25 May 2012

International summer school on new trends in computational approaches for many-body systems

Refresher in quantum mechanics and many-body systems

[1] Introduction (Power Point)

[2] Density matrix

2.1 Density matrix and ordinary quantum mechanics

Expectation value in a pure state

(i) $$\boxed{\langle\Psi|O|\Psi\rangle = Tr[\rho O] \quad \text{where } \rho = |\Psi\rangle\langle\Psi|}$$

Proof: $Tr[\rho O] = Tr[O\rho]$

$$= \sum_i \langle i|O|\Psi\rangle\langle\Psi|i\rangle$$

$$= \langle\Psi|O|\Psi\rangle \text{ using completeness relation } \sum_i |i\rangle\langle i| = 1$$

N.B. $\rho_{ij} \equiv |i\rangle\langle i|\Psi\rangle\langle\Psi|j\rangle\langle j|$ in a general basis is not diagonal

For a pure state $\boxed{\rho^2 = \rho}$ (2)

We can represent statistical mixtures where p_n is the probability to be in $|\Psi_n\rangle$

(3) $$\boxed{\sum_n p_n \langle \Psi_n | O | \Psi_n \rangle = Tr[\rho O] \quad \text{where} \quad \rho = \sum_n p_n |\Psi_n\rangle\langle\Psi_n|}$$

Reduced density matrix (often in quantum information)

$|\Psi(R_A, R_B)\rangle$ where $R_{A,B}$ are the sets of coordinates respectively associated with subsystem A and B.

Define reduced ρ:

(4) $$\boxed{\rho_A = Tr_B[\rho]} \quad \text{where } \rho = |\Psi(R_A, R_B)\rangle\langle\Psi(R_A, R_B)|$$

↑ Trace over the coordinates of B

Then

$$\langle \Psi | O_A | \Psi \rangle = Tr_A[\rho_A O_A]$$

if O_A depends only on coordinates of A.

2.2 Density matrix in statistical physics

Number of ways to arrange the copies in such a way that n_1 of the copies are in microstate 1, n_2 in microstate 2 etc...

$$(5) \quad \frac{N!}{n_1!\, n_2! \cdots (N - n_1 - n_2 \cdots)!} = \Omega(n_1, \cdots n_i, \cdots N)$$

The probability of having state 1 occupied is $\frac{n_1}{N} \equiv \mathcal{P}_1$

Most likely values of n_1, n_2 etc... are those that can be realized in the largest number of ways. Hence, optimize Eqn. (5). Using Stirling $\ln N! = N \ln N - N$

$$(6) \quad \ln \Omega = N \ln N - \sum_{i=1}^{\eta} n_i \ln n_i$$

where η is the size of the Hilbert space. Above we removed the constraint $\sum_i^{\eta} n_i = N$. We can add it with a Lagrange multiplier.

$$(7) \quad \ln \Omega = \sum_{i=1}^{\eta} n_i \ln N - \sum_{i=1}^{\eta} n_i \ln n_i = - \sum_{i=1}^{\eta} \mathcal{P}_i \ln \mathcal{P}_i$$

with $\mathcal{P}_i = \frac{n_i}{N}$

Optimizing with the normalization constraint we recover the microcanonical ensemble (all microstates equiprobable).
With normalization and $\sum_{i=1}^{\eta} \mathcal{P}_i E_i \equiv E$ we find

$$\frac{\partial \left(\ln \Omega - \beta \sum_{i=1}^{\eta} \mathcal{P}_i E_i - \lambda \sum_{i=1}^{\eta} \mathcal{P}_i \right)}{\partial \mathcal{P}_j} = 0$$

where β and λ are Lagrange multipliers

$$-\ln \mathcal{P}_j - 1 - \beta E_j - \lambda = 0$$

$$(8) \quad \boxed{\mathcal{P}_i = e^{-\beta E_j - 1 - \lambda} = e^{-\beta E_i} / Z}$$

Proof: $\sum_{i}^{\eta} \mathcal{P}_i = 1 \Rightarrow e^{1+\lambda} = \sum_{i=1}^{\eta} e^{-\beta E_i} \equiv Z$

Thermodynamics:

$$\langle E \rangle = \sum_i \mathcal{P}_i E_i$$

$$d\langle E \rangle = \sum_i (d\mathcal{P}_i) E_i + \sum_i \mathcal{P}_i \, dE_i$$

Using $\mathcal{P}_i = \frac{e^{-\beta E_i}}{Z}$ we find

$$d\langle E \rangle = \sum_i d\mathcal{P}_i \left(-\frac{1}{\beta} \ln (\mathcal{P}_i Z) \right) + \sum_i \mathcal{P}_i \, dE_i$$

With $\sum_i d\mathcal{P}_i = 0$,

$$d\langle E \rangle = -\frac{1}{\beta} \sum_i d\mathcal{P}_i \ln \mathcal{P}_i + \sum_i \mathcal{P}_i \, dE_i$$

$$= -k_B T \sum_i d\left(\mathcal{P}_i \ln \mathcal{P}_i \right) + \sum_i \mathcal{P}_i \, dE_i$$

$$d\langle E\rangle = T\,dS + \underbrace{\sum_i \mathcal{P}_i\, dE_i}_{\text{Mechanical}} \qquad \text{where} \quad \boxed{S \equiv -k_B \sum_i \mathcal{P}_i \ln \mathcal{P}_i} \tag{9}$$

In the energy eigenbasis,

$$\rho = \sum_i \mathcal{P}_i \, |i\rangle\langle i|$$

$$\ln \rho = \sum_i \ln \mathcal{P}_i \, |i\rangle\langle i|$$

$$\rho \ln \rho = \sum_{ij} |i\rangle\langle i|\rho|j\rangle\langle j|\ln\rho|k\rangle\langle k|$$

$$\mathrm{Tr}[\rho \ln \rho] = \sum_i \langle i|\rho|i\rangle\langle i|\ln\rho|i\rangle$$

where we also used the fact that ρ is diagonal.

(10) In general, $\boxed{S \equiv -k_B \,\mathrm{Tr}[\rho \ln \rho]}$

$$= -k_B \sum_i \mathcal{P}_i \ln \mathcal{P}_i$$

In equilibrium, entropy is maximal

2.3 Legendre transform

Example: change between Lagrangian and Hamiltonian

Thermodynamics:

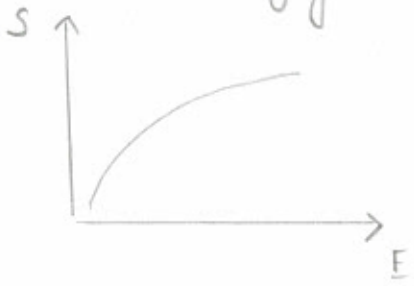
(11) $dE = T dS - p dV + \mu dN + \mathcal{M} dH$

$\mathcal{M}$ ↑ Broken symmetries

Entropy maximal in equilibrium. S is a function of mechanical variables: (neglect broken symmetries)

(12) $S(E, V, N) = \frac{1}{T} dE + \frac{p}{T} dV - \frac{\mu}{T} dN$

Conjugate variables



$\frac{\partial^2 S}{\partial E^2} \leq 0$

for systems whose energy is unbounded

Note:

(13) $p = -\left(\frac{\partial E}{\partial V}\right)_{S,N}$ E is a thermodynamic potential.

