Chapter 3:
GREEN'S FUNCTIONS AND FIELD THEORY (FERMIONS)

Review

7. GREEN'S FUNCTIONS

Definition. The time-ordered product of operators in the Heisenberg picture

Consider $A_H(t)$ and $B_H(t)$.

They don't necessarily commute.

Now define

$$T\left[A_H(t)\, B_H(t')\right] \equiv \begin{cases} A_H(t)\, B_H(t') & \text{if } t > t' \\ \pm\, B_H(t')\, A_H(t) & \text{if } t < t' \end{cases}$$

- The earlier time stands to the right.
- Sign $(\pm)$ depends on bosonic or fermionic character of the operators.

7a. Definition of the Green's function

The Green's function (or, also called 1-particle matrix element) is $G_{\alpha\beta}(\mathbf{x},t;\mathbf{x}',t')$ where αβ are spin indices;
x,**x'** are two positions;
t,t' are two times. The definition is …

$$i\,G_{\alpha\beta}(\vec{x}t\,;\vec{x}'t') = \frac{\langle \Psi_0 |\, T[\psi_\alpha(\vec{x},t)\,\psi_\beta^\dagger(\vec{x}',t')]\,| \Psi_0\rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

where $|\Psi_0\rangle$ is the ground state in the Heisenberg picture.

(We could require $\langle \Psi_0 | \Psi_0\rangle = 1$.)

Notations

- $|\Psi_0\rangle$ = Heisenberg ground state;
  $H|\Psi_0\rangle = E_0|\Psi_0\rangle$
- $\psi_\alpha(\vec{x},t)$ = Heisenberg field operator;
  $\psi_\alpha(\vec{x},t) = e^{iHt}\,\psi_\alpha(\vec{x},0)\,e^{-iHt}$ $(\hbar = 1)$
  $\psi_\beta^\dagger(\vec{x}',t') = e^{iHt'}\,\psi_\beta^\dagger(\vec{x}',0)\,e^{-iHt'}$
- $T[\psi_\alpha(xt)\,\psi_\beta^\dagger(\vec{x}'t')]$

$$= \begin{cases} \psi_\alpha(\vec{x},t)\,\psi_\beta^\dagger(\vec{x}'t') & \text{if } t'<t \\ -\,\psi_\beta^\dagger(x't')\,\psi_\alpha(xt) & \text{if } t'>t \end{cases}$$

assuming fermions

$$iG_{\alpha\beta}(xt;x't') = \begin{cases} e^{iE_0(t-t')}\langle\Psi_0|\,\psi_\alpha(\vec{x}0)\,e^{-iH(t-t')}\,\psi^\dagger_\beta(x'0)\,|\Psi_0\rangle \\ -e^{-iE_0(t-t')}\langle\Psi_0|\,\psi^\dagger_\beta(x'0)\,e^{+iH(t-t')}\,\psi_\alpha(x0)\,|\Psi_0\rangle \end{cases}$$

Comment. $\psi_\alpha(\bar{x},0) = \psi_{S\alpha}(\vec{x})$

7b. RELATION TO OBSERVABLES

Some quantities in the theory can be calculated from $G_{\alpha\beta}(x,x')$.

Let J be a one-particle operator...

$$J = \int d^3x\; \mathcal{J}(\vec{x})$$

$$\mathcal{J}(\vec{x}) = \sum_{\alpha,\beta} \psi^\dagger_\beta(\vec{x})\, J_{\beta\alpha}(\vec{x})\, \psi_\alpha(x)$$

The first quantized operator would be $\sum_{k=1}^{N} J_{\beta\alpha}(\vec{r}_k)$.

