Zero Temperature Signle Particle Green's Function

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Schrodinger Picture and Heisenberg Picture

Schrodinger Picture

- States are time dependent $|\Psi_S(t)\rangle$, operators are not $\hat{O}_S$
- Equation of motion: $i\frac{\partial}{\partial t}|\Psi_S(t)\rangle = \hat{\mathcal{H}}|\Psi_S(t)\rangle$

Heisenberg Picture

- States are time-independent $|\Psi_H\rangle$,
  operators are time dependent $\hat{O}_H(t) = e^{i\hat{\mathcal{H}}t}\hat{O}_S e^{-i\hat{\mathcal{H}}t}$
- Equation of motion: $i\frac{\partial}{\partial t}\hat{O}_H = [\hat{O}_H, \hat{\mathcal{H}}]$

Definition of Green's Function

Formal Definition: Expectation Value of Field Operators

$$iG_{\alpha\beta}(rt, r't') = \langle\Psi_0|\hat{T}[\hat{\psi}_\alpha(rt)\hat{\psi}^\dagger_\beta(r't')]|\Psi_0\rangle$$

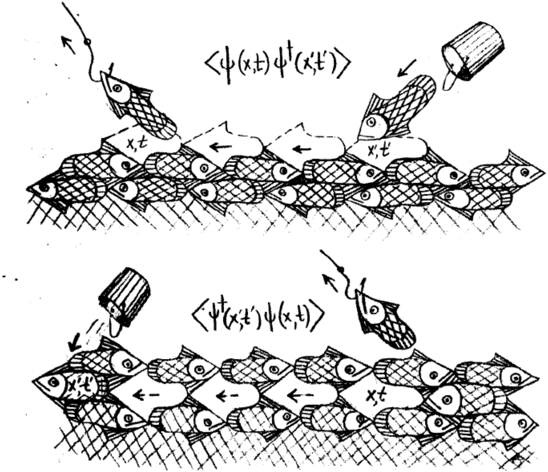
Parts

- $|\Psi_0\rangle$: Many-body ground state in Heisenberg picture
- $\hat{\psi}_\alpha(rt)$: Field operator in Heisenberg picture

Time-Ordered Product

$$\hat{T}[\hat{\psi}_\alpha(rt)\hat{\psi}^\dagger_\beta(r't')] = \begin{cases} \hat{\psi}_\alpha(rt)\hat{\psi}^\dagger_\beta(r't') & t > t' \\ -\hat{\psi}^\dagger_\beta(r't')\hat{\psi}_\alpha(rt) & t < t' \end{cases}$$

Probability Amplitude of Particle Propagation



Quantum System of Many-Body Systes: Alexander Zagoskin

Observables from Single Particle Greens' Function

- Expectation value of any single-particle operator in ground state
- The ground state energy of the system
- The excitation spectrum of the system
  (will be clear in Lehmann representation)

Expectation Value of Single-Particle Operator

$$\hat{J}(r) = \sum_{\alpha\beta} \hat{\psi}_\alpha^\dagger(r) J_{\alpha\beta}(r) \hat{\psi}_\beta(r)$$

$$\begin{aligned}
\langle J(r) \rangle &= \langle \Psi_0 | \hat{J}(r) | \Psi_0 \rangle \\
&= \lim_{r' \to r} \sum_{\alpha\beta} J_{\alpha\beta}(r) \langle \Psi_0 | \hat{\psi}_\beta^\dagger(r') \hat{\psi}_\alpha(r) | \Psi_0 \rangle \\
&= -i \lim_{t' \to t^+} \lim_{r' \to r} \sum_{\alpha\beta} J_{\beta\alpha}(r) G_{\alpha\beta}(rt, r't') \\
&= -i \lim_{t' \to t^+} \lim_{r' \to r} tr[J(r) G(rt, r't')]
\end{aligned}$$