What is pressure at fixed T?
Is there an other thermodynamic potential?

(14) $T = \left(\frac{\partial E}{\partial S}\right)_{V,N}$

(15) $$p = -\left(\frac{\partial E}{\partial V}\right)_{T,N} + T\left(\frac{\partial S}{\partial V}\right)_{T,N} = -\left.\frac{\partial (E-TS)}{\partial V}\right|_{T,N}$$

(16) $\bar{F} = E - TS$ is a thermodynamic potential.
It can be seen as a function of T, V, N only if we define

(17) $$\bar{F} = \left(E(S,V,N) - TS\right)$$ and eliminate the variable S using

(18) $$\left(\frac{\partial E}{\partial S}\right)_{V,N} = T$$

The last two equations define the Legendre transform of $E(S,V,N)$ to $\bar{F}(T,V,N)$

We can also define

(19) $$\bar{\mathcal{F}}(S,V,N,T) = E(S,V,N) - TS$$

and replace (18) by the equivalent $$\left.\frac{\partial \bar{\mathcal{F}}}{\partial S}\right|_{T,V,N} = 0 \quad (20)$$

or more generally by an extremum condition if the derivative does not exist (as in a phase transition)

This is particularly useful to establish variational principles in cases elsewhere in this school.

3 Second quantization

3.1 Representation of antisymmetric states (fermions)

Similar results for bosons are easy to find.

Define the creation operator

$\Psi^+(r)$ an operator that adds one particle in state $|r\rangle$ and antisymmetrizes with all others.

Examples:

$$\Psi^+(r)\,|0\rangle = |r\rangle$$

↓ complete Hilbert space for one particle

$$(20)\quad \Psi^+(r)\,\Psi^+(r')\,|0\rangle = \frac{1}{\sqrt{2}}\left(|r\rangle|r'\rangle - |r'\rangle|r\rangle\right)$$

$$\equiv |r, r'\rangle = -|r', r\rangle$$

This is easy to satisfy with the anticommutation relations

$$(21)\quad \left\{\Psi^+(r),\ \Psi^+(r')\right\} = 0$$

i.e. $\Psi^+(r)\,\Psi^+(r') + \Psi^+(r')\,\Psi^+(r) = 0$

Note Pauli if $r = r'$

Exercise: With the above anticommutation relations, show that

$$\Psi^+(r_1)\,\Psi^+(r_2)\,\Psi^+(r_3)\,|0\rangle$$

$$= -\Psi^+(r_3)\,\Psi^+(r_2)\,\Psi^+(r_1)\,|0\rangle$$

Generalize to an arbitrary long list of creation operators where only two indices are interchanged

Since $\langle r|r'\rangle = \delta(r-r') = \langle 0|\Psi(r)\,\Psi^+(r')|0\rangle$

we define:

$$\Psi(r)\,|0\rangle = 0 \tag{22}$$

$$\{\Psi(r),\ \Psi^+(r')\} = \delta(r-r') \tag{23}$$

then $\langle 0|\Psi(r)\,\Psi^+(r')|0\rangle = \delta(r-r')\langle 0|0\rangle + \langle 0|\Psi^+(r')\,\Psi(r)|0\rangle$

$= \delta(r-r')$

Exercise: Use (20), both in first and second quantization to evaluate $\langle r\,r'|y\,y'\rangle$

3.2 Change of basis

$$|r\rangle = \sum_\alpha |\alpha\rangle\langle\alpha|r\rangle \quad\Rightarrow\quad \Psi^+(r) = \sum_\alpha c^+_\alpha\,\langle\alpha|r\rangle \tag{24}$$

3.3 Second quantized operators

One body operators:

$\Psi^+(r)\,\Psi(r)$ is the density and $\int d^3r\ \Psi^+(r)\,\Psi(r) \equiv N$ counts the number of particles.

Using

$$[AB, C] = ABC + ACB - ACB - CAB$$
$$= A\{B,C\} - \{A,C\}B$$

we have

$$[\Psi^+(r)\,\Psi(r),\ \Psi^+(r')] = \Psi^+(r')\,\delta(r-r')$$

$$\left[\int d^3r\,\Psi^+(r)\,\Psi(r)\ ,\ \Psi^+(r')\right] = \Psi^+(r')$$

$$[N, \psi^+(r')] = \psi^+(r')$$

Theorem: $[A, B] = \beta B \Rightarrow$ if $A|\alpha\rangle = \alpha|\alpha\rangle$
then $A(B|\alpha\rangle) = (\alpha+\beta)(B|\alpha\rangle)$

Proof: $(AB - BA)|\alpha\rangle = \beta B|\alpha\rangle$

$$A(B|\alpha\rangle) - B\alpha|\alpha\rangle = \beta B|\alpha\rangle$$

Thus since $N|0\rangle = 0$, $N\psi^+(r)|0\rangle = \psi^+(r)|0\rangle$
$N\psi^+(r)\psi^+(r')|0\rangle = 2\psi^+(r)\psi^+(r')|0\rangle$

One-body operator

In the diagonal basis: $\sum_\alpha c^+_\alpha \langle\alpha|\mathcal{O}|\alpha\rangle c_\alpha$

($c^+_\alpha c_\alpha$: number operator)

$$\sum_\alpha c^+_\alpha \langle\alpha|\mathcal{O}|\alpha\rangle c_\alpha \left(c^+_{\alpha_1} c^+_{\alpha_2}|0\rangle\right)$$

$$= \langle\alpha_1|\mathcal{O}|\alpha_1\rangle + \langle\alpha_2|\mathcal{O}|\alpha_2\rangle$$

Hence:

(25) $\boxed{\int d^3r\, \psi^+(r) V(r) \psi(r)}$ potential energy

$$\int \frac{d^3k}{(2\pi)^3} c^+(k) \frac{\hbar^2 k^2}{2m} c(k)$$

(26) $\rightarrow \boxed{\int d^3r\, \psi^+(r) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \psi(r)}$

