Clase 12

Viernes 16/10/2020

La clase pasada vimos:

Operadores en segunda cuantización: Demostración para operadores de una partícula

Relación de la función de Green de una partícula con observables físicos: (3) El espectro de excitación del sistema, o Representación de Lehmann ⟵ hoy seguimos

Representación de Lehmann

time-independent, translationally invariant

$$G_{\alpha\beta}(\vec{k}, t-t') = \delta_{\alpha\beta}\, G(\vec{k}, t-t')$$

$$i\,G(\vec{k}, t-t') = \langle \Phi^0_H |\, T\left[c_{\vec{k}}(t)_H \; c^{+}_{\vec{k}}(t')_H \right] | \Phi^0_H \rangle$$

$$= \Theta(t-t') \langle c_{\vec{k}}(t)_H \; c^{+}_{\vec{k}}(t')_H \rangle_H - \Theta(t'-t) \langle c^{+}_{\vec{k}}(t')_H \; c_{\vec{k}}(t)_H \rangle_H$$

$= \Theta(t-t') \langle e^{iHt} c_{\vec{k}}$ [redacted] $e^{-iHt} e^{iHt'} c^{+}_{k} e^{-iHt'} \rangle - \Theta(t'-t) \langle e^{iHt'} c^{+}_{k} e^{-iHt'} e^{iHt} c_{k} e^{-iHt} \rangle$

$$= \Theta(t-t')\, e^{i E_0^{(N)}(t-t')} \langle c_{\vec{k}}\, e^{-iH(t-t')}\, c^{+}_{k} \rangle - \Theta(t'-t)\, e^{-i E_0^{(N)}(t'-t)} \langle c^{+}_{k}\, e^{-iH(t'-t)}\, c_{k} \rangle$$

Insertamos la identidad en el espacio de Fock:

Insertamos la identidad en el espacio de Fock:

$$\mathbb{1} = |vac\rangle\langle vac| + \sum_n |\psi_n^{(1)}\rangle\langle\psi_n^{(1)}| + \dots + \sum_n |\psi_n^{(N)}\rangle\langle\psi_n^{(N)}| + \dots$$

donde $|\Psi_n^{(N)}\rangle$ son las autofunciones del Hamiltoniano de un sistema de N partículas.

$$= \theta(t-t')\, e^{iE_0^N(t-t')} \sum_n \langle c_k\, e^{-iH(t-t')} |\psi_n^{N+1}\rangle\langle\psi_n^{N+1}| c_k^+ |\Phi\rangle - \theta(t'-t)\, e^{-iE_0^N(t-t')}$$

$$\times \sum_n \langle\Phi_H| c_k^+ e^{-iH(t'-t)} |\psi_n^{N-1}\rangle\langle\psi_n^{N-1}| c_k |\Phi_H^0\rangle$$

$$= \theta(t-t') \sum_n e^{i(E_0^{(N)} - E_n^{(N+1)})(t-t')} \langle\Phi^0| c_k |\psi_n^{N+1}\rangle\langle\psi_n^{N+1}| c_k^+ |\Phi^0\rangle - \theta(t'-t) \sum_n e^{-i(E_0^N - E_n^{N-1})(t-t')}$$

$$\times \sum_n \langle\Phi^0| c_k^+ |\psi_n^{N-1}\rangle\langle\psi_n^{N-1}| c_k |\Phi^0\rangle$$

$$= \theta(t-t')\, e^{iE_0^N(t-t')} \sum_n \langle c_k\, e^{-iH(t-t')} |\psi_n^{N+1}\rangle\langle\psi_n^{N+1}| c_k^+ |\Phi^0\rangle - \theta(t'-t)\, e^{-iE_0^N(t-t')}$$

$$\times \sum_n \langle \Phi_N | c_k^+ e^{-iH(t'-t)} |\psi_n^{N-1}\rangle\langle\psi_n^{N-1}| c_k |\Phi_N^0\rangle$$

$$= \theta(t-t') \sum_n e^{i(E_0^{(N)} - E_n^{(N+1)})(t-t')} \langle\Phi^0| c_k |\psi_n^{N+1}\rangle\langle\psi_n^{N+1}| c_k^+ |\Phi^0\rangle - \theta(t'-t) \sum_n e^{-i(E_0^N - E_n^{N-1})(t-t')}$$

$$\times \sum_n \langle\Phi^0| c_k^+ |\psi_n^{N-1}\rangle\langle\psi_n^{N-1}| c_k |\Phi^0\rangle$$