Density and Energy

$$\langle \hat{n}(r) \rangle = -itrG(rt, rt^{+})$$

$$N = -i \sum_k \int \frac{d\omega}{2\pi} e^{i\omega 0^{+}} trG(k, \omega)$$

$$\langle \hat{T} \rangle = -i \int d^3 r \lim_{r' \to r} -\frac{\hbar^2 \nabla^2}{2m} trG(rt, r't^{+})$$

$$E = \langle H \rangle = -\frac{1}{2} i \int d^3 r \lim_{t' \to t^{+}} \lim_{r' \to r} [i\hbar \frac{\partial}{\partial t} - \frac{\hbar^2 \nabla^2}{2m}] trG(rt, r't')$$

Potential energy operator is not single-particle operator, non-trivial result.
Fetter and Walecka P67-P68

Example: Free Fermi Gas

$$G(rt, r't') = -i\langle\Psi_0|\hat{T}[\hat{\psi}_\alpha(rt)\hat{\psi}^\dagger_\beta(r't')]|\Psi_0\rangle$$
$$= \langle\Psi_0|[\hat{\psi}_\alpha(rt)\hat{\psi}^\dagger_\beta(r't')]|\Psi_0\rangle\theta(t-t')$$
$$+i\langle\Psi_0|[\hat{\psi}^\dagger_\beta(r't')\hat{\psi}_\alpha(rt)]|\Psi_0\rangle\theta(t'-t)$$

$$\theta(t-t') = \int \frac{d\omega'}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega' + i0^+}$$

For transitionally invariant system:

$$G(rt, r't') = G(r-r', t-t')$$
$$= \sum_k \int \frac{d\omega}{2\pi} e^{ik(r-r')} e^{-i\omega(t-t')} G(k,\omega)$$

Free Fermi Gas Cont. 1

$$\hat{H}_0 = \sum_{k,\sigma} \epsilon_k a^\dagger_{k,\sigma} a_{k,\sigma}$$

$$|\Psi_0\rangle = a^\dagger_{k1\uparrow} a^\dagger_{k1\downarrow} a^\dagger_{k2\uparrow} a^\dagger_{k2\downarrow} ... a^\dagger_{kF\uparrow} a^\dagger_{kF\downarrow} |0\rangle$$

$$\begin{aligned}
a^\dagger_{k,\sigma}(t)|\Psi_0\rangle &= e^{i\hat{\mathcal{H}}_0 t} a^\dagger_{k,\sigma} e^{-i\hat{\mathcal{H}}_0 t}|\Psi_0\rangle \\
&= e^{i\hat{\mathcal{H}}_0 t} e^{iE_0 t}\theta(k - k_F)|\Psi_0\rangle|k\sigma\rangle \\
&= e^{i(E_0+\epsilon_k)t} e^{-iE_0 t}\theta(k - k_F)|\Psi_0\rangle|k\sigma\rangle \\
&= e^{i\epsilon_k t}\theta(k - k_F) a^\dagger_{k,\sigma}|\Psi_0\rangle = e^{i\epsilon_k t}\theta(k - k_F)|N + 1\rangle \\
a_{k,\sigma}(t)|\Psi_0\rangle &= e^{-i\epsilon_k t}\theta(k_F - k) a_{k,\sigma}|\Psi_0\rangle
\end{aligned}$$

Free Fermi Gas Cont. 2

$$G(k,t-t') = -i\langle\Psi_0|\hat{T}[a_{k,\sigma}(t)a^{\dagger}_{k,\sigma}(t')]|\Psi_0\rangle$$

$$= -ie^{-i\epsilon_k(t-t')}(\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k))$$

$$G(k,\omega) = \int d(t-t')e^{i\omega(t-t')}G(k,t-t')$$

$$= -i\int d(t-t')e^{i(\omega-\epsilon_k)(t-t')}(\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k$$

$$= \int \frac{d\omega'}{2\pi}\int d(t-t')e^{i(-\epsilon_k+\omega-\omega')(t-t')}[\frac{\theta(k-k_F)}{\omega'+i0^+} + \frac{\theta(k_F-k)}{\omega'-i0^+}]$$

$$= \int \frac{d\omega'}{2\pi}2\pi\delta(-\epsilon_k+\omega-\omega')[\frac{\theta(k-k_F)}{\omega'+i0^+} + \frac{\theta(k_F-k)}{\omega'-i0^+}]$$

$$= \frac{\theta(k-k_F)}{\omega-\epsilon_k+i0^+} + \frac{\theta(k_F-k)}{\omega-\epsilon_k-i0^+}$$