↑ Change of basis

Restoring spin:

$$(27)\quad \vec{S} = \int d^3r\ \Psi^+_\alpha(\vec{r}) \left(\frac{1}{2}\vec{\sigma}_{\alpha\beta}\right) \Psi_\beta(\vec{r})$$

Two-body operator

$$(28)\quad \int V_c(\vec{r}-\vec{r}') \frac{1}{2}\left(\rho(\vec{r})\rho(\vec{r}') - \delta(\vec{r}-\vec{r}')\rho(\vec{r})\right) d^3r\, d^3r'$$

with spin $\rho(\vec{r}) = \sum_\sigma \Psi^+_\sigma(\vec{r})\ \Psi_\sigma(\vec{r})$

$$(29)\quad \boxed{\sum_{\sigma\sigma'} \int \frac{1}{2} V_c(\vec{r}-\vec{r}')\ \Psi^+_\sigma(\vec{r})\ \Psi^+_{\sigma'}(\vec{r}')\ \Psi_{\sigma'}(\vec{r}')\ \Psi_\sigma(\vec{r})\ d^3r\, d^3r'}$$

3.4 Solution for quadratic Hamiltonian

$$(30)\quad H_0 = \sum_\sigma \int d^3r\ \Psi^+_\sigma(r)\ V(r)\ \Psi_\sigma(r)$$

We are in the diagonal basis. The solution is simple: $|\Phi\rangle = \Psi^+_\sigma(r)\,\Psi^+_{\sigma'}(r')\ldots|0\rangle$

$$(31)\quad H_0|\Phi\rangle = \left[V(r) + V(r') + \ldots\right]|\Phi\rangle$$

In general case

$$(32)\quad H_0 = \sum_\sigma \int d^3r\ \Psi^+_\sigma(r)\ \mathcal{D}\ \Psi_\sigma(r)$$

where $\mathcal{D} = -\frac{\hbar^2\nabla^2}{2m} + V(r)$ or similar

Expand in some basis

$$(33)\qquad \Psi^{+}_{\sigma}(\vec{r}) = \sum_i c^{+}_{i\sigma} \langle i,\sigma | \vec{r},\sigma \rangle$$

$$= \sum_i c^{+}_{i\sigma} \varphi^{*}_{i\sigma}(\vec{r})$$

$$(34)\qquad \mathcal{H}_0 = \sum_{\substack{i,j \\ \sigma}} \left(\int d^3r \, \varphi^{*}_{i\sigma}(r) \, \mathcal{D} \, \varphi_{j\sigma}(r) \right) c^{+}_{i\sigma} c_{j\sigma}$$

In the eigenbasis: $(35)\quad \mathcal{D}\,\varphi_{i\sigma}(\vec{r}) = \epsilon_i \, \varphi_{i\sigma}(r)$

using orthogonality

$$(36)\qquad \mathcal{H}_0 = \sum_{i\sigma} \epsilon_i \, c^{+}_{i\sigma} c_{i\sigma}$$

Solution: $|\phi\rangle = c^{+}_{1\sigma} c^{+}_{1-\sigma} c^{+}_{2\sigma} c^{+}_{2-\sigma} \cdots |0\rangle$

3.5 Solution if quadratic and quartic

The potential energy (29) in the same basis as above is

$$(37)\qquad \sum_{\substack{ijkl \\ \sigma\sigma'}} \left[\int d^3r \int d^3r' \, \frac{1}{2} V_c(r-r') \, \varphi^{*}_{i\sigma}(r) \, \varphi^{*}_{j\sigma'}(r') \, \varphi_{k\sigma'}(r') \, \varphi_{l\sigma}(r) \right] c^{+}_{i\sigma} c^{+}_{j\sigma'} c_{k\sigma'} c_{l\sigma}$$

Clearly, $|\phi\rangle$ above is no longer a good solution. The interaction term is not just a number operator.

For example

$$(38)\qquad \sum_{\substack{ijkl\\ \sigma\sigma'}} c^{\dagger}_{i\sigma} c^{\dagger}_{j\sigma'} c_{k\sigma'} c_{l\sigma} \left(c^{\dagger}_{1\uparrow} c^{\dagger}_{1\downarrow} |0\rangle \right)$$

We need $k = l = 1$ to have non-zero term, and $\sigma = \uparrow$ $\sigma' = \downarrow$ or $\sigma = \downarrow$ $\sigma' = \uparrow$

$$(39)\qquad = \sum_{ij} \left(c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow} c_{1\downarrow} c_{1\uparrow} + c^{\dagger}_{i\downarrow} c^{\dagger}_{j\uparrow} c_{1\uparrow} c_{1\downarrow} \right) c^{\dagger}_{1\uparrow} c^{\dagger}_{1\downarrow} |0\rangle$$

Using anti-commutation:

$$(40)\qquad = \sum_{ij} \left(c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow} - c^{\dagger}_{i\downarrow} c^{\dagger}_{j\uparrow} \right) |0\rangle \neq c^{\dagger}_{i\uparrow} c^{\dagger}_{1\downarrow} |0\rangle$$

Thus, the general solution, if there are only two-particles of not spin 0 will be of the form

$$(42)\qquad \sum_{ij} A_{ij} \left(c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow} - c^{\dagger}_{i\downarrow} c^{\dagger}_{j\downarrow} \right) |0\rangle$$

and for a general number of particles, a linear combination of states with differently populated single-particle orbitals.

4 Hartree-Fock

4.1 Theory of everything - (no phonons)

4.2 Variational theorem:

(44) $\langle \Psi | H | \Psi \rangle \geq \langle \Psi_0 | H | \Psi_0 \rangle$

↑ True ground state

Proof: $\langle \Psi | H | \Psi \rangle = \sum_{ij} a_i^* \langle \varphi_i | H | \varphi_j \rangle a_j$

With $|\varphi_i\rangle$ an energy eigenstate

$= \sum_i |a_i|^2 E_i \geq \sum_i |a_i|^2 E_0$

$\geq E_0$ if the state is normalized.