$$\theta(\tau) = \lim_{\eta\to 0^+} \frac{-1}{2\pi i} \int_{-\infty}^{\infty} d\omega\, \frac{e^{-i\omega\tau}}{\omega + i\eta}, \quad \theta(-\tau) = \lim_{\eta\to 0^+} \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega\, \frac{e^{-i\omega\tau}}{\omega - i\eta}$$

$$iG(\vec{k}, t-t') = i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sum_n \frac{e^{-i(\omega + E_n^{N+1} - E_0^N)(t-t')}}{\omega + i0^+} |\langle\psi_n^{N+1}| c_k^+ |\Phi^0\rangle|^2$$

$$+ i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sum_n \frac{e^{-i(\omega + E_0^N - E_n^{N-1})(t-t')}}{\omega + i0^+} |\langle\psi_n^{N-1}| c_k |\Phi^0\rangle|^2$$

$$iG(\vec{k}, t-t') = i \int_{-\infty}^{\infty} \frac{d\varpi}{2\pi} \sum_n \frac{e^{-i\left(\varpi + E_n^{N+1} - E_0^N\right)(t-t')}}{\varpi + i0^+} \left|\langle \Psi_n^{N+1} | c_k^+ | \Phi^0 \rangle\right|^2$$

$$+ i \int_{-\infty}^{\infty} \frac{d\varpi}{2\pi} \sum_n \frac{e^{-i\left(\varpi + E_0^N - E_n^{N+1}\right)(t-t')}}{\varpi + i0^+} \left|\langle \Psi_n^{N-1} | c_k | \Phi^0 \rangle\right|^2$$

Sustituyendo:

$$\omega \equiv \varpi + E_n^{N+1} - E_0^N \qquad \text{en la primera integral}$$

$$\omega \equiv \varpi + E_0^N - E_n^{N-1} \qquad \text{en la segunda integral}$$

$$iG(\vec{k}, t-t') = i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \left(\sum_n \frac{\left|\langle \Psi_n^{N+1} | c_k^+ | \Phi^0 \rangle\right|^2}{\omega - E_n^{N+1} + E_0^N + i0^+} + \sum_n \frac{\left|\langle \Psi_n^{N-1} | c_k | \Phi^0 \rangle\right|^2}{\omega + E_n^{N-1} - E_0^N - i0^+} \right)$$

Identificamos:

$\Rightarrow G(\vec{k}, \omega)$

Podemos reescribir los denominadores de la siguiente forma.

En la primera integral tenemos:

$$\omega - E_n^{(N+1)} + E_0^N + i\eta = \omega - \underbrace{\left(E_n^{(N+1)} - E_0^{(N+1)}\right)}_{w_n^{(N+1)} > 0} - \underbrace{\left(E_0^{(N+1)} - E_0^N\right)}_{\cong \left.\frac{\partial E_0}{\partial N}\right|_N = \mu^{(N)}} + i\eta$$

Y en la segunda integral:

$$\omega + E_n^{(N-1)} - E_0 - i\eta = \omega + \underbrace{\left(E_n^{(N-1)} - E_0^{(N-1)}\right)}_{w_n^{(N-1)}} - \underbrace{\left(E_0^N - E_0^{(N-1)}\right)}_{\mu^{(N-1)}} - i\eta.$$

Para N grande: $\mu^{(N)} \cong \mu^{(N-1)} \equiv \mu$ (cuando hay un gap de energía eso no vale)

Otro punto importante:

$\langle \Psi_n^{(N+1)} | c_{\mathbf{k}}^{\dagger} | \Psi_0 \rangle$ es no nulo sólo si $\Psi_n^{(N+1)}$ es autoestado del momento con $\mathbf{P}_n = \mathbf{k}$

