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- Let's resume our discussion of the Green's function (from 135 and thereabouts...)

- We found that the Green's function can be used to calculate the ground state expectation value of (certain) observables.
  - What else can we learn from it?

- We will explore this issue by examining the <u>analytic structure</u> of the Green's function considered as a function of <u>frequency</u>.

- Recall the <u>noninteracting</u> Green's function

$$\boxed{\begin{aligned} iG^0_{\alpha\beta}(\vec{x}t,\vec{x}'t') &= \delta_{\alpha\beta}\frac{1}{V}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}\, e^{-i\omega_k^0(t-t')}\Big[\theta(t-t')\theta(|\vec{k}|-k_f) \\ &\qquad -\theta(t'-t)\theta(k_f-|\vec{k}|)\Big] \\ &\overset{V\to\infty}{=} \int\frac{d^3k}{(2\pi)^3}\int_{-\infty}^{\infty}d\omega\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}e^{-i\omega(t-t')}\left[\frac{\theta(|\vec{k}|-k_f)}{\omega-\omega_k^0+i\eta}+\frac{\theta(k_f-|\vec{k}|)}{\omega-\omega_k^0-i\eta}\right]\delta_{\alpha\beta}\end{aligned}}$$

Thus, the Fourier transform $\left(\omega_k^0 \equiv \epsilon_k^0 = \frac{k^2}{2m}\right)$

$$\boxed{G^0_{\alpha\beta}(\vec{k},\omega) = \frac{1}{\omega-\epsilon_k^0+i\eta\,\mathrm{sgn}(|\vec{k}|-k_f)}\delta_{\alpha\beta}} \qquad \boxed{\mathrm{sgn}(z) = \begin{cases} +1 & \text{if } z>0 \\ 0 & \text{if } z=0 \\ -1 & \text{if } z<0\end{cases}}$$

has simple poles with unit residue at the "on-shell" frequencies $\omega=\epsilon_k^0$.

- How should we interpret this and what is the generalization to the interacting Green's function, which for the spin-independent case takes the form (from the solution to Dyson's equation):

$$\boxed{G_{\alpha\beta}(\vec{k},\omega) = \frac{1}{\omega-\epsilon_k^0-\Sigma^*(\vec{k},\omega)}\delta_{\alpha\beta}} \quad ?$$

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- To proceed, we'll return to the definition of G in terms of Heisenberg field operators:

$$\boxed{iG_{\alpha\beta}(\vec{x}t, x't') = \langle \Psi_0^N | T[\hat{\psi}_{H\alpha}(\vec{x}t)\hat{\psi}^+_{H\beta}(\vec{x}'t')|\Psi_0^N\rangle}$$

- The "H" subscripts are a reminder that these are Heisenberg field operators with time dependence

$$\boxed{\hat{\psi}_{H\alpha}(\vec{x}t) = e^{i\hat{H}t}\hat{\psi}_\alpha(\vec{x})e^{-i\hat{H}t}} \quad \boxed{\hat{\psi}^+_{H\beta}(\vec{x}'t') = e^{i\hat{H}t'}\hat{\psi}^+_\beta(\vec{x}')e^{-i\hat{H}t'}}$$

- The eigenstates of $\hat{H}$ are labeled $|\Psi_n^N\rangle$ where "N" is the number of particles (fermions) and $n=0,1,2,\ldots$ labels the spectrum for a given N (with $n=0$ the ground state).

- If we insert a complete set of eigenstates between the operators, which will give a nonzero result?
  - That is, how many particles can be in the intermediate states?
  - We'll find out using the number operator $\hat{N}$:

$$\boxed{\hat{N} = \sum_\gamma \int d^3x\, \hat{\psi}^+_\gamma(\vec{x})\hat{\psi}_\gamma(\vec{x})}$$

  - So how many particles do the states $(\hat{\psi}^+_{H\beta}(\vec{x}'t')|\Psi_0^N\rangle)$ or $(\hat{\psi}_{H\alpha}(\vec{x}t)|\Psi_0^N\rangle)$ contain?
  - Let's first note that

$$\boxed{\begin{aligned}\hat{\psi}_{H\alpha}(\vec{x}t)|\Psi_0^N\rangle &= e^{i\hat{H}t}\hat{\psi}_\alpha(\vec{x})e^{-i\hat{H}t}|\Psi_0^N\rangle \\ &= e^{i(\hat{H}-E_0^N)t}\hat{\psi}_\alpha(\vec{x})|\Psi_0^N\rangle\end{aligned}}$$

where we'll label the eigenvalues of $\hat{H}$ as $\boxed{\hat{H}|\Psi_n^N\rangle = E_n^N|\Psi_n^N\rangle}$

$\Rightarrow$ we can isolate the time dependence trivially.

