

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

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Abstract...

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

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

with states and operators defined as

$$|\psi_I\rangle = e^{iH_0t} |\psi_S(t)\rangle$$
$$O_I(t) = e^{iH_0t} O_S e^{-iH_0t}$$

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

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

1.2 Finite temperature

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

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

where

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

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

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

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

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

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

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 .

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

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

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

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

1.6 Feynman Diagrams

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

$$1 + \left[\text{Diagram 1} + \text{Diagram 2} \right] + \left[\text{Diagram 3} + \text{Diagram 4} + \text{Diagram 5} + \text{Diagram 6} + \dots \right]$$

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

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

2 Model

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

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