 \\
&-4i\omega_5^2\left(\beta^2\omega_5^2-3i\beta\omega_5+6\right)\omega_4^2-8\omega_5^3\left(\beta\omega_5-i\right)\omega_4+24i\omega_5^4\Big)\omega_3^7 \\
&+\Big(5\beta^2\omega_5\left(\beta\omega_5+2i\right)\omega_4^6+\left(13\beta^3\omega_5^3+10i\beta^2\omega_5^2+12\beta\omega_5+96i\right)\omega_4^5 \\
&+\omega_5\left(11\beta^3\omega_5^3-22i\beta^2\omega_5^2-60\beta\omega_5+136i\right)\omega_4^4+\omega_5^2\left(3\beta^3\omega_5^3-34i\beta^2\omega_5^2-84\beta\omega_5-48i\right)\omega_4^3 \\
&-4i\omega_5^3\left(3\beta^2\omega_5^2-17i\beta\omega_5+12\right)\omega_4^2+8\omega_5^4\left(14i-3\beta\omega_5\right)\omega_4+72i\omega_5^5\Big)\omega_3^6 \\
&-\Big(10\beta^2\omega_5\left(\beta\omega_5+2i\right)\omega_4^7+\left(32\beta^3\omega_5^3+42i\beta^2\omega_5^2+4\beta\omega_5+96i\right)\omega_4^6 \\
&+\omega_5\left(37\beta^3\omega_5^3-6i\beta^2\omega_5^2-88\beta\omega_5+200i\right)\omega_4^5+2\omega_5^2\left(9\beta^3\omega_5^3-35i\beta^2\omega_5^2-76\beta\omega_5-12i\right)\omega_4^4 \\
&+\omega_5^3\left(3\beta^3\omega_5^3-54i\beta^2\omega_5^2-160\beta\omega_5-192i\right)\omega_4^3-4i\omega_5^4\left(3\beta^2\omega_5^2-27i\beta\omega_5-20\right)\omega_4^2 \\
&-24\omega_5^5\left(\beta\omega_5-9i\right)\omega_4+72i\omega_5^6\Big)\omega_3^5+\left(\omega_4+\omega_5\right)\Big(10\beta^2\omega_5\left(\beta\omega_5+2i\right)\omega_4^7 \\
&+4\left(7\beta^3\omega_5^3+12i\beta^2\omega_5^2-6\beta\omega_5+8i\right)\omega_4^6+\omega_5\left(27\beta^3\omega_5^3+16i\beta^2\omega_5^2-88\beta\omega_5+24i\right)\omega_4^5 \\
&+2\omega_5^2\left(5\beta^3\omega_5^3-17i\beta^2\omega_5^2-18\beta\omega_5-44i\right)\omega_4^4+\omega_5^3\left(\beta^3\omega_5^3-26i\beta^2\omega_5^2-48\beta\omega_5-144i\right)\omega_4^3 \\
&-4i\omega_5^4\left(\beta^2\omega_5^2-13i\beta\omega_5-4\right)\omega_4^2-8\omega_5^5\left(\beta\omega_5-13i\right)\omega_4+24i\omega_5^6\Big)\omega_3^4 \\
&-\omega_4\omega_5\left(\omega_4+\omega_5\right)^2\Big(5\beta^2\left(\beta\omega_5+2i\right)\omega_4^6+4\beta\left(3\beta^2\omega_5^2+8i\beta\omega_5-9\right)\omega_4^5+\left(9\beta^3\omega_5^3+24i\beta^2\omega_5^2-92\beta\omega_5-120i\right)\omega_4^4 \\
&+2\omega_5\left(\beta^3\omega_5^3-i\beta^2\omega_5^2-2\beta\omega_5-28i\right)\omega_4^3+4\beta\omega_5^3\left(4-i\beta\omega_5\right)\omega_4^2-8\omega_5^3\left(\beta\omega_5+4i\right)\omega_4+16i\omega_5^4\Big)\omega_3^3 \\
&+\omega_4^2\omega_5\left(\omega_4+\omega_5\right)^2\Big(\beta^2\left(\beta\omega_5+2i\right)\omega_4^6+\beta\left(3\beta^2\omega_5^2+14i\beta\omega_5-20\right)\omega_4^5+\left(3\beta^3\omega_5^3+24i\beta^2\omega_5^2-112\beta\omega_5-168i\right)\omega_4^4 \\
&+\omega_5\left(\beta^3\omega_5^3+14i\beta^2\omega_5^2-120\beta\omega_5-160i\right)\omega_4^3+2i\omega_5^2\left(\beta^2\omega_5^2+10i\beta\omega_5+60\right)\omega_4^2+8\omega_5^3\left(\beta\omega_5+4i\right)\omega_4 \\
&-16i\omega_5^4\Big)\omega_3^2-2i\omega_4^3\omega_5\left(\omega_4+\omega_5\right)^3\Big(\beta\left(\beta\omega_5+2i\right)\omega_4^4+2\left(\beta^2\omega_5^2+14i\beta\omega_5-26\right)\omega_4^3+\omega_5\left(\beta^2\omega_5^2+32i\beta\omega_5-24\right)\omega_4^2 \\
&+2\omega_5^2\left(3i\beta\omega_5+26\right)\omega_4+8\omega_5^3\Big)\omega_3-12\omega_4^4\omega_5\left(\omega_4+\omega_5\right)^5\left(\omega_4\left(\beta\omega_5+2i\right)-2i\omega_5\right)\Big)
\end{aligned} \tag{3.21}$$

3.3 Conclusion

The debates about whether it's necessary or not to include greater than second perturbation terms in the dual-fermion expansion thus shall continue.

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