LECTURE 1

Why Green's functions?

I. The ground state energy as an integral over coupling constant.

Consider Hamiltonian $H(\lambda) = H_0 + \lambda H_1$

$$H(\lambda)\,|\Psi_G\rangle = E_G\,|\Psi_G\rangle$$

functions of λ

$$E_G(\lambda) = \langle \Psi_G(\lambda)|\,H(\lambda)\,|\Psi_G(\lambda)\rangle$$

$$\underline{\frac{\partial E_G}{\partial\lambda}} = \langle \Psi_G(\lambda)|H_1|\Psi_G(\lambda)\rangle + \left\langle \frac{\partial \Psi_G(\lambda)}{\partial\lambda}\right|H(\lambda)\left|\Psi_G(\lambda)\right\rangle$$

$$+ \left\langle \Psi_G(\lambda)\right|H(\lambda)\left|\frac{\partial\Psi_G(\lambda)}{\partial\lambda}\right\rangle$$

$$= \underline{\langle\Psi_G|H_1|\Psi_G\rangle} + E_G\underbrace{\left[\left\langle\frac{\partial\Psi_G}{\partial\lambda}\middle|\Psi_G\right\rangle + \left\langle\Psi_G\middle|\frac{\partial\Psi_G}{\partial\lambda}\right\rangle\right]}_{0}$$

$$\frac{\partial}{\partial\lambda}\langle\Psi_G|\Psi_G\rangle = \frac{\partial}{\partial\lambda}1 = 0$$

normalization

So, we can obtain E_G by integration:

$$\boxed{\Delta E_G = E_G(1) - E_G(0) = \int_0^1 d\lambda\,\frac{\partial E_G(\lambda)}{\partial\lambda} = \int_0^1 d\lambda\,\langle\Psi_G(\lambda)|H_1|\Psi_G(\lambda)\rangle}$$

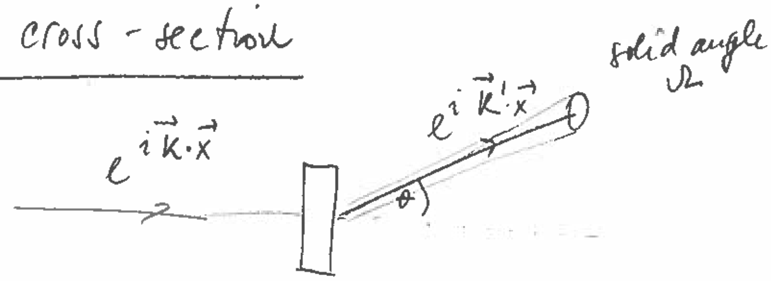
For lattice vibrations [Eq 1.1.6 from the book]

$$H_1 = \frac{1}{2} M \sum_{i \neq j} D_{ij} \cdot u_i u_j$$

So

$$\boxed{\Delta E_G = \frac{1}{2} M \sum_{i \neq j} D_{ij} \int_0^1 d\lambda \, \langle \Psi_G(\lambda) | u_i u_j | \Psi_G(\lambda) \rangle}$$

II. The neutron scattering cross-section



$$\frac{d^2\sigma}{d\Omega \, d\omega} = \sum_F \frac{K'}{K} \left(\frac{M}{2\pi} \right)^2$$

$$|\langle K' \psi_F | H' | K \psi_G \rangle|^2 \, \delta(\omega + E_G - E_F)$$

interaction between neutron and target

ground state and final state energies

energy supplied by neutron ($\hbar = 1$)

We assume

$$H' = \sum_j V(\vec{x} - \vec{X}_j) \qquad \vec{X}_j \text{ - ionic positions}$$

$$\langle K' \psi_F | H' | K \psi_G \rangle = \langle \psi_F | \int d^3x \, e^{i\vec{q}\cdot\vec{x}} H' | \psi_G \rangle$$

$$= V_q \sum_j \langle \psi_F | e^{i\vec{q}\cdot\vec{X}_j} | \psi_G \rangle \qquad \vec{q} = \vec{K} - \vec{K}'$$

$$V_q = \int d^3x \, e^{i\vec{q}\cdot\vec{x}} \, V(\vec{x})$$

$$\frac{d^2\sigma}{d\Omega d\omega} = \sum_F \frac{k'}{k}\left(\frac{M}{2\pi}\right)^2 |V_q|^2 \sum_{j,\ell} \langle \psi_G | e^{-i\vec{q}\cdot\vec{X}_j} | \psi_F \rangle \langle \psi_F | e^{i\vec{q}\cdot\vec{X}_\ell} | \psi_G \rangle$$
$$\otimes\, \delta(\omega + E_G - E_F)$$

Use integral representation of δ-function

$$\delta(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega t}\,dt \quad \Rightarrow \quad \delta(\omega + E_G - E_F) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(\omega + E_G - E_F)t}\,dt$$

Consider term

$$e^{i(E_G - E_F)t}\langle \psi_G | e^{-i\vec{q}\cdot\vec{X}_j} | \psi_F \rangle = \langle \psi_G | e^{iHt}\, e^{-i\vec{q}\cdot\vec{X}_j}\, e^{-iHt} | \psi_F \rangle$$
$$= \underline{\langle \psi_G | e^{-i\vec{q}\,\vec{X}_j(t)} | \psi_F \rangle}$$

$$\vec{X}_j(t) \equiv e^{iHt}\, \vec{X}_j\, e^{-iHt}$$

$\vec{X}_j$ operator in Heisenberg picture.

- Use completness of states $\sum_F |\psi_F\rangle\langle\psi_F| = 1$ to perform sum on F:

$$\boxed{\frac{d^2\sigma}{d\Omega d\omega} = \frac{k'}{2\pi k}\left(\frac{M}{2\pi}\right)^2 |V_q|^2 \int_{-\infty}^{\infty} dt\, e^{i\omega t} \underbrace{\sum_{j\ell} \langle \psi_G | e^{-i\vec{q}\cdot\vec{X}_j(t)}\, e^{i\vec{q}\cdot\vec{X}_\ell(0)} | \psi_G \rangle}_{F(\vec{q},t)}}$$

For small vibration we write

$$\vec{X}_j(t) = \underset{\substack{\uparrow \\ \text{equilibrium position}}}{\vec{R}_j} + \vec{u}_j(t) \leftarrow \text{small vibration}$$

• Expand to leading order in $\vec{u}$.

$$F(\vec{q},t) \simeq F_0(\vec{q}) + q^2 \sum_{je} e^{i\vec{q}\cdot(\vec{R}_e-\vec{R}_j)} \underbrace{\langle \psