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Title

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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

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

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

with states and operators defined as

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

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

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

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

$$\nu_n = 2\pi n k_B T \quad (Boson)$$
$$\omega_n = \pi(2n+1)k_B T \quad (Fermion)$$

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

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

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