The ground state expectation value of $\mathcal{J}(\vec{x})$

$$= \sum_{\alpha\beta} J_{\beta\alpha}(\vec{x})\, \frac{\langle\Psi_0|\,\psi^\dagger_\beta(x')\,\psi_\alpha(x)\,|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \quad \text{where } \vec{x}' = \vec{x}$$

$$= \sum_{\alpha\beta} (\pm i)\, J_{\beta\alpha}(\vec{x})\, G_{\alpha\beta}(\vec{x}t;\vec{x}'t') \quad \begin{cases}\text{bosons}\\ \text{fermions}\end{cases}$$

with limits $\vec{x}' \to \vec{x}$ and $t' \to t$ with $t' > t$

Examples

- Particle number density

$$\langle \hat{n}(\vec{x}) \rangle_0 = \pm i\, G_{\alpha\alpha}(\vec{x}t; \vec{x}t+0)$$

$\sum_{\alpha}$ implied

- Spin density

$$\langle \hat{\sigma}_i(\vec{x}) \rangle_0 = \pm i\, (\sigma_i)_{\beta\alpha}\, G_{\alpha\beta}(\vec{x}t; \vec{x}t+0)$$

$\sum_{\alpha\beta}$ implied

- Total kinetic energy

$$\langle \hat{T} \rangle_0 = \pm i \int d^3x \lim_{x' \to x} \frac{-\hbar^2 \nabla^2}{2m} G_{\alpha\alpha}(xt; x't+0)$$

There are some tricks for calculating the ground state energy.

$$\langle \hat{V} \rangle = \pm \frac{i}{2} \int d^3x \lim_{x' \to x} \lim_{t' \to t} \left(i\hbar \frac{\partial}{\partial t} - \frac{\hbar^2 \nabla^2}{2m} \right) G_{\alpha\alpha}(\vec{x}t; \vec{x}'t')$$

So, by this or other formulas we can determine the ground state energy $E = \langle T + V \rangle_0$

Lesson #1: If we know the Green's function, then we can calculate some interesting quantities.

Lesson #2. Of course we do not know the Green's function; but we can estimate it, approximately, using perturbation theory.

7c. Example : "free fermions" in a box

What is the Green's function for free particles in a box, with periodic boundary conditions, that do not interact with each other?

The ground state: fill the lowest available states up to the Fermi energy.

This could be interesting, e.g., as the first approximation for nuclear structure: protons and neutrons confined inside a sphere.

Particles and holes

We have $\hat{\Psi}(\vec{x}) = \sum_{\vec{k}\lambda} \psi_{\vec{k}\lambda}(\vec{x})\, c_{\vec{k}\lambda}$

where

$$\psi_{\vec{k}\lambda}(\vec{x}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{x}} u_\lambda \qquad \begin{cases} u_{1/2} = \begin{pmatrix}1\\0\end{pmatrix} \\ u_{-1/2} = \begin{pmatrix}0\\1\end{pmatrix} \end{cases}$$

Now define

$$c_{\vec{k}\lambda} = \begin{cases} a_{\vec{k}\lambda} \text{ for } k > k_F & \text{annihilates particles} \\ b^\dagger_{-\vec{k}\lambda} \text{ for } k < k_F & \text{creates holes} \end{cases}$$

A hole with momentum $-\hbar\mathbf{k}$,
is created by annihilating an electron with momentum $\hbar\mathbf{k}$ below the Fermi surface.

The field operator in the Schroedinger picture is

$$\hat{\Psi}_s(\vec{x}) = \sum_{\substack{\vec{k}\lambda \\ (k>k_F)}} \psi_{\vec{k}\lambda}(\vec{x})\, a_{\vec{k}\lambda} + \sum_{\substack{\vec{k}\lambda \\ (k<k_F)}} \psi_{\vec{k}\lambda}(\vec{x})\, b^{\dagger}_{-\vec{k}\lambda}$$

$\hat{\Psi}_s$ annihilates particles and creates holes

$\hat{\Psi}_s^{\dagger}$ creates particles and annihilates holes

"creating a hole" is the same as "annihilating a particle below the Fermi energy" .

Calculate the one-particle Green's function, for free particles ($H = H_0$)

$$i\,G^0_{\alpha\beta}(xt;x't') = \langle \Phi_0 | T[\hat\psi_\alpha(xt)\,\hat\psi^+_\beta(x't')] | \Phi_0\rangle$$

$$\hat\psi_\alpha(xt) = \sum_{\vec k\lambda} \psi_{\vec k\lambda\alpha}(\vec x)\, e^{-i\omega_k t}\,[\,a_{\vec k\lambda}\,\theta(k-k_F) + b^+_{-\vec k\lambda}\,\theta(k_F-k)\,]$$

$$\hat\psi^+_\beta(x't') = \sum_{k'\lambda'} \psi^+_{k'\lambda'\beta}\, e^{i\omega_{k'} t}\,[\,a^+_{k'\lambda'}\,\theta(k'-k_F) + b_{-k'\lambda'}\,\theta(k_F-k')\,]$$

Check your understanding: what is $\psi_{\mathbf{k}\lambda\alpha}(\mathbf{x})$?

- The ground state has no particles and no holes; $a|\Phi_0\rangle = 0$ and $b|\Phi_0\rangle = 0$
- For $t > t'$, order is $\hat\psi_\alpha \hat\psi^+_\beta$;

  $\hat\psi^+_\beta$ creates a particle $\Rightarrow \psi^+_{k'\lambda'\beta}\, e^{i\omega' t'}\,\theta(k'-k_F)$

  $\hat\psi_\alpha$ annihilates it $\Rightarrow \psi_{k\lambda\alpha}\, e^{-i\omega t}\,\theta(k-k_F)\,\delta(\vec k,\vec k')\,\delta_{\lambda\lambda'}$
- For $t < t'$, order is $\hat\psi^+_\beta \hat\psi_\alpha$;

  $\hat\psi_\alpha$ creates a hole $\Rightarrow \psi_{k\lambda\alpha}\, e^{-i\omega t}\,\theta(k_F-k)$

  $\hat\psi^+_\beta$ annihilates it $\Rightarrow \psi^+_{k'\lambda'\beta}\, e^{i\omega' t'}\,\theta(k_F-k')\,\delta(\vec k,\vec k')\,\delta_{\lambda\lambda'}$
- $\sum_{\vec k\lambda}\sum_{\vec k'\lambda'} \delta(\vec k,\vec k')\,\delta_{\lambda\lambda'} \longrightarrow \sum_{\vec k\lambda}$
- $\sum_\lambda u_{\lambda\alpha}\, u^+_{\lambda\beta} = \delta_{\alpha\beta}$ (spin sum)

Result $\quad i\,G^0_{\alpha\beta}(\vec x t;\vec x' t')$

$$= \delta_{\alpha\beta}\,\frac{1}{\Omega}\sum_{\vec k} e^{i\vec k\cdot(\vec x-\vec x')}\,e^{-i\omega_k(t-t')}\,[\,\theta(t-t')\,\theta(k-k_F) - \theta(t'-t)\,\theta(k_F-k)\,]$$

important sign

Result $\quad iG^0_{\alpha\beta}(\vec{x}t;\vec{x}'t)$

$$= \delta_{\alpha\beta}\frac{1}{\Omega}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}e^{-i\omega_k(t-t')}$$

$$\left[\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k)\right]$$

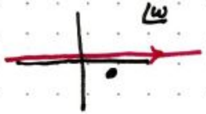
↑ important sign

Now take the limit $\Omega\to\infty$;

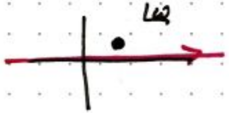
$$\sum_{\vec{k}} \to \frac{\Omega}{(2\pi)^3}\int d^3k$$

<u>Now employ some tricks with contour integration</u>

$$e^{-i\omega_k(t-t')}\theta(t-t') = \frac{-1}{2\pi i}\int_{-\infty}^{\infty}\frac{e^{-i\omega(t-t')}d\omega}{\omega-\omega_k+i\epsilon}$$



$$e^{-i\omega_k(t-t')}\theta(t'-t) = \frac{+1}{2\pi i}\int_{-\infty}^{\infty}\frac{e^{-i\omega(t-t')}d\omega}{\omega-\omega_k-i\epsilon}$$



$$iG^0_{\alpha\beta} = \delta_{\alpha\beta}\int\frac{d^3k}{(2\pi)^3}e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}\int\frac{i\,d\omega}{2\pi}e^{-i\omega(t-t')}$$

$$\left[\frac{\theta(k-k_F)}{\omega-\omega_k+i\epsilon} + \frac{\theta(k_F-k)}{\omega-\omega_k-i\epsilon}\right]$$

propagator for a particle

and propagator for a hole

Finally, $\quad G^0_{\alpha\beta}(xt;x't') = \int\frac{d^4k}{(2\pi)^4}e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}e^{-i\omega(t-t')}$

$$\times\ \delta_{\alpha\beta}\left[\frac{\theta(k-k_F)}{\omega-\omega_k+i\epsilon} + \frac{\theta(k_F-k)}{\omega-\omega_k-i\epsilon}\right]$$

~~7d. The Lehmann representation (skip)~~

7e. The physical interpretation of the Green's function

The "propagator".

(1) Start with the ground state at time t' in the interaction picture;

(2) create a particle at x';

(3) let the system evolve to time t;

(4) annihilate a particle at x;

(5) and calculate the overlap with the ground state;

(6) rewrite the overlap in the Heisenberg picture;

The result is the Green's function, for t > t'.

In words, it's the matrix element for a particle to propagate from (x',t') to (x,t) in the ground state.

Let t > t'.

Consider, in the interaction picture,

$$\langle \Psi_I(t) \,|\, \psi_\alpha(\mathbf{x},t)\, \psi_\beta^\dagger(\mathbf{x}',t') \,|\, \Psi_I(t')\rangle$$

$$|\Psi_I(t')\rangle$$

$$\hat{\psi}_\beta^+(\vec{x}', t')\,|\Psi_I(t')\rangle$$

$$\hat{U}(t,t')\,\hat{\psi}_\beta^+(x' t')\,|\Psi_I(t')\rangle$$

$$\hat{\psi}_\alpha(x t)\,\hat{U}(t t')\,\hat{\psi}_\beta^+(x' t')\,|\Psi_I(t')\rangle$$

$$\langle\Psi_I(t)|\,\hat{\psi}_\alpha(x t)\,\hat{U}(t t')\,\hat{\psi}_\beta^+(x' t')\,|\Psi_I(t')\rangle$$

$$\langle\Psi_0|\,\psi_\alpha(x,t)\,\psi_\beta^+(x',t')\,|\Psi_0\rangle$$

Homework Problem due Friday February 12

Problem 20.

(a) Evaluate Equation (7.8) for the free Green's function, (7.44).

(b) Do the same for Equation (7.10).

(7.8) $< n(\mathbf{x}) > = \pm\, i \;\mathrm{tr}\; G_{\alpha\alpha}(\mathbf{x}t,\mathbf{x}t^{+})$

(7.10) $< T > = \pm\, i \int d^3x \lim_{\mathbf{x}' \to \mathbf{x}} \left[(-\hbar^2 \nabla^2 /2m)\; \mathrm{tr}\; G_{\alpha\alpha}(\mathbf{x}t,\mathbf{x}'t^{+}) \right]$

(7.44) $G^0_{\alpha\beta}(\mathbf{x}t,\mathbf{x}'t') = (2\pi)^{-4} \int d^3k \int_{-\infty}^{\infty} d\omega\;\; e^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}')}\, e^{-i\omega(t-t')}\;\; G^0_{\alpha\beta}(\mathbf{k},\omega)$

where $G^0_{\alpha\beta}(\mathbf{k},\omega) = \delta_{\alpha\beta}\; [\; \theta(k-k_F) / (\omega - \omega_k + i\eta) + \theta(k_F-k) / (\omega - \omega_k - i\eta) \;]$