Expanding as in Eq. (33)

(45) $\Psi_\sigma^+(r) = \sum_{i=1}^{\infty} c_{i\sigma}^+ \varphi_i^*(r)$

we look for the best single-particle state of the form

(47) $|\Phi\rangle = c_{1\sigma}^+ c_{1-\sigma}^+ c_{2\sigma}^+ c_{-2\sigma}^+ \cdots c_{\frac{N}{2}\sigma}^+ c_{\frac{N}{2}-\sigma}^+ |0\rangle$

The variational parameters are the $\varphi_i(r)$ and $\varphi_i^*(r)$

(48) $\langle r_{1\uparrow} r_{2\uparrow} \cdots r_{\frac{N}{2}\uparrow} r_{\frac{N}{2}+1\downarrow} r_{\frac{N}{2}+2\downarrow} \cdots | \Phi \rangle$

$= \langle 0 | \Psi_\uparrow(r_1) \Psi_\uparrow(r_2) \cdots \Psi_{N\downarrow} | \Phi \rangle$

is called a Slater determinant

4.3 Wick's theorem

Note that $\langle 0 | c_{1\sigma} c^{+}_{2\sigma'} | 0 \rangle = 0$

In general if $|\bar{\Phi}_1\rangle = c^{+}_{1\sigma_1} c^{+}_{2\sigma_2} \cdots |0\rangle$

and $|\bar{\Phi}_2\rangle$ also has the form of an eigenstate of a one-body Hamiltonian, then

$\langle \bar{\Phi}_1 | \bar{\Phi}_2 \rangle = 0$ unless all occupied states are identical in both $|\bar{\Phi}_i\rangle$

and

$\langle \bar{\Phi} | \bar{\Phi} \rangle = 1$

To evaluate the expectation value of H, we need

(49) $\langle \bar{\Phi} | c^{+}_{i\sigma} c_{j\sigma'} | \bar{\Phi} \rangle = \delta_{ij}\delta_{\sigma\sigma'} - \langle \bar{\Phi} | c_{j\sigma'} c^{+}_{i\sigma} | \bar{\Phi} \rangle$

but $\langle \bar{\Phi} | c_{j\sigma'} c^{+}_{i\sigma} | \bar{\Phi} \rangle = \delta_{ij}\delta_{\sigma\sigma'}$ if i,j unoccupied

$= 0$ otherwise

Thus,

(50) $\langle \bar{\Phi} | c^{+}_{i\sigma} c_{j\sigma'} | \bar{\Phi} \rangle = \begin{cases} \delta_{ij}\delta_{\sigma\sigma'} & \text{if } i\sigma, j\sigma' \text{ occupied} \\ 0 & \text{if } i\sigma, j\sigma' \text{ unoccupied} \end{cases}$

We also need

(51) $\langle \bar{\Phi} | c^{+}_{i\sigma} c^{+}_{j\sigma'} c_{k\sigma'} c_{l\sigma} | \bar{\Phi} \rangle$

$= \delta_{jk}\delta_{il} - \delta_{\sigma\sigma'}\delta_{ik}\delta_{jl}$ if i,j,k,l occupied

$= 0$ otherwise

$= \langle \bar{\Phi} | c^{+}_{i\sigma} c_{l\sigma} | \bar{\Phi} \rangle \langle \bar{\Phi} | c^{+}_{j\sigma'} c_{k\sigma'} | \bar{\Phi} \rangle$

$- \langle \bar{\Phi} | c^{+}_{i\sigma} c_{k\sigma'} | \bar{\Phi} \rangle \langle \bar{\Phi} | c^{+}_{j\sigma'} c_{l\sigma} | \bar{\Phi} \rangle$

This generalizes to an arbitary number of operators.

Let $\langle \Phi | c_a^\dagger c_{a'} | \Phi \rangle$ where a contains spin and space label.

be defined as $G^<_{aa'}$

We have

(52) $$\langle \Phi | c_a^\dagger c_b^\dagger c_{b'} c_{a'} | \Phi \rangle$$

$$= G^<_{aa'} G^<_{bb'} - G^<_{ab'} G^<_{ba'} = \det [G]$$

where

$$G = \begin{bmatrix} G^<_{aa'} & G^<_{ab'} \\ G^<_{ba'} & G^<_{bb'} \end{bmatrix}$$

(53) $$\langle \Phi | c_a^\dagger c_b^\dagger c_c^\dagger c_{c'} c_{b'} c_{a'} | \Phi \rangle$$

$$= \det \begin{bmatrix} G^<_{aa'} & G^<_{ab'} & G^<_{ac'} \\ G^<_{ba'} & G^<_{bb'} & G^<_{bc'} \\ G^<_{ca'} & G^<_{cb'} & G^<_{cc'} \end{bmatrix}$$

This will be useful for CTQMC

Exercise: Find the Hartree-Fock equations.

5 Model Hamiltonians

- DFT particularly good for s, p electron materials. It assumes that the single Slater-determinant representation is good.
- If only a few d or f bands near the Fermi level, one can write down a model Hamiltonian that is solved beyond the independant particle approximation.

5.1 Hubbard model

Assume that one has found a set of bands.
Then

$$(54)\quad \Psi^{\dagger}(r) = \sum_{n} \int_{B.Z.} \frac{d^3k}{(2\pi)^3}\, C^{\dagger}_{k n \sigma}\, \varphi^{*}_{k n \sigma}(\vec{r})$$

where k is a quasi-momentum index, n a band index and $\varphi_{k n \sigma}(\vec{r})$ a Bloch function. N is the number of lattice sites.

Assume there is a single d-band near the Fermi level. We take into account interactions only within this band.

Dropping the band index, we write

$$(55)\quad \Psi^{\dagger}(r) = \sum_{i} C^{\dagger}_{i\sigma}\, w_{i\sigma}(r)$$

where i stands for R_i in a one-atom per unit cell case.

Then

$$(56)\quad \sum_\sigma \int d^3r\, \Psi^\dagger_\sigma(r)\, \mathcal{O}\, \Psi_\sigma(r)$$

$$= \sum_\sigma \sum_{ij} \int d^3r\, w^*_{i\sigma}(r)\, \mathcal{O}\, w_{j\sigma}(r)\; c^\dagger_{i\sigma} c_{j\sigma}$$

$$= \sum_\sigma \sum_{ij} \langle i|\mathcal{O}|j\rangle\, c^\dagger_{i\sigma} c_{j\sigma}$$

The analogous change of variable for the interacting part leads to

$$(57)\quad \sum_{\sigma\sigma'} \sum_{ijkl} \frac{1}{2} \langle i|\langle j|\, V\, |l\rangle|k\rangle\, c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{k\sigma'} c_{l\sigma}$$

Assume that the largest contribution comes from $i=j=k=l$. Then the interaction becomes

$$(58)\quad \sum_{\sigma\sigma'} \sum_i \frac{U}{2}\, c^\dagger_{i\sigma} c^\dagger_{i\sigma'} c_{i\sigma'} c_{i\sigma}$$

where $U = \langle i|\langle i|\, V\, |i\rangle|i\rangle$

Since $c^\dagger_{i\sigma} c^\dagger_{i\sigma} = 0$ we are left with $\sigma' = -\sigma$ and the same term appears twice so

$$(59)\quad \sum_\sigma \sum_i \frac{U}{2}\, c^\dagger_{i\sigma} c^\dagger_{i-\sigma} c_{i-\sigma} c_{i\sigma} = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

where $n_{i\uparrow} = c^\dagger_{i\uparrow} c_{i\uparrow}$

Taken together:

$$(60)\quad \mathcal{H}_{\text{Hubbard}} = \sum_\sigma \sum_{ij} t_{ij}\, c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Solutions exist in • $d=1$ (Bethe Ansatz)

• $d=\infty$ (Dynamical mean-field theory)

It is used to understand the Mott transition

$U \to 0$ Eigenstate $c^+_{k_0\uparrow} c^+_{k_0\downarrow} \cdots\cdots |0\rangle$

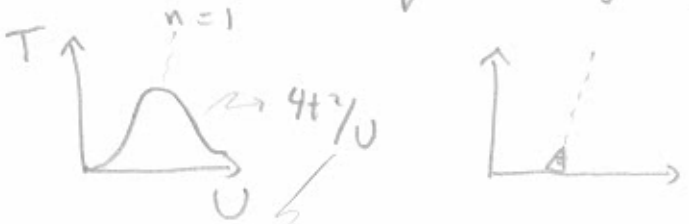
Wave nature of the electron

$t \to 0$ Eigenstate $c^+_{i\uparrow} c^+_{i\downarrow} \cdots\cdots |0\rangle$

Particle nature.

Localized if $n=1$

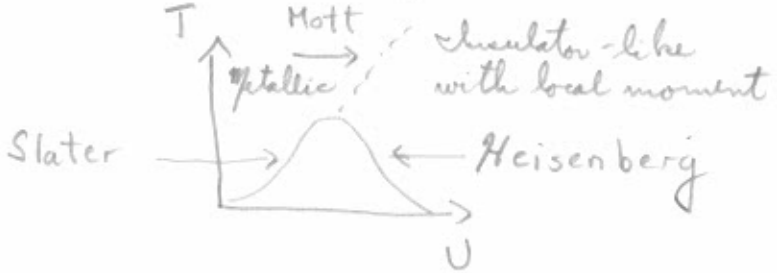
At intermediate coupling, highly entangled, i.e. cannot write the state as direct product of single-particle states.



Antiferromagnetic coupling. Start from large U

↑ ↓ Second order degenerate perturbation theory ↑↓ ⟷ ↑↓

↑ ↑ Pauli forbids double occupancy



Anderson model:

$$H = \sum_{\sigma} \epsilon f_{\sigma}^{+} f_{\sigma} + U\left(f_{\uparrow}^{+} f_{\uparrow} f_{\downarrow}^{+} f_{\downarrow}\right) + \sum_{k,\sigma} \epsilon_k c_{k\sigma}^{+} c_{k\sigma}$$

$$+ \sum_{k\sigma} V_k c_{k\sigma}^{+} f_{\sigma} + V_k^{*} c_{k\sigma}^{+} f_{\sigma}$$

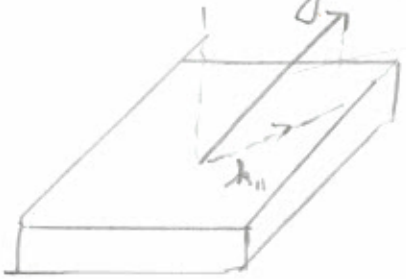
impurity hybridized with a bath of non-interacting electrons

Chapter 3 : Green's functions

3 reasons to define this correlation function

- Directly related to photoemission cross-section
- Arises naturally in the calculation of other observables
- Necessary for perturbation theory (Wick's theorem)

1 Photoemission



$$\frac{\hbar^2 k^2}{2m} = E_{pn} + \hbar\omega + \mu - W$$

Matrix element

$$(61)\quad -\frac{1}{V}\sum_{k'} \langle n|\langle k|\langle 0|_{em}\ \vec{j}_{k'}\cdot\vec{A}_{-k'}\ |m\rangle|0\rangle|\,|_{q}\rangle_{em}$$

$|n\rangle$: System; $|k\rangle$: Outgoing electron

$$(62)\quad \vec{j}_{k'=0} = \frac{e}{V}\sum_{p}\frac{\vec{p}}{m}c_p^+ c_p \qquad p = k_\parallel \text{ conserved}$$

$$(63)\quad \frac{\partial^2\sigma}{\partial\Omega\,\partial\omega} \sim \sum_{mn} e^{-\beta(E_m-\mu N_m)}\,|\langle n|c_{k_\parallel}|m\rangle|^2$$

$$\delta(\hbar\omega+\mu-(E_m-E_n))$$

$$(64)\quad \boxed{K \equiv H-\mu N}$$

$$(65)\quad \sim \sum_{mn} e^{\frac{-\beta K_m}{Z}}\,|\langle n|c_{k_\parallel}|m\rangle|^2\,\delta(\hbar\omega-(K_m-K_n))$$

$$\sim \int dt\, e^{i\omega t}\sum_{mn}\langle m|e^{\frac{-\beta K}{Z}}c^+_{k_\parallel}|n\rangle\langle n|e^{iKt/\hbar}\,c_{k_\parallel}e^{-iKt/\hbar}|m\rangle$$

(66) $$\nu \int dt\, e^{i\omega t} \langle c^{+}_{k_\parallel} c_{k_\parallel}(t) \rangle$$

where (67) $$\langle \mathcal{O} \rangle = \frac{Tr\left[e^{-\beta K}\mathcal{O}\right]}{Tr\left[e^{-\beta K}\right]}$$

(68) $$C_{k_\parallel}(t) = e^{iKt/\hbar} C_{k_\parallel} e^{-iKt/\hbar}$$

2. Perturbation theory

Let $K = K_0 + K_1$

Define $e^{-\beta K} \equiv e^{-\beta K_0} U_I(\beta, 0)$

↑ where U_I is the evolution operator in the interaction representation.

The equation for U_I is obtained from

$$\frac{\partial}{\partial \tau} e^{-\tau K} = -K e^{-\tau K} = -K\left(e^{-\tau K_0} U_I(\tau,0)\right)$$

$$= -K_0\left(e^{-\tau K_0} U_I(\tau,0)\right) + e^{-\tau K_0} \frac{\partial U_I}{\partial \tau}(\tau,0)$$

Subtracting the two eqns. and multiplying by $e^{\tau K_0}$

$$\frac{\partial U_I}{\partial \tau}(\tau,0) = -\left(e^{\tau K_0} K_1 e^{-\tau K_0}\right) U_I(\tau,0)$$

(69) $$\frac{\partial U_I}{\partial \tau}(\tau,0) = -K_1(\tau)\, U_I(\tau,0)$$

where $K_1(\tau)$ evolves as Heisenberg equation of motion, but in imaginary time and with K_0

At different times, K_1 do not commute in general, since the operator can change from one operator to another.

Since $U(0,0) = 1$

(70)
$$U_I(\beta,0) - 1 = -\int_0^\beta d\tau\, K_1(\tau)\, U_I(\tau,0)$$

Iteratively

(71)
$$U_I(\beta,0) = 1 - \int_0^\beta d\tau\, K_1(\tau) + \int_0^\beta d\tau \int_0^\tau d\tau'\, K_1(\tau) K_1(\tau') - \int_0^\beta d\tau \int_0^\tau d\tau' \int_0^{\tau'} d\tau''\, K_1(\tau) K_1(\tau') K_1(\tau'') \ldots$$

Later times are always to the left.

If all integrals end at β, all time orders are included and we overcount $N!$ for term of N^{th} order

Hence

(72)
$$\boxed{U_I(\beta,0) = T_\tau \left[e^{-\int_0^\beta K_1(\tau)\, d\tau} \right]}$$

where T_τ is the time ordering operator.

If K_1 is time independant, we recover the expected result.

3 Matsubara Green's function

3.1 Definition

expected when we do perturbation theory

(73) $\mathcal{G}(r, r'; \tau) = -\langle T_\tau \Psi(r,\tau)\, \Psi^+(r';0)\rangle$ ← Drop spin index for simplicity

$= -\langle \Psi(r,\tau)\, \Psi^+(r';0)\rangle \theta(\tau)$

$+ \langle \Psi^+(r',0)\, \Psi(r,\tau)\rangle \theta(-\tau)$

Expectation value defined in (67)

(N.B.) Change of sign for fermions

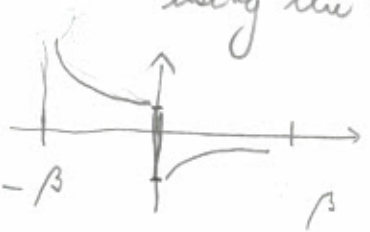
(74) $\Psi(r,\tau) = e^{K\tau}\, \Psi(r)\, e^{-K\tau}$

(75) $\Psi^+(r,\tau) = e^{K\tau}\, \Psi^+(r)\, e^{-K\tau}$ (not the adjoint)

3.2 Antiperiodicity

(76) $\mathcal{G}(r, r''; \tau) = -\mathcal{G}(r, r'; \tau + \beta)$

using the cyclic property of the trace



Exercise Using the anticommutation relations, show that the jump at $\tau = 0$ is unity

Repeat this function periodically (not the true value outside $-\beta \le \tau \le \beta$ but anyway we do not need it there) and use Fourier theorem:

Then,

$$(77)\quad \mathcal{G}(r,r';\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\omega_n\tau}\,\mathcal{G}(r,r';i\omega_n)$$

$$\omega_n = (2n+1)\frac{\pi}{\beta} = (2n+1)\pi T \qquad (k_B = 1)$$

$$(78)\quad \mathcal{G}(r,r';i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau}\,\mathcal{G}(r,r';\tau)$$

3.3 Spectral representation and links with observables (photoemission)

(Lehman representation)

$$(79)\quad \int_0^\beta \mathcal{G}(r,r';\tau)\,d\tau = -\int_0^\beta d\tau\, e^{i\omega_n\tau}\langle \Psi(r,\tau)\,\Psi^+(r',0)\rangle$$

$$= -\int_0^\beta d\tau\, e^{i\omega_n\tau}\sum_{m,n}\frac{e^{-K_n\beta}}{Z}\langle m|e^{K_m\tau}\Psi(r)e^{-K_n\tau}|n\rangle$$

$$= -\sum_{m,n}\frac{e^{-K_m\beta}}{Z}\,\frac{\langle n|\Psi(r)|n\rangle\langle n|\Psi^+(r')|m\rangle}{i\omega_n + K_m - K_n}\left[e^{i\omega_n\beta}\,e^{(K_m-K_n)\beta} - 1\right]$$

Since $e^{i\omega_n\beta} = -1$, we are left with

$$= \sum_{m,n}\frac{\left(e^{-K_n\beta} + e^{-K_m\beta}\right)}{Z}\,\frac{\langle m|\Psi(r)|n\rangle\langle n|\Psi^+(r')|m\rangle}{i\omega_n + K_m - K_n}$$

The case of photoemissions: Change variables (unitary transformation) to go to momentum variables $\Psi(r) \to c_k$. The unitary transformation is Fourier transforms.

Then

(80) $$\mathcal{G}(k, i\omega_n) = \int_0^\beta \mathcal{G}(k,\tau)\, d\tau$$
$$= \sum_{m,n} \frac{e^{-\kappa_n\beta} + e^{-\kappa_m\beta}}{Z} \frac{|\langle n|c_k|m\rangle|^2}{i\omega_n + \kappa_m - \kappa_n}$$

Analytically continue $i\omega_n \to \omega + i\eta$ (this gives the so-called retarded Green's function). Then using

(81) $$\lim_{\eta\to 0} \frac{1}{\omega - \epsilon + i\eta} = \mathcal{P}\frac{1}{\omega-\epsilon} - i\pi\delta(\omega-\epsilon)$$

we obtain:

(82) $$G^R(k,\omega) = \mathcal{G}(k, i\omega_n \to \omega + i\eta)$$

(83) $$-2\,\mathrm{Im}\, G^R(k,\omega) = \sum_{m,n} \frac{e^{-\kappa_n\beta} + e^{-\kappa_m\beta}}{Z} |\langle n|c_k|m\rangle|^2 \, 2\pi\delta(\omega - (\kappa_n - \kappa_m))$$
$$= \left[\sum_{m,n} \frac{e^{-\kappa_n\beta}}{Z} |\langle n|c_k|m\rangle|^2 \, 2\pi\delta(\omega - (\kappa_n - \kappa_m))\right] \frac{1}{f(\omega)}$$

where $f(\omega) = \dfrac{1}{e^{\beta\omega}+1}$ is the Fermi-Dirac distribution.

Hence, the photo-emission cross-section Eq. (65) is proportional to

(84) $$\frac{\partial^2\sigma}{\partial\Omega\,\partial\omega} \sim \left[-2\,\mathrm{Im}\, G^R(k,\omega)\right] f(\omega)$$

where the "spectral weight" is defined by

$$(85) \qquad -2\,\mathrm{Im}\,G^R(k,\omega) = A(k,\omega)$$

This has the interpretation of a momentum resolved DOS.

For example, at $T=0$: only the ground state survives and Eq. (23) becomes:

$$(86) \qquad A(k,\omega) = 2\pi \left[\sum_n |\langle n|c_k|0\rangle|^2 \delta(\omega - (K_n - K_0)) + \sum_m |\langle m|c_k|0\rangle|^2 \delta(\omega - (K_0 - K_m)) \right]$$

The first term contributes at $\omega < 0$ if k is below the Fermi surface. The second term at $\omega > 0$ if k is above the Fermi surface.

Exercise: From (83), using the anticommutation relations, show that

$$\int \frac{d\omega}{2\pi} A(k,\omega) = 1$$

3.4 Non-interacting case:

(87) $$K_0 = \sum_{\substack{k \\ \sigma}} (\epsilon_k - \mu)\, c^+_{k\sigma}\, c_{k\sigma}$$

(88) $$\frac{\partial c_{k\sigma}}{\partial \tau} = [K_0,\, c_{k\sigma}] = (\epsilon_k - \mu)\, c_{k\sigma}$$

(89) $$\frac{\partial \mathcal{G}^0_{k\sigma}(\tau)}{\partial \tau} = (\epsilon_k - \mu)\mathcal{G}^0_{k\sigma} - \delta(\tau)$$

↑ Derivative of θ function and anticommutation relation.

With $\int_0^\beta d\tau\, e^{i\omega_n \tau}$ and integration by parts

(90) $$\mathcal{G}^0_{k\sigma}(i\omega_n) = \frac{1}{i\omega_n - (\epsilon_k - \mu)}$$

3.5 Self-energy

From (80) (83) (85) in general we have

(91) $$\mathcal{G}(k, i\omega_n) = \int \frac{d\omega}{2\pi} \frac{A(k,\omega)}{i\omega_n - \omega}$$

The high frequency expansion

(92) $$\mathcal{G}(k, i\omega_n) = \frac{\int \frac{d\omega}{2\pi} A(k,\omega)}{i\omega_n} + \frac{\int \frac{d\omega}{2\pi} A(k,\omega)\,\omega}{(i\omega_n)^2} + \cdots$$

and

(93) $$\int \frac{d\omega}{2\pi} A(k,\omega) = 1$$ reveals that in general we can write

This means that in general we can write:

(94) $$\mathcal{G}_\sigma(k, i\omega_n) = \frac{1}{i\omega_n - (\epsilon_k - \mu) - \Sigma(k, i\omega_n)}$$

where Σ goes to a constant at $i\omega_n = \infty$.

- It reflects the fact that there is more than one pole in the presence of interactions.
- Take $\Sigma(k, i\omega_n) = -i\Gamma$ with Γ a constant.

Then

$$-2\,\mathrm{Im}\,G^R = -2\,\mathrm{Im}\left[\frac{1}{\omega + i\eta + i\Gamma - (\epsilon_k - \mu)}\right]$$

$$= \frac{2\Gamma}{[\omega - (\epsilon_k - \mu)]^2 + \Gamma^2}$$

The $\mathrm{Im}\,\Sigma^R(k, \omega)$ has the meaning of a lifetime
$\mathrm{Re}\,\Sigma^R(k, \omega)$ renormalizes the real part of the dispersion relation.

A frequency dependent self-energy means that $c_k^+ |0\rangle$ does not corresponds to an eigenstate. It has non-zero projection on many eigenstates. Conversely, eigenstates are linear combinations of many independent-particle states (Slater determinants).

The frequency dependence of Σ also follows from that of G where many poles contribute according to the Lehman representation.

4. Generating functional formalism

4.1 $Z[\varphi]$ and G

Define

$$(95)\quad \boxed{Z[\varphi] \equiv \mathrm{Tr}\left[e^{-\beta K} T_\tau e^{-S[\varphi]} \right]}$$

where

$$(97)\quad \boxed{S[\varphi] \equiv \int d^3r_1 d\tau_1 d^3r_2 d\tau_2 \sum_\sigma \psi^+_\sigma(r_1,\tau_1)\, \varphi_\sigma(r_1,\tau_1;r_2,\tau_2)\, \psi_\sigma(r_2,\tau_2)}$$

We use the shorthand

$$(98)\quad \boxed{S[\varphi] \equiv \psi^+_{\bar{\sigma}}(\bar{1})\, \varphi_{\bar{\sigma}}(\bar{1},\bar{2})\, \psi_{\bar{\sigma}}(\bar{2})}$$

$1 \to (\vec{r}_1, \tau_1)$ and overbar means integration

Define the functional derivative (generalization of partial derivative)

$$(99)\quad \frac{\delta}{\delta \varphi_\sigma(3,4)} \psi^+_{\bar{\sigma}}(\bar{1})\, \varphi_{\bar{\sigma}}(\bar{1},\bar{2})\, \psi_{\bar{\sigma}}(\bar{2}) = \psi^+(3)\,\psi(4)$$

Then

$$(100)\quad G_\sigma(1,2)_\varphi = \frac{-\mathrm{Tr}\left[e^{-\beta K} T_\tau e^{-S[\varphi]} \psi_\sigma(1)\,\psi^+_\sigma(2) \right]}{\mathrm{Tr}\left[e^{-\beta K} T_\tau e^{-S[\varphi]} \right]}$$

$$\equiv -\langle \psi_\sigma(1)\,\psi^+_\sigma(2) \rangle_\varphi$$

Inside T_τ, field operators for fermions anticommute

$$(101)\quad \boxed{G_\sigma(1,2)_\varphi = -\frac{\delta \ln Z[\varphi]}{\delta \varphi(2,1)}}$$

Physical quantities such as $\mathcal{H}$ and partition function are evaluated at $\varphi = 0$

The advantage is formal. We can in particular evaluate higher order correlation functions and formulate variational principles.

4.2 Higher order correlation functions

(102) $$\frac{\delta^2 \ln Z}{\delta \varphi_\sigma(2,1)\,\delta \varphi_{\sigma'}(3,4)} = \langle \Psi_\sigma(1)\Psi^+_\sigma(2)\Psi^+_{\sigma'}(3)\Psi_{\sigma'}(4)\rangle_\varphi - \langle \Psi_\sigma(1)\Psi^+_\sigma(2)\rangle_\varphi \langle \Psi^+_{\sigma'}(3)\Psi_{\sigma'}(4)\rangle_\varphi$$

where the last term comes from derivative of the denominator in Eq. (100)

By specializing the indices, this corresponds to spin-spin or charge-charge correlation functions.