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- Since $\boxed{[\hat{N},\hat{H}]=0}$ (problem set #2), neither $\hat{H}$ nor $e^{i\hat{H}t}$ changes the number of particles, so we can simply ask about the number of particles in $\hat{\psi}_\alpha(\vec{x})|\Psi_0^N\rangle$.

$\Rightarrow$ What is $\hat{N}\left(\hat{\psi}_\alpha(\vec{x})|\Psi_0^N\rangle\right)$?

Just as in the homework,

$$\boxed{\hat{N}\hat{\psi}_\alpha(\vec{x}) = \hat{\psi}_\alpha\hat{N} - \hat{\psi}_\alpha(\vec{x})} \quad \left(\text{or } \boxed{[\hat{N},\hat{\psi}_\alpha(\vec{x})] = -\hat{\psi}_\alpha(\vec{x})}\right)$$

$$\text{or } \boxed{\begin{aligned}\hat{N}\left(\hat{\psi}_\alpha(\vec{x})|\Psi_0^N\rangle\right) &= \hat{\psi}_\alpha(\vec{x})(\hat{N}-1)|\Psi_0^N\rangle \\ &= (N-1)\left(\hat{\psi}_\alpha(\vec{x})|\Psi_0^N\rangle\right)\end{aligned}}$$

$\Rightarrow \left(\hat{\psi}_\alpha(\vec{x})|\Psi_0^N\rangle\right)$ is an eigenstate of the number operator with $N-1$ particles.

- This does not mean it is equal to $|\Psi_0^{N-1}\rangle$ or any of the other $|\Psi_n^{N-1}\rangle$, but it must be a combination of them.
- Similarly, $\hat{\psi}^\dagger_\alpha(\vec{x})$ increases the number of particles by precisely one (to $N+1$).

- So now we can insert appropriate intermediate states with each time ordering:

$$\boxed{\begin{aligned}iG_{\alpha\beta}(\vec{x}t,\vec{x}'t') = \sum_n\Big[&\theta(t-t')\langle\Psi_0^N|\hat{\psi}_\alpha(\vec{x})e^{i(E_0^N-\hat{H})t}|\Psi_n^{N+1}\rangle\langle\Psi_n^{N+1}|e^{i(\hat{H}-E_0^N)t'}\hat{\psi}^\dagger_\beta(\vec{x}')|\Psi_0^N\rangle \\ &-\theta(t'-t)\langle\Psi_0^N|\hat{\psi}^\dagger_\beta(\vec{x}')e^{i(E_0^N-\hat{H})t'}|\Psi_n^{N-1}\rangle\langle\Psi_n^{N-1}|e^{i(\hat{H}-E_0^N)t}\hat{\psi}_\alpha(\vec{x})|\Psi_0^N\rangle\Big] \\ = \sum_n\Big[&\theta(t-t')e^{-i(E_n^{N+1}-E_0^N)(t-t')}\langle\Psi_0^N|\hat{\psi}_\alpha(\vec{x})|\Psi_n^{N+1}\rangle\langle\Psi_n^{N+1}|\hat{\psi}^\dagger_\beta(\vec{x}')|\Psi_0^N\rangle \\ &-\theta(t'-t)e^{i(E_n^{N-1}-E_0^N)(t-t')}\langle\Psi_0^N|\hat{\psi}^\dagger_\beta(\vec{x}')|\Psi_n^{N-1}\rangle\langle\Psi_n^{N-1}|\hat{\psi}_\alpha(\vec{x})|\Psi_0^N\rangle\Big]\end{aligned}}$$

- Note that we have made manifest that it depends on $t-t'$ $\Rightarrow$ Fourier transform!

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Fourier transforms:

$$\boxed{\begin{aligned} G_{\alpha\beta}(\vec{x}t,\vec{x}'t') &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\, e^{-i\omega(t-t')}\, G_{\alpha\beta}(\vec{x},x';\omega) \\ G_{\alpha\beta}(\vec{x},\vec{x}';\omega) &= \int_{-\infty}^{\infty} d(t-t')\, e^{+i\omega(t-t')}\, G_{\alpha\beta}(\vec{x}t,\vec{x}'t') \end{aligned}}$$

To carry this out, we'll use

$$\boxed{\int_{-\infty}^{\infty} d(t-t')\ \theta(t-t')\, e^{-i(E_n^{N+1}-E_0^N)(t-t')}\, e^{i\omega(t-t')} = \frac{i}{\omega-(E_n^{N+1}-E_0^N)+i\eta}}$$

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

and the analogous formula for $\theta(t'-t)$.