Lo notamos como: $\Psi_n^{(N+1)}(\mathbf{k})$

Análogamente con $\langle \Psi_n^{(N-1)} | c_{\mathbf{k}} | \Psi_0 \rangle$

$\Psi_n^{(N-1)}$ tiene que tener momento $\mathbf{P}_n = -\mathbf{k}$

$\longrightarrow \Psi_n^{(N-1)}(-\mathbf{k})$

Juntando todo:

$$G(\mathbf{k},\omega) = \lim_{\eta\to 0^+} \frac{1}{\langle\Psi_0 \mid \Psi_0\rangle} \left\{ \sum_n \frac{\left|\langle\Psi_n^{(N+1)}(\mathbf{k}) \mid c_{\mathbf{k}}^{\dagger} \mid \Psi_0\rangle\right|^2}{\omega - \mu - w_{n,\mathbf{k}}^{(N+1)} + i\eta} + \sum_n \frac{\left|\langle\Psi_n^{(N-1)}(-\mathbf{k}) \mid c_{\mathbf{k}} \mid \Psi_0\rangle\right|^2}{\omega - \mu + w_{n,-\mathbf{k}}^{(N-1)} - i\eta} \right\}$$

Representación de Lehmann

Conclusión: la función de Green tiene polos en

$$\omega = \mu + w_{n,\mathbf{k}}^{(N+1)} - i\eta$$ ← de un sistema de N+1 partículas

$$\omega = \mu - w_{n,-\mathbf{k}}^{(N-1)} + i\eta$$ ← de un sistema de N-1 partículas

Llevándolo a la forma genérica:

$$G(\mathbf{k},\omega) = \lim_{\eta\to 0+} \int_0^\infty d\epsilon \left[\frac{A(\mathbf{k},\epsilon)}{\omega-\mu-\epsilon+i\eta} + \frac{B(\mathbf{k},\epsilon)}{\omega-\mu+\epsilon-i\eta}\right]$$

Obtenemos las siguientes **Funciones Espectrales**:

$$A(\mathbf{k},\epsilon) = \sum_n \frac{\left|\langle \Psi_n^{(N+1)}(\mathbf{k}) \mid c_{\mathbf{k}}^\dagger \mid \Psi_0\rangle\right|^2}{\langle \Psi_0 \mid \Psi_0\rangle} \delta(\epsilon - w_{n,\mathbf{k}}^{(N+1)})$$

$$B(\mathbf{k},\epsilon) = \sum_n \frac{\left|\langle \Psi_n^{(N-1)}(-\mathbf{k}) \mid c_{\mathbf{k}} \mid \Psi_0\rangle\right|^2}{\langle \Psi_0 \mid \Psi_0\rangle} \delta(\epsilon - w_{n,-\mathbf{k}}^{(N-1)})$$

- Las Funciones Espectrales son reales y positivas:

$$A^*(\mathbf{k},\epsilon) = A(\mathbf{k},\epsilon) \quad \geq \quad 0$$

$$B^*(\mathbf{k},\epsilon) = B(\mathbf{k},\epsilon) \quad \geq \quad 0.$$

- También se ve fácilmente que:

$$w_n^{(N\pm 1)} > 0 \quad \longrightarrow \quad A(\mathbf{k},\epsilon) = 0 = B(\mathbf{k},\epsilon) \text{ for } \epsilon < 0$$

- Se obtiene una “sum rule”:

$$\int_0^\infty \mathrm{d}\epsilon \, (A(\mathbf{k},\epsilon) + B(\mathbf{k},\epsilon)) = 1$$

Demostración:

Sum rule: $$\int_0^\infty d\epsilon\,(A(\mathbf{k},\epsilon)+B(\mathbf{k},\epsilon))=1$$

Teníamos: $$A(\mathbf{k},\epsilon)=\sum_n \frac{\left|\langle\Psi_n^{(N+1)}(\mathbf{k})\mid c_{\mathbf{k}}^\dagger\mid\Psi_0\rangle\right|^2}{\langle\Psi_0|\,\Psi_0\rangle}\delta(\epsilon-w_{n,\mathbf{k}}^{(N+1)})$$

$$\int d\epsilon\,A(\mathbf{k},\epsilon)=\sum_n\frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\langle\Psi_0\mid c_{\mathbf{k}}\mid\Psi_n^{(N+1)}\rangle\langle\Psi_n^{(N+1)}\mid c_{\mathbf{k}}^\dagger|\,\Psi_0\rangle$$

$$=\quad\frac{\langle\Psi_0\mid c_{\mathbf{k}}c_{\mathbf{k}}^\dagger|\,\Psi_0\rangle}{\langle\Psi_0|\,\Psi_0\rangle}=\frac{\langle\Psi_0\mid 1-c_{\mathbf{k}}^\dagger c_{\mathbf{k}}|\,\Psi_0\rangle}{\langle\Psi_0|\,\Psi_0\rangle}=1-\langle n_{\mathbf{k}}\rangle$$

