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

Review

7. GREEN'S FUNCTIONS

The time-ordered product of operators in the Heisenberg picture

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

They don't necessarily commute.

Now define

$$T[A_H(t)\, B_H(t')]$$

$$\equiv \begin{cases} A_H(t)\, B_H(t') & \text{if } t>t' \\ (\pm 1)\, B_H(t')\, A_H(t) & \text{if } t<t' \end{cases}$$

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

7a. Definition of the Green's function

The Green's function (or, also called 1 particle matrix element) is $G_{\alpha\beta}(\vec{x}t\,;\,\vec{x}'t')$ where $\alpha\beta$ are spin indices, $\vec{x}\vec{x}'$ are two positions, tt' are two times; is defined by

$$i\,G_{\alpha\beta}(\vec{x}t;\vec{x}'t') = \frac{\langle \Psi_0 | T\left[\psi_{H\alpha}(\vec{x}t)\,\psi^{+}_{H\beta}(\vec{x}'t')\right] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

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

(We could require $\langle \Psi_0 | \Psi_0 \rangle = 1$ but not necessary.)

Notations

- $|\Psi_0\rangle$ = the Heisenberg ground state;

$$H\,|\Psi_0\rangle = E_0\,|\Psi_0\rangle$$

- $\psi_{H\alpha}(\vec{x}t)$ = the Heisenberg field operator

$$\psi_{H\alpha}(\vec{x}t) = e^{iHt/\hbar}\,\psi_{S\alpha}(\vec{x})\,e^{-iHt/\hbar}$$

$$\psi^{+}_{H\beta}(\vec{x}'t') = e^{iHt'/\hbar}\,\psi^{+}_{S\beta}(\vec{x}')\,e^{-iHt'/\hbar}$$

- $T\left[\psi_{H\alpha}(\vec{x}t)\,\psi^{+}_{H\beta}(\vec{x}'t')\right]$

$$= \begin{cases} \psi_{H\alpha}(\vec{x}t)\,\psi^{+}_{H\beta}(\vec{x}'t') & \text{if } t > t'; \\ -\,\psi^{+}_{H\beta}(\vec{x}'t')\,\psi_{H\alpha}(\vec{x}t) & \text{if } t < t' \end{cases}$$

assuming fermions

$$iG_{\alpha\beta}(\vec{x}t;\vec{x}'t') = \begin{cases} e^{iE_0(t-t')/\hbar}\langle\Psi_0|\,\psi_{s\alpha}(\vec{x})\,e^{-iH(t-t')/\hbar}\,\psi_{s\beta}(\vec{x}')|\Psi_0\rangle \\ -e^{-iE_0(t-t')/\hbar}\langle\Psi_0|\,\psi^{+}_{s\beta}(\vec{x}')\,e^{+iH(t-t')/\hbar}\,\psi_{\alpha}(\vec{x})|\Psi_0\rangle \end{cases}$$

7b. Relation to observables

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

Let $\hat{J}$ be a one-particle operator;

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

$$\hat{\mathcal{J}}(\vec{x}) = \sum_{\alpha,\beta} \hat{\psi}^{+}_{\beta}(\vec{x})\, J_{\beta\alpha}(\vec{x})\, \hat{\psi}_{\alpha}(\vec{x})$$

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

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

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

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

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

$t' \to t$ 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

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

$\sum_{\alpha\beta}$ implied

- Total kinetic energy

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

There are some tricks for calculating the ground state energy.

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

So by this (or other formulas) we can determine the ground state energy $E = \langle \hat{T} + \hat{V} \rangle$.

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

The Green's function for free particles in a box with periodic boundary conditions ;

"free particles" means they don't interact with each other,

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

This is interesting, e.g., as the first approximation for nuclear structure: protons and neutrons in a box.

Particles and holes

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

where $\psi_{\vec{k}\lambda}(\vec{x}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{x}}\, \eta_\lambda$

$\eta_{1/2} = \binom{1}{0}$

$\eta_{-1/2} = \binom{0}{1}$

Now define

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

The field operator in the Schroedinger picture is

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

So $\hat{\Psi}_s$ annihilates ~~creates~~ 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 ($H=H_0$)

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

(interaction picture or Heisenberg picture; the same because $H_1=0$)

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

annihilates particles — creates holes

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

creates particles — annihilates holes

Understand the terminology:
"particle" means a particle above the Fermi energy;
"hole" means a particle below the Fermi energy.

- The ground state has no particles, no holes
  $\therefore\ a_{k\lambda}|\Phi_0\rangle = 0$ and $b_{\lambda k}|\Phi_0\rangle = 0$
- For $t>t'$: $\hat\psi^\dagger$ creates a particle
  $\hat\psi$ annihilates it
  $$\Rightarrow\ \psi_{k\lambda\alpha}(x)\,e^{-i\omega_k t}\,\psi^\dagger_{k'\lambda'\beta}(x')\,e^{i\omega_{k'}t'}$$
  $$\delta(\vec{k},\vec{k}')\,\delta_{\lambda\lambda'}\,\theta(k-k_F)$$
- For $t<t'$: $\hat\psi$ creates a hole
  $\hat\psi^\dagger$ annihilates it
  $$\Rightarrow\ \psi^\dagger_{k'\lambda'\beta}(x')\,e^{i\omega_{k'}t'}\,\psi_{k\lambda\alpha}(x)\,e^{-i\omega_k t}$$
  $$\delta(\vec{k},\vec{k}')\,\delta_{\lambda\lambda'}\,\theta(k_F-k)$$
- $\sum_{\vec{k}\lambda}\sum_{\vec{k}'\lambda'}\delta(\vec{k},\vec{k}')$ becomes $\sum_{\vec{k}\lambda}$
- $\sum_{\lambda=\pm 1/2} u_{\lambda\alpha}\,u^\dagger_{\lambda\beta} = \delta_{\alpha\beta}$ (spin sum)

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

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

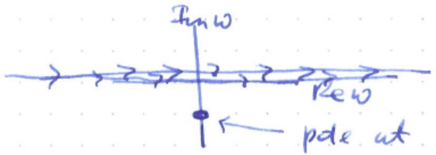
$$\left[\theta(t-t')\,\theta(k-k_F) - \theta(t'-t)\,\theta(k_F-k)\right]$$

note this sign!

Now take the limit $V\to\infty$.

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

Also $\quad \theta(\xi) = \dfrac{i}{2\pi}\displaystyle\int_{-\infty}^{\infty}\frac{d\omega\, e^{-i\omega\xi}}{\omega+i\eta}$ $\quad (\eta = 0+)$



pole at $\omega = -i\eta$

$\xi>0$ close contour below

$\xi<0$ close contour above

... a bit of analysis ...

$$iG^0_{\alpha\beta} = \delta_{\alpha\beta}\int\frac{d^3k}{(2\pi)^3}e^{i\vec k\cdot(\vec x-\vec x')}\int\frac{i\,d\omega}{2\pi}e^{-i\omega(t-t')}\left[\frac{\theta(k-k_F)}{\omega-\omega_k+i\eta} + \frac{\theta(k_F-k)}{\omega-\omega_k-i\eta}\right]$$

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

where $\quad G^0_{\alpha\beta}(\vec k,\omega) = \delta_{\alpha\beta}\left[\dfrac{\theta(k-k_F)}{\omega-\omega_k+i\eta} + \dfrac{\theta(k_F-k)}{\omega-\omega_k-i\eta}\right]$

propagating particle; t>t' $\quad$ propagating hole;t<t'

7d. The Lehmann representation

<u>Some general features of the</u>
<u>interacting 1-particle Green's function</u>

$$iG_{\alpha\beta}(xt; x't') = \langle \Psi_0 | T[\hat{\psi}_{H\alpha}(\vec{x}t)\,\hat{\psi}^{\dagger}_{H\beta}(\vec{x}'t')] | \Psi_0 \rangle$$

$$= \sum_n \Big\{ \theta(t-t') \langle \Psi_0 | \hat{\psi}_{\alpha}^{(H)}(xt) | \Psi_n \rangle \langle \Psi_n | \hat{\psi}^{\dagger (H)}_{\beta}(x't') | \Psi_0 \rangle$$

$$- \theta(t'-t) \langle \Psi_0 | \hat{\psi}^{\dagger (H)}_{\beta}(x't') \underbrace{| \Psi_n \rangle \langle \Psi_n |}_{\text{complete set of states}} \hat{\psi}_{\alpha}^{(H)}(xt) | \Psi_0 \rangle \Big\}$$

By translation invariance,

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

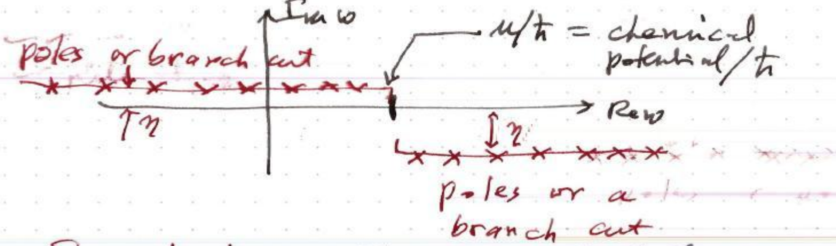
$$G_{\alpha\beta}(\vec{k},\omega) = V \sum_n \frac{\langle \Psi_0 | \hat{\psi}_{\alpha}(0) | n\vec{k} \rangle \langle n\vec{k} | \hat{\psi}^{\dagger}_{\beta}(0) | \Psi_0 \rangle}{\omega - (E_n - E_0)/\hbar + i\eta}$$

$$+ V \sum_n \frac{\langle \Psi_0 | \hat{\psi}^{\dagger}_{\beta}(0) | n, -\vec{k} \rangle \langle n, -\vec{k} | \hat{\psi}_{\alpha}(0) | \Psi_0 \rangle}{\omega + (E_n - E_0)/\hbar - i\eta}$$

$$G(\vec{k}\omega) = \int_0^{\infty} d\omega' \left\{ \frac{A(\vec{k},\omega')}{\omega - \mu/\hbar - \omega' + i\eta} + \frac{B(\vec{k},\omega')}{\omega - \mu/\hbar + \omega' - i\eta} \right\}$$

where $A(\vec{k},\omega')$ and $B(\vec{k},\omega')$ are real and positive.

Analytic structure of $G(\vec{k},\omega)$ in the complex ω plane (Fig. 7.1)



Important — If we can calculate $G(\vec{k},\omega)$ then we can determine excitation energies from the analytic structure of the 1PGF.

7e. Physical interpretation of the Green's function

Physical interpretation of the Green's function

— the "propagator"

Start with the ground state at time t';

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

create an additional particle at $\vec{x}'$;

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

let the system evolve (or propagate) to time t,

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

Calculate the overlap with the state $\psi^+_\alpha(\vec{x}t)\,|\Psi_I(t)\rangle$

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

$$= \langle \Psi_0|\,\hat{\psi}_{H\alpha}(xt)\,\hat{\psi}^+_{H\beta}(x't')\,|\Psi_0\rangle = \text{Green's function for } t > t'$$