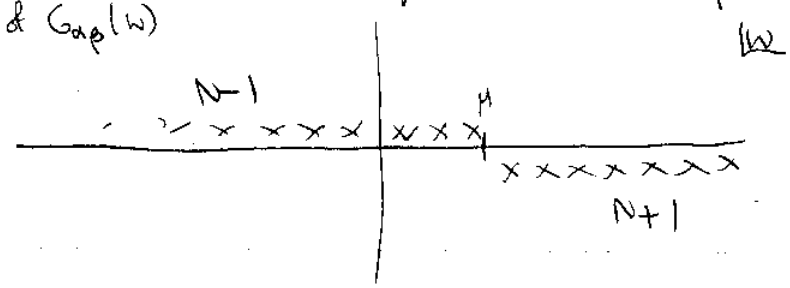
$$\Rightarrow \boxed{\begin{aligned} G_{\alpha\beta}(\vec{x},\vec{x}';\omega) = &\sum_n \frac{\langle\Psi_0^N|\hat\psi_\alpha(\vec{x})|\Psi_n^{N+1}\rangle\langle\Psi_n^{N+1}|\hat\psi_\beta^\dagger(\vec{x}')|\Psi_0^N\rangle}{\omega-(E_n^{N+1}-E_0^N)+i\eta} \\ &-\sum_n \frac{\langle\Psi_0^N|\hat\psi_\beta^\dagger(\vec{x}')|\Psi_n^{N-1}\rangle\langle\Psi_n^{N-1}|\hat\psi_\alpha(\vec{x})|\Psi_0^N\rangle}{\omega+(E_n^{N-1}-E_0^N)-i\eta} \end{aligned}}$$

which reveals the analytic structure in the (complex) ω plane:

- For each eigenstate $|\Psi_n^{N+1}\rangle$ of the $(N+1)$-particle system, there is a pole in the lower half plane at $\boxed{\omega = E_n^{N+1}-E_0^N}$ with residue $\boxed{\langle\Psi_0^N|\hat\psi_\alpha(\vec{x})|\Psi_n^{N+1}\rangle\langle\Psi_n^{N+1}|\hat\psi_\beta^\dagger(\vec{x}')|\Psi_n^0\rangle}$

- for each $N-1$ particle eigenstate $|\Psi_n^{N-1}\rangle$ the pole is at $-(E_n^{N-1}-E_0^N)$

poles of $G_{\alpha\beta}(\omega)$



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Now the chemical potential for the N+1 system is:
$\mu^{N+1} = E_0^{N+1} - E_0^{N}$ and $E_{n\neq 0}^{N+1} > E_0^{N+1}$, so the poles start at μ^{N+1} and go to $+\infty$ in the lower half plane.
Similarly, they go from $\mu^{N} = E_0^{N} - E_0^{N-1}$ to $-\infty$ in the upper half plane.

• We define $\boxed{\epsilon_n^{N+1} \equiv E_n^{N+1} - E_0^{N+1}}$, which is the excitation energy of the (N+1)-particle system and $\boxed{\epsilon_n^{N-1} = E_n^{N-1} - E_0^{N-1}}$, which is the excitation energy of the (N-1)-particle system

• For N large, $\mu^{N+1} = \mu^{N} = \mu$ up to $\mathcal{O}(\frac{1}{N})$ corrections, so the poles are at:

$$\boxed{\begin{aligned} \omega &= \mu + \epsilon_n^{N+1} - i\eta \\ \text{and} \quad \omega &= \mu - \epsilon_n^{N-1} + i\eta \end{aligned}}$$

so if we identify the location of poles, we find the excitation energies of the system with one more or one less particle.

• Now let's restrict our attention to uniform systems.
• Write the field operators in momentum representation:

$$\boxed{\hat{\psi}(\vec{x}) = \frac{1}{\sqrt{\Omega}} \sum_{\vec{k}\lambda} e^{i\vec{k}\cdot\vec{x}} a_{\vec{k}\lambda} \eta_\lambda} \quad \boxed{\hat{\psi}^\dagger(\vec{x}) = \frac{1}{\sqrt{\Omega}} \sum_{\vec{k}\lambda} e^{-i\vec{k}\cdot\vec{x}} a_{\vec{k}\lambda}^\dagger \eta_\lambda^\dagger}$$

• The momentum operators $\vec{P}$ is

$$\boxed{\vec{P} \equiv \int d^3x\, \psi_\alpha^\dagger(\vec{x}) (-i\hbar\vec{\nabla}) \hat{\psi}(\vec{x}) = \sum_{\vec{k}\lambda} \hbar\vec{k}\, a_{\vec{k}\lambda}^\dagger a_{\vec{k}\lambda}}$$

and $[\hat{H}, \vec{P}] = 0$, which means that the intermediate states $|\Psi_n^{N+1}\rangle$ and $|\Psi_n^{N-1}\rangle$ can be chosen as eigenstates of total momentum.