4.3 Equations of motion

(103) $$\frac{\partial \Psi_\sigma(r,\tau)}{\partial \tau} = [K, \Psi_\sigma(r,\tau)]$$

$$= \frac{\nabla^2}{2m}\Psi_\sigma(r,\tau) + \mu \Psi_\sigma(r,\tau) - \sum_{\sigma_1}\int d^3_{r'} V_c(\vec{r}-\vec{r}')\, \Psi^+_{\sigma_1}(r',\tau)\Psi_{\sigma_1}(r',\tau)\Psi_\sigma(r,\tau)$$

The interaction term can be written with an integral over imaginary time as well if we define

(104) $$V(1,1') \equiv V_c(r-r')\delta(\tau_1-\tau'_1)$$

Then, if we take into account the φ dependence as well instead of Eq. (89) we have

$$(104)\quad \left(\frac{\partial}{\partial \tau_1} - \frac{\nabla_1^2}{2m} - \mu\right) G_\sigma(1,2)_\varphi$$

$$= -\delta(1-2) - \varphi_\sigma(1,\bar{2})\, G_\sigma(\bar{2},2)_\varphi$$

$$+ \langle T_\tau \left[\psi^+_{\bar{\sigma}}(\bar{2}^+)\, V(1-\bar{2})\, \psi_{\bar{\sigma}}(\bar{2})\, \psi_\sigma(1)\, \psi^+_\sigma(2)\right]\rangle_\varphi$$

Define

$$(105)\quad G^{-1}_{0\sigma}(1,2) = -\left(\frac{\partial}{\partial \tau_1} - \frac{\nabla_1^2}{2m} - \mu\right)\delta(1-2)$$

the (104) takes the form

$$(106)\quad \left(G^{-1}_{0\sigma}(1,\bar{2}) - \varphi(1,\bar{2})\right) G(\bar{2},2)_\varphi = \delta(1-2)$$

$$\underbrace{- V(1-\bar{2}) \langle T_\tau \left[\psi^+_{\bar{\sigma}}(\bar{2}^+)\, \psi_{\bar{\sigma}}(\bar{2})\, \psi(1)\, \psi^+(2)\right]\rangle_\varphi}$$

if we define this as

$$\Sigma(1,\bar{2})_\varphi\, G(\bar{2},2)_\varphi$$

in the end we will have $G = \dfrac{1}{G_0^{-1} - \Sigma}$ when evaluated at $\varphi = 0$

4.4 An impressionistic view for approximations

$$(107)\quad (G_0^{-1} - \varphi)\, G = 1 - V \langle T_c\, \psi^+ \psi\, \psi \psi^+ \rangle_\varphi$$

$$(108)\quad \Sigma G = -V \langle T_c\, \psi^+ \psi\, \psi \psi^+ \rangle_\varphi$$

so that

$$(109)\quad (G_0^{-1} - \varphi - \Sigma)\, G = G^{-1} G = 1$$

At $\varphi = 0$ $\quad G = G_0 + G_0 \Sigma G$

is known as Dyson's equation

Σ, G are functionals of φ.

To compute the self-energy, we need

$$(110)\quad \Sigma G = -V \langle T_c\, \psi^+ \psi\, \psi \psi^+ \rangle = -V \left[\frac{\delta G}{\delta \varphi} - G G \right]$$

To evaluate $\frac{\delta G}{\delta \varphi}$ we proceed as follows:

$$(111)\quad \frac{\delta (G G^{-1})}{\delta \varphi} = 0 \qquad \frac{\delta G}{\delta \varphi} G^{-1} + G \frac{\delta G^{-1}}{\delta \varphi} = 0$$

$$(112)\quad \frac{\delta G}{\delta \varphi} = -\, G \frac{\delta G^{-1}}{\delta \varphi} G$$

Using (109) for G^{-1}, we are left with

$$(113)\quad \frac{\delta G}{\delta \varphi} = G \frac{\delta \varphi}{\delta \varphi} G + G \left(\frac{\delta \Sigma}{\delta \varphi} \right) G$$

↑ Like particles that propagate without interactions

↘ Effect of interactions.

By analogy with Dyson, we want to bring in the denominator

Thus, use the chain rule: $\frac{\delta \Sigma}{\delta \varphi} = \frac{\delta \Sigma}{\delta G} \frac{\delta G}{\delta \varphi}$

(114) $$\boxed{\frac{\delta G}{\delta \varphi} = G \frac{\delta \varphi}{\delta \varphi} G + G \left(\frac{\delta \Sigma}{\delta G} \frac{\delta G}{\delta \varphi} \right) G}$$

↑ irreducible vertex

(115) 

Substituting (113) in (110)

(116) $$\Sigma = -V \left[G \frac{\delta \varphi}{\delta \varphi} G + G \frac{\delta \Sigma}{\delta \varphi} G - GG \right] G^{-1}$$

(117) $$\boxed{\Sigma = -V \left[G \frac{\delta \varphi}{\delta \varphi} - G + G \frac{\delta \Sigma}{\delta \varphi} \right]}$$

Use this in (114) as leading order in V.

This is Hartree-Fock

Once we have $\frac{\delta G}{\delta \varphi}$ we can improve the approximation for Σ by replacing $\frac{\delta \Sigma}{\delta \varphi}$ in (117) by $\frac{\delta \Sigma^{H.F.}}{\delta G} \frac{\delta G}{\delta \varphi}$

The result is the GW approximation if we keep the most important term in $\frac{\delta G}{\delta \varphi}$, i.e.

(118) 

$$\chi = \chi_0 + \chi_0 V(q) \chi \qquad V(q) \sim \frac{1}{q^2}$$

(119) Σ = H.F. + 

4.5 Kadanoff-Baym functional and variational formulation of the many-body problem

(120) $\Omega[\varphi] \equiv -T \ln Z[\varphi]$

(121) $\frac{1}{T}\frac{\delta\Omega[\varphi]}{\delta\varphi} = G$

Define the Legendre transform of that equation. Then

(122) $\tilde{\Omega}[G] = \Omega[\varphi] - \mathrm{Tr}[\varphi G]$

where (123) $\mathrm{Tr}\, A = T\sum_{i\omega_n}\sum_{\alpha} A_{\alpha\alpha}(i\omega_n)$

General properties of Legendre transforms show that

(123) $\boxed{\frac{1}{T}\frac{\delta\tilde{\Omega}[G]}{\delta G} = -\varphi = G^{-1} - G_0^{-1} + \Sigma}$

The physical solution is at $\varphi = 0$

We thus have a variational principle

$$\frac{\delta\tilde{\Omega}[G]}{\delta G} = 0$$

We can guess as follows the value of $\tilde{\Omega}$. Proceed as if we were integrating (123):

(124) $\boxed{\tilde{\Omega}[G] = \Phi[G] - \mathrm{Tr}\left[(G_0^{-1} - G^{-1})G\right] + \mathrm{Tr}\ln(-G)}$

where $\boxed{\frac{1}{T}\frac{\delta\Phi}{\delta G} = \Sigma}$

This can be seen as an integration constant.

This is the Kadanoff-Baym functional

Φ is the Luttinger-Ward functional

This reduces to the correct result when $\Sigma_1 = 0$