Y análogamente se obtiene:

$$\int d\epsilon\,B(\mathbf{k},\epsilon)=\langle n_{\mathbf{k}}\rangle$$ ///

Para el gas de fermiones no interactuantes tenemos:

$$
\begin{aligned}
A(\mathbf{k},\epsilon) &= \theta(k-k_F)\delta(\epsilon-w_{\mathbf{k}}^{(N+1)}) &&= (1-\langle n_{\mathbf{k}}\rangle)\,\delta(\epsilon-w_{\mathbf{k}}^{(N+1)}) \\
B(\mathbf{k},\epsilon) &= \theta(k_F-k)\delta(\epsilon-w_{-\mathbf{k}}^{(N-1)}) &&= \langle n_{\mathbf{k}}\rangle\delta(\epsilon-w_{-\mathbf{k}}^{(N-1)}).
\end{aligned}
$$

Se satisface la *sum rule*?

Usando la definición:

$$G(\mathbf{k},\omega) = \lim_{\eta\to 0^+} \int_0^\infty d\epsilon \left[\frac{A(\mathbf{k},\epsilon)}{\omega-\mu-\epsilon+i\eta} + \frac{B(\mathbf{k},\epsilon)}{\omega-\mu+\epsilon-i\eta}\right]$$

Podemos volver al dominio tiempo en la función de Green:

$$\begin{aligned} iG(\mathbf{k},t-t') &= \theta(t-t')\int_0^\infty d\epsilon\, A(\mathbf{k},\epsilon)e^{-i(\epsilon+\mu)(t-t')} \\ &\quad -\theta(t'-t)\int_0^\infty d\epsilon\, B(\mathbf{k},\epsilon)e^{-i(\mu-\epsilon)(t-t')} \end{aligned}$$

Sale inmediatamente que:

$$\begin{aligned} \lim_{\tau\to 0^+} iG(\mathbf{k},\tau) &= \int_0^\infty d\epsilon\, A(\mathbf{k},\epsilon) = 1-\langle n_{\mathbf{k}}\rangle \\ \lim_{\tau\to 0^-} iG(\mathbf{k},\tau) &= -\int_0^\infty d\epsilon\, B(\mathbf{k},\epsilon) = -\langle n_{\mathbf{k}}\rangle. \end{aligned}$$

Util representación de la distribución de momentos $\langle n_{\mathbf{k}}\rangle$

Muestra Fermi edge

Notar la discontinuidad en el 0: $\lim_{\tau\to 0^+} G(\mathbf{k},\tau) - \lim_{\tau\to 0^-} G(\mathbf{k},\tau) = -i$

Estructura analítica de la función de Green

$$\lim_{\eta\to 0^+} \frac{1}{x - x_0 \pm i\eta} = P\frac{1}{x - x_0} \mp i\pi\delta(x - x_0)$$

$$\begin{aligned} G(\mathbf{k},\omega) &= \lim_{\eta\to 0^+}\left\{-\int_0^\infty \mathrm{d}\epsilon \frac{A(\mathbf{k},\epsilon)}{\epsilon-(\omega-\mu)-i\eta} + \int_0^\infty \mathrm{d}\epsilon \frac{B(\mathbf{k},\epsilon)}{\epsilon-(\mu-\omega)-i\eta}\right\} \\ &= P\int_0^\infty \mathrm{d}\epsilon \frac{A(\mathbf{k},\epsilon)}{\omega-\mu-\epsilon} + P\int_0^\infty \mathrm{d}\epsilon \frac{B(\mathbf{k},\omega)}{\omega-\mu+\epsilon} \\ &\quad -i\pi A(\mathbf{k},\omega-\mu) + i\pi B(\mathbf{k},\mu-\omega). \end{aligned}$$

Como A y B son reales sale que:

$$\operatorname{Re} G(\mathbf{k},\omega) = P\int_0^\infty \mathrm{d}\epsilon \frac{A(\mathbf{k},\epsilon)}{\omega-\mu\epsilon} + P\int_0^\infty \mathrm{d}\epsilon \frac{B(\mathbf{k},\epsilon)}{\omega-\mu+\epsilon}$$

cambia de signo en $\omega = \mu$

$$\operatorname{Im} G(\mathbf{k},\omega) = -\pi A(\mathbf{k},\omega-\mu) + \pi B(\mathbf{k},\mu-\omega) = \begin{cases} -\pi A(\mathbf{k},\omega-\mu) & \omega > \mu \\ +\pi B(\mathbf{k},\mu-\omega) & \omega < \mu \end{cases}$$