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- This means that

$$\boxed{\langle \Psi_0^N | a_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | a_{\vec{k}'}^{\dagger} e^{-i\vec{k}'\cdot\vec{x}'} | \Psi_0^N \rangle \propto \delta_{\vec{k}\vec{k}'}}$$

and $G(\vec{x},\vec{x}';\omega)$ is a function of $\vec{x}-\vec{x}'$ only (as expected).

- We can also derive this using $\boxed{\hat{\psi}(\vec{x}) = e^{-i\hat{\vec{p}}\cdot\vec{x}} \hat{\psi}_\alpha(0) e^{i\hat{\vec{p}}\cdot\vec{x}}}$

- In any case, we fourier transform $G(\vec{x}-\vec{x}';\omega)$ to get

$$\boxed{G(\vec{k},\omega) = \sum_n \frac{|\langle \Psi_n^{N+1}| a_{\vec{k}}^{\dagger} | \Psi_0^N \rangle|^2}{\omega - \mu - \epsilon_n^{N+1} + i\eta} + \frac{|\langle \Psi_n^{N-1} | a_{\vec{k}} | \Psi_0^N \rangle|^2}{\omega - \mu + \epsilon_n^{N-1} - i\eta}}$$

where we see that the residues are now positive-definite squares of matrix elements.

- We've suppressed the spin indices through all this; what is the matrix structure of $G_{\alpha\beta}(\vec{k},\omega)$?
  - For spin-1/2, $G_{\alpha\beta}$ is a two-by-two matrix, which has the <u>general</u> expression

$$\boxed{G_{\alpha\beta}(\vec{k},\omega) = a\,\delta_{\alpha\beta} + b(\vec{\sigma})_{\alpha\beta}\cdot\vec{k} = a\underline{\mathbb{1}} + b\vec{\sigma}\cdot\vec{k}}$$

since there is no preferred direction and $\vec{k}$ is the only variable available to combine with $\vec{\sigma}$.

$\therefore\ a = a(\vec{k}^2,\omega)\ ,\ b = b(\vec{k}^2,\omega)$

- If $\hat{H}$ has good parity ($\vec{x} \to -\vec{x}$), then G must have the property, but this means that $b \equiv 0$ and $G_{\alpha\beta} \propto \delta_{\alpha\beta}$ in general.

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- Let's check that the special case of $G^0(\vec{k},\omega)$ is reproduced.
  - In this case, $|\Psi_0^N\rangle = |F\rangle$ and $|\Psi_n^{N+1}\rangle$ is just an added particle above the fermi sea $\Rightarrow \theta(|\vec{k}|-k_f)$

- So the matrix elements are

$$\boxed{|\langle \Psi_n^{N+1}|a_{\vec{k}}^\dagger|\Psi_0^n\rangle|^2 = \theta(|\vec{k}|-k_f)}$$

and $\boxed{|\langle \Psi_n^{N-1}|a_{\vec{k}}|\Psi_0^n\rangle|^2 = \theta(k_f-|\vec{k}|)}$

Further, we have

$$\boxed{\begin{aligned} \omega-\mu-\epsilon_n^{N+1}+i\eta &= \omega-\epsilon_F^0-(\epsilon_k^0-\epsilon_F^0)+i\eta = \omega-\epsilon_k^0+i\eta \\ \omega-\mu+\epsilon_n^{N-1}+i\eta &= \omega-\epsilon_f^0+(\epsilon_F^0-\epsilon_k^0)-i\eta = \omega-\epsilon_k^0-i\eta \end{aligned}}$$

which yields

$$\boxed{G^0(\vec{k},\omega) = \left[\frac{\theta(k-k_f)}{\omega-\epsilon_k^0+i\eta} + \frac{\theta(k_f-k)}{\omega-\epsilon_k^0-i\eta}\right]}$$ as before.