Lehmann Representation

$$
\begin{aligned}
G(rt, r't') &= -i\langle\Psi_0|\hat{T}[\hat{\psi}(r,t)\hat{\psi}^\dagger(r',t')]|\Psi_0\rangle \\
&= -i\sum_n [\theta(t-t')\langle\Psi_0|\hat{\psi}(r,t)|n\rangle\langle n|\hat{\psi}^\dagger(r',t')|\Psi_0\rangle \\
&- \theta(t'-t)\langle\Psi_0|\hat{\psi}^\dagger(r',t')|n\rangle\langle n|\hat{\psi}(r,t)|\Psi_0\rangle \\
&= -i\sum_n [\theta(t-t')e^{-i(E_n^{N+1}-E_0^N)(t-t')}\langle\Psi_0|\hat{\psi}(r)|n\rangle\langle n|\hat{\psi}^\dagger(r')|\Psi_0\rangle \\
&- \theta(t'-t)e^{-i(E_n^{N-1}-E_0^N)(t'-t)}\langle\Psi_0|\hat{\psi}^\dagger(r')|n\rangle\langle n|\hat{\psi}(r)|\Psi_0\rangle
\end{aligned}
$$

Lehmann Representation cont.

$$G(r,r',\omega) = \sum_n [\frac{\langle \Psi_0|\hat{\psi}(r)|n\rangle\langle n|\hat{\psi}^\dagger(r')|\Psi_0\rangle}{\omega - (E_n^{N+1} - E_0^N) + i0^+}$$
$$+ \frac{\langle \Psi_0|\hat{\psi}^\dagger(r')|n\rangle\langle n|\hat{\psi}(r)|\Psi_0\rangle}{\omega - (E_0^N - E_n^{N-1}) - i0^+}$$

Remarks

- Poles of G are excitation energies
- All frequency dependence in denominator

Single Site Hubbard Model

$$H = Un\uparrow n\downarrow - \mu(n\uparrow + n\downarrow)$$

$$F0 = \{|0\rangle\}, F1 = \{|\uparrow\rangle, |\downarrow\rangle\}, F2 = \{|\uparrow\downarrow\rangle\}$$

F0 Ground State

$$G\uparrow(\omega) = G\downarrow(\omega) = \frac{1}{\omega + \mu + i0^+}$$

F2 Ground State

$$G\uparrow(\omega) = G\downarrow(\omega) = \frac{1}{\omega - U + \mu - i0^+}$$

Lehmann Representation: Spectral functions

$$G(k,\omega) = \int d\omega' [\frac{A(k,\omega')}{\omega - \mu - \omega' + i0^+} + \frac{B(k,\omega')}{\omega - \mu + \omega' - i0^+}]$$

$$A(k,\omega) = \sum_n \delta(\omega - (E_n^{(N+1)} - E_0^N))|\langle n, k|\hat{\psi}^\dagger|\Psi_0\rangle|^2, positive$$

$$B(k,\omega) = \sum_n \delta(\omega - (E_0^N - E_n^{(N-1)}))|\langle n, -k|\hat{\psi}|\Psi_0\rangle|^2, positive$$

Remarks

- Infinite system:
  $E_n^{N+1} - E_0^N = (E_n^{N+1} - E_0^{N+1}) - (E_0^{N+1} - E_0^N) = E_n - E_0 + \mu$
- B, A: Photoemission and inverse photoemission spectroscopy
- Asymptotic behavior: $G(k,\omega) \sim \frac{1}{\omega}$
- Density of states, $N(\omega) = \sum_n \delta(\omega - \epsilon_n) = \sum_k A(k,\omega) + B(k,\omega)$

Dyson Equation

Green's function as propogator

$$G = G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 \Sigma G_0 + \ldots$$

$$G = G_0 + G_0 \Sigma G$$

Dyson Equation

$$G^{-1} = G_0^{-1} - \Sigma$$

Dyson Equation in DFT+DMFT

$$G_0 = (\omega - \mu - H_0)^{-1}$$

$$G = (G_0^{-1} - \Sigma)^{-1} = (\omega - \mu - H_0 - \Sigma)^{-1}$$