Porque: $A(\mathbf{k},\epsilon) = 0 = B(\mathbf{k},\epsilon)$ for $\epsilon < 0$

Despejando A y B tenemos:

$$A(\mathbf{k},\epsilon) = -\frac{1}{\pi}\mathrm{Im}\, G(\mathbf{k},\epsilon+\mu)$$

$$B(\mathbf{k},\epsilon) = +\frac{1}{\pi}\mathrm{Im}\, G(\mathbf{k},\mu-\epsilon)$$

Reemplazando en: $\mathrm{Re}\, G(\mathbf{k},\omega) = P\int_0^\infty \mathrm{d}\epsilon \frac{A(\mathbf{k},\epsilon)}{\omega-\mu\epsilon} + P\int_0^\infty \mathrm{d}\epsilon \frac{B(\mathbf{k},\epsilon)}{\omega-\mu+\epsilon}$ →

$$\mathrm{Re}\, G(\mathbf{k},\omega) = -\frac{1}{\pi}P\int_0^\infty \mathrm{d}\epsilon \frac{\mathrm{Im}\, G(\mathbf{k},\epsilon+\mu)}{\omega-\mu-\epsilon} + \frac{1}{\pi}P\int_0^\infty \mathrm{d}\epsilon \frac{\mathrm{Im}\, G(\mathbf{k},\mu-\epsilon)}{\omega-\mu+\epsilon}$$

$\epsilon_{new} = \mu+\epsilon_{old}$ $\epsilon_{new} = \mu-\epsilon_{old}$

$$\mathrm{Re}\, G(\mathbf{k},\omega) = -\frac{1}{\pi}P\int_\mu^\infty \mathrm{d}\epsilon \frac{\mathrm{Im}\, G(\mathbf{k},\epsilon)}{\omega-\epsilon} + \frac{1}{\pi}P\int_{-\infty}^\mu \mathrm{d}\epsilon \frac{\mathrm{Im}\, G(\mathbf{k},\epsilon)}{\omega-\epsilon}$$

Relación de dispersión

Supongamos que calculamos una función de Green aproximada.

En general no respetará la estructura analítica correcta, por ejemplo

que no se satisfaga

$$\mathrm{Re}\, G(\mathbf{k},\omega) = -\frac{1}{\pi} P \int_{\mu}^{\infty} \mathrm{d}\epsilon \, \frac{\mathrm{Im}\, G(\mathbf{k},\epsilon)}{\omega - \epsilon} + \frac{1}{\pi} P \int_{-\infty}^{\mu} \mathrm{d}\epsilon \, \frac{\mathrm{Im}\, G(\mathbf{k},\epsilon)}{\omega - \epsilon}.$$

Podríamos meterla acá y sacar las funciones espectrales:

$$A(\mathbf{k},\epsilon) = -\frac{1}{\pi} \mathrm{Im}\, G(\mathbf{k},\epsilon + \mu)$$

$$B(\mathbf{k},\epsilon) = +\frac{1}{\pi} \mathrm{Im}\, G(\mathbf{k},\mu - \epsilon)$$

satisface

Y recalcular la parte real de la G:

$$\mathrm{Re}\, G(\mathbf{k},\omega) = P \int_{0}^{\infty} \mathrm{d}\epsilon \, \frac{A(\mathbf{k},\epsilon)}{\omega - \mu\epsilon} + P \int_{0}^{\infty} \mathrm{d}\epsilon \, \frac{B(\mathbf{k},\epsilon)}{\omega - \mu + \epsilon}$$

Palabras finales

We will close this chapter with a remark on the theory of superconducting systems.

The single-particle Green's function is the expectation value $\langle\psi^\dagger\psi\rangle$ and $\langle\psi\psi^\dagger\rangle$, respectively.

In superconductors, on the other hand, expectation values of the type $\langle\psi^\dagger(\mathbf{r}'t')\psi^\dagger(\mathbf{r}t)\rangle$ and $\langle\psi(\mathbf{r}'t')\psi(\mathbf{r}t)\rangle$, the so-called anomalous propagators, are of fundamental importance.

The order parameter Δ is for example an expectation value of this sort.

The properties of the single-particle Green's function discussed here (analytic structure, equation of motion and diagrammatic expansion) can easily be carried over to the anomalous propagators.