- Side note: One often defines advanced and retarded functions that are analytic in the upper-half or lower-half planes, respectively by

$$\boxed{\begin{aligned} iG^R_{\alpha\beta}(\vec{x}t,\vec{x}'t') &= \langle\Psi_0|\{\hat{\psi}_{H\alpha}(\vec{x}t),\hat{\psi}^\dagger_{H\beta}(\vec{x}'t')\}|\Psi_0\rangle\,\theta(t-t') \\ iG^A_{\alpha\beta}(\vec{x}t,\vec{x}'t') &= -\langle\Psi_0|\{\hat{\psi}_{H\alpha}(\vec{x}t),\hat{\psi}^\dagger_{H\beta}(\vec{x}'t')\}|\Psi_0\rangle\,\theta(t'-t) \end{aligned}}$$

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- As our system gets large ($N \to \infty$), the poles in $G(\vec{k},\omega)$ become arbitrarily closely spaced
  - The uncertainty priciple says that if our observation lasts time T, we can only resolve $\Delta E \lesssim \hbar/T$
  - But the level spacing (pole spacing) $\Delta \mathcal{E} \ll \Delta E$ for large systems.

$\Rightarrow$ instead of individual levels, we see a <u>level density</u>, averaged over small energy intervals.

- Define the <u>spectral</u> <u>densities</u>

$$\boxed{\begin{aligned} \rho^+(\vec{k},\omega) &= \sum_n |\langle \Psi_n^{N+1} | a_{\vec{k}}^\dagger | \Psi_0^N \rangle|^2 \, 2\pi\delta(\epsilon_n^{N+1}-\omega) \\ \rho^-(\vec{k},\omega) &= \sum_n |\langle \Psi_n^{N-1} | a_{\vec{k}} | \Psi_0^N \rangle|^2 \, 2\pi\delta(\epsilon_n^{N-1}-\omega) \end{aligned}}$$

and

$$\boxed{\rho(\vec{k},\omega) = \theta(\omega)\rho^+(\vec{k},\omega) + \theta(-\omega)\rho^-(\vec{k},-\omega)}$$

- The Green's function then takes the form:

$$\boxed{G(\vec{k},\omega) = \int_0^\infty \frac{d\omega'}{2\pi}\left[\frac{\rho^+(\vec{k},\omega')}{\omega-\mu-\omega'+i\eta} + \frac{\rho^-(\vec{k},\omega')}{\omega-\mu+\omega'-i\eta}\right]}$$

which you can verify by plugging in ρ^+ and ρ^-.

- Note that G now has a branch cut along the entire real axis in the complex ω plane.
  - We can write dispersion relations for G, G^A, and G^R (see Negele and Orland, Chap. 5).

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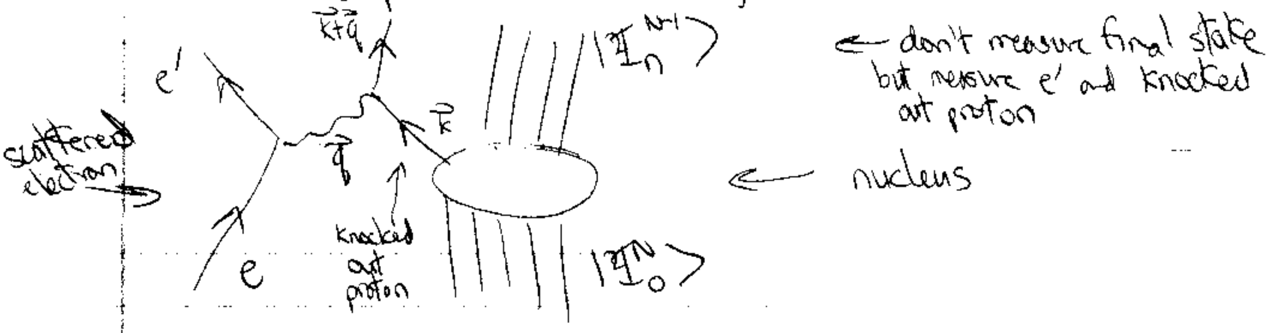
· Can we measure the spectral density?

Suppose we do semi-inclusive experiments, such as $(e,e'p)$ without looking at the final state:



If the impulse approximation is valid, which means we can neglect the interactions of the knocked out fermion (neglect "final state interactions"), then the removed proton must have had momentum $\vec{k}$ in the nucleus.

· The cross section σ is

$$\boxed{\begin{aligned}\sigma &= 2\pi \sum_n |\langle \Psi_n^{N-1}| a_{\vec{k}} |\Psi_0^N\rangle|^2 \delta(E_n^{N-1} + E_p - E_0^N - E_\gamma) \\ &= \rho^-(\vec{k}, E_\gamma + \mu^N - E_p)\end{aligned}}$$

· By varying the kinematics and adding corrections to the impulse approximation, we can extract ρ^-.

· (Caveat: EFT shows a limit to what can be extracted without relying on models.)