P 523

LECTURE 7

2. One-electron Green's function

$$G^{(N)}(\vec{p},t) = -i\langle \Psi_G^{(N)} | T[c_p(t)\, c_p^+(0)] | \Psi_G^{(N)} \rangle$$

Where $|\Psi_G^{(N)}\rangle$ is the ground state of N electrons described by H, and

$$T[c(t)\, c^+(t')] = \begin{cases} c(t)\, c^+(t') & \text{for } t > t' \\ -c^+(t')\, c(t) & \text{for } t < t' \end{cases}$$

notice the (-) sign for fermions.

• Important: Because electrons do not interact with one another in our model (e.g. no Culomb repulsion) it is sufficient to consider GF representing a single electron injected into an empty system:

$$G(\vec{p},t) = -i\langle 0 | T[c_p(t)\, c_p^+(0)] | 0 \rangle$$

"independent electron approximation" the same as one uses in band theory of solids.

∘ Calculate G:

$t>0$: $G(\vec{p},t) = -i \langle 0| e^{iHt} c_p e^{-iHt} c_p^{+} |0\rangle$

$= -i \langle 0| c_p e^{-iHt} c_p^{+} |0\rangle$

$\equiv -i \langle \vec{p}| e^{-iHt} |\vec{p}\rangle$

$e^{iHt}|0\rangle = |0\rangle$
since $a_p|0\rangle = 0$

$t<0$: $G(\vec{p},t) = +i \langle 0| c_p^{+} e^{-iHt} c_p e^{iHt} |0\rangle = 0$

Note that in this case we have

$$G(\vec{p},t) = G^R(\vec{p},t) \equiv -i\theta(t) \langle 0| \{ c_p(t), c_p^{+}(0) \} |0\rangle$$

notice the anticommutator

We will be interested in "density of one-electron states"

$$\rho(\varepsilon) = \sum_m \delta(\varepsilon - \varepsilon_m)$$

where ε_m are energy eigenvalues of H:

$$H|\Psi_m\rangle = \varepsilon_m |\Psi_m\rangle$$

This can be obtained from $G(\vec{p},t)$ by noticing

$t>0$: $\sum_p G(\vec{p},t) = -i \sum_p \langle \vec{p}| e^{-iHt} |\vec{p}\rangle = -i \, Tr(e^{-iHt})$

$$= -i \sum_m \langle \Psi_m | e^{-iHt} | \Psi_m \rangle$$

$$= -i \sum_m e^{-i\varepsilon_m t} \underbrace{\langle \Psi_m | \Psi_m \rangle}_{1}$$

Tr is invariant under change of basis

Introduce FT in time:

$$G(\vec{p}, \varepsilon) = \int_{-\infty}^{\infty} dt\, e^{i\varepsilon t}\, G(\vec{p}, t)$$

$$\sum_p G(\vec{p}, \varepsilon) = \int_0^{\infty} dt\, e^{i\varepsilon t} \sum_m \left(-i e^{-i\varepsilon_m t}\right) e^{-\eta t}$$

$$= -i \sum_m \int_0^{\infty} dt\, e^{i(\varepsilon - \varepsilon_m + i\eta)t}$$

$$= \sum_m \frac{1}{\varepsilon - \varepsilon_m + i\eta} \qquad / \mathrm{Im}$$

$\eta > 0$ infinitesimal convergence factor

$$\mathrm{Im} \sum_p G(\vec{p}, \varepsilon) = -\pi \sum_m \delta(\varepsilon - \varepsilon_m)$$

$$\boxed{\rho(\varepsilon) = -\frac{1}{\pi}\, \mathrm{Im}\, G(\vec{p}, \varepsilon)}$$

Calculation of $G(\vec{p},t)$

To set up an Equation of motion we define

$$F(\vec{p},\vec{p}\,';t) = -i\langle 0|T[c_p(t)\,c^+_{p'}(0)]|0\rangle$$

$$G(\vec{p},t) = F(\vec{p},\vec{p};t)$$

$$i\frac{\partial}{\partial t}F(\vec{p},\vec{p}\,';t) = i\delta(t)\left[F(\vec{p},\vec{p}\,';0^+) - F(\vec{p},\vec{p}\,';0^-)\right]$$
$$-i\langle 0|T[[c_p(t),H]\,c^+_{p'}(0)]|0\rangle$$

(i) $$F(p,p';0^+) - F(p,p';0^-) = -i\langle 0|c_p c^+_{p'} + c^+_{p'}c_p|0\rangle$$
$$= -i\langle 0|\delta_{pp'}|0\rangle = -i\delta_{pp'}$$

(ii) $$[c_p, H] = \varepsilon_p c_p + \sum_q U(\vec{q})\,c_{p+q}$$ (by direct calculation)

$\Downarrow$

$$\boxed{\left(i\frac{\partial}{\partial t} - \varepsilon_p\right)F(p,p';t) = \delta_{pp'}\delta(t) + \sum_q U(q)\,F(p+q,p';t)} \quad (*)$$

- We are going to solve for $F(p,p';t)$ by transforming into an integral equation and iterating.

