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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.

1 Introduction

1.1 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

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

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

with states and operators defined as

$$\left|\psi_I\right\rangle = e^{iH_0t}\left|\psi_S(t)\right\rangle$$

$$O_I(t) = e^{iH_0t}O_S e^{-iH_0t}$$

The evolution of the wave function is thus

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

so that

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

using T-operator we obtain time-ordered exponential

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

1.2 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

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

1.3 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

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

1.4 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.

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

1.5 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

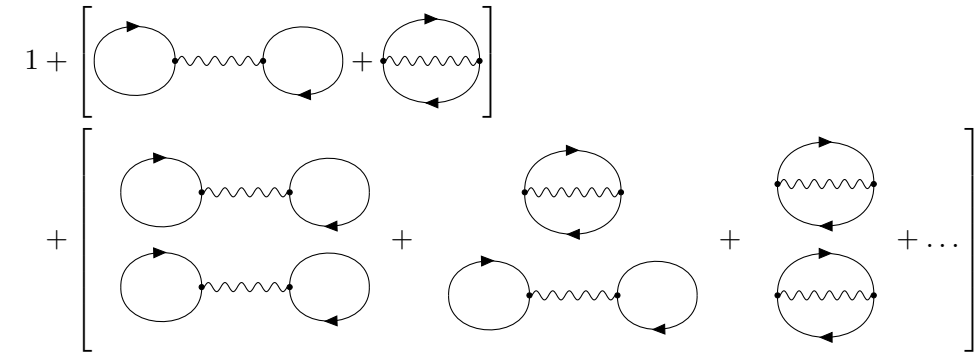
$$\begin{aligned}\nu_n &= 2\pi n k_B T \quad (Boson)\\ \omega_n &= \pi(2n+1)k_B T \quad (Fermion)\end{aligned}$$

Fourier expansion and its inverse then

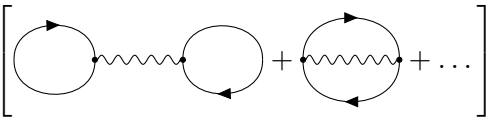
$$\begin{aligned}\mathcal{G}(\tau) &= T\sum_n \mathcal{G}(i\alpha_n)e^{-i\alpha_n\tau}\\ \mathcal{G}(i\alpha_n) &= \int_0^\beta d\tau\mathcal{G}(\tau)e^{i\alpha_n\tau}, \quad \alpha_n = \nu_n,\omega_n\end{aligned}$$

1.6 Feynman Diagrams

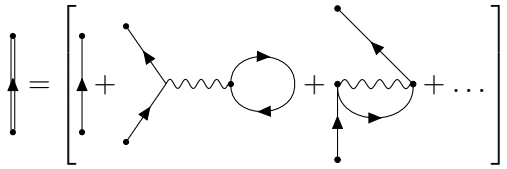
$Z = Z_0 \sum \{\text{Disconnected Feynman diagrams}\} \equiv$



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



$\mathcal{G}(1,2) = \sum \{\text{Two leg diagrams}\} \equiv$



2 Theory

2.1 Strongly correlated system

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.

2.2 The Hubbard model

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 Hubbard model can be thus be written

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

with the corresponding imaginary-time action

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

and its Fourier transform

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

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

2.3 Dynamical mean-field theory

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.

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

with the following action

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

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

2.4 Dual fermion approach

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

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

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

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

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

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

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

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

One can see that the n-th coefficient from the Taylor series of $V[f_i^*, f_i]$ is proportional to $\gamma^{(n)}$, starting from $n = 4$.

3 What was done

3.1 Preparations

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

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

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

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

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

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

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

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

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

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

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

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

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

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

where variables $1, 2\dots n; 1', 2'\dots n'$ are shortcuts for the (σ_i, τ_i) and the summation over time ordering ($(2n)!$ permutations $\tau_{i_1} > \tau_{i_2} > \dots > \tau_{i_{2n}} > 0$) is also implied.
The vertex functions $\gamma^{(2n)}$ are defined as follows

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

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

3.2 Calculations

We require energy conservation in the form $\omega_1 + \cdots + \omega_{2n} = 0$.

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

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

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

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