• <u>Zero-order</u>: $F^0(p,p';t) = \delta_{pp'}\, G^0(p,t)$

Solving directly for $G^0(p,t) = -i \langle 0| T[c_p(t)\, c_p^+(0)] |0\rangle$ with $H_0 = \sum_p \varepsilon_p c_p^+ c_p$ we find

$$\boxed{G^0(p,t) = -i\,\theta(t)\, e^{-i\varepsilon_p t}}$$

• <u>Integral equation</u>

$$\boxed{F(p,p';t) = \delta_{pp'}\, G^0(p,t) + \int_{-\infty}^{\infty} dt'\, G^0(p,t-t') \sum_q U(q)\, F(p+q,p';t)}$$

- check by substituting into (*) and using the fact that G^0 satisfies $\left(i\frac{\partial}{\partial t} - \varepsilon_p\right) G^0(p,t) = \delta(t)$.

• Simplify by Fourier transforming in time:

$$F(p,p';t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\varepsilon\, e^{-i\varepsilon t}\, F(p,p';\varepsilon)$$

$$G^0(p,\varepsilon) = \int_{-\infty}^{\infty} dt\, e^{i\varepsilon t - \delta t}\, G^0(p,t) = \frac{1}{\varepsilon - \varepsilon_p + i\delta}$$

$$\boxed{F(p,p';\varepsilon) = \delta_{pp'}\, G^0(p,\varepsilon) + G^0(p,\varepsilon) \sum_q U(q-p)\, F(q,p';\varepsilon)} \quad (**)$$

BORN SERIES: Iterative solution of Eq. (**)

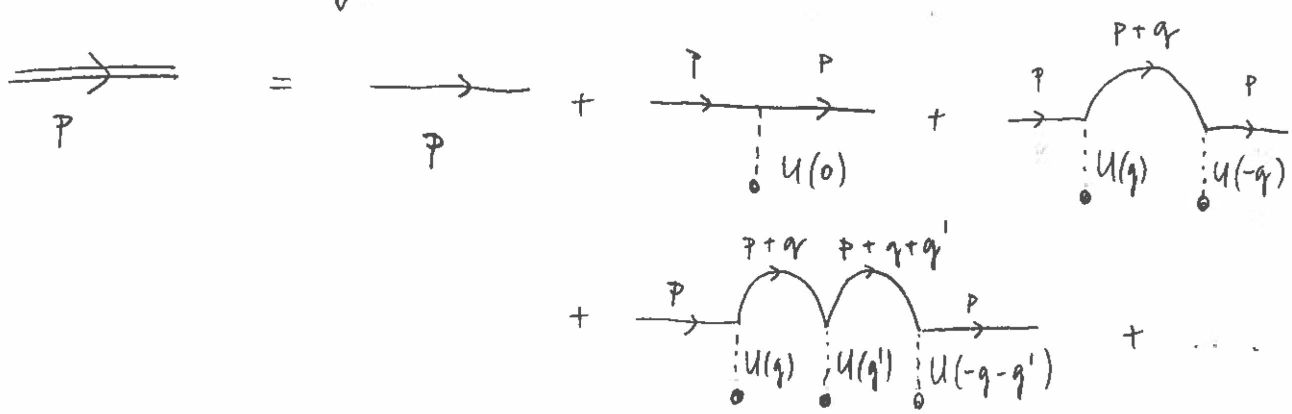
Write $F(p,p') = \sum_{n=0}^{\infty} F^{(n)}(p,p')$ $\qquad F^{0}(p,p') = \delta_{pp'}\, G(p)$

$$F^{(n)}(p,p') = G^{0}(p) \sum_{q} U(q-p)\, F^{(n-1)}(q,p') \qquad n = 1, 2 \ldots$$

For $G(p) = F(p,p)$ we thus obtain:

$$\boxed{\begin{aligned} G(p) = \; & G^{0}(p) + G^{0}(p)\, U(0)\, G^{0}(p) \\ & + G^{0}(p) \sum_{q} U(q)\, G^{0}(p+q)\, U(-q)\, G^{0}(p) + \ldots \end{aligned}}$$

Diagrammatically this can be represented as



Feynman diagrams in frequency space (ε = frequency or energy)

- The T-matrix expansion

$$G(p) = G^0(p) + G^0(p)\, T(p)\, G^0(p) = G^0(p)\left[1 + T(p)\, G^0(p)\right]$$

$$T(p) = U(0) + \sum_q U(q)\, G^0(p+q)\, U(-q) + \cdots$$

$=$ 

Closed solution for short-range potential

Assume $U(\vec{x}) = U\,\delta(\vec{x}) \;\longrightarrow\; U(\vec{q}) = \dfrac{U}{V}$ ← system volume

Analyze $T(p)$

2nd order $\quad \left(\dfrac{U}{V}\right)^2 \sum_q G^0(p+q) = \left(\dfrac{U}{V}\right)^2 V\, g_0(\varepsilon)$

$$g_0(\varepsilon) = \frac{1}{V}\sum_q G^0(q)$$

3rd order $\quad \left(\dfrac{U}{V}\right)^3 \sum_{q,q'} G^0(p+q)\, G^0(p+q+q') \qquad q' \to q' - p - q$, $\quad q \to q - p$

$$= \left(\frac{U}{V}\right)^3 \left[V\, g_0(\varepsilon)\right]^2$$

$$T(p) = \sum_{n=0}^{\infty} \left(\frac{U}{V}\right)^{n+1} \left[V g_0(\varepsilon)\right]^n = \frac{U}{V} \sum_{n=0}^{\infty} \left[U g_0(\varepsilon)\right]^n$$

$$= \frac{U}{V} \frac{1}{1 - U g_0(\varepsilon)}$$

$$G(p,\varepsilon) = G^0(p,\varepsilon)\left[1 + \frac{U}{V} \frac{G^0(p,\varepsilon)}{1 - U g_0(\varepsilon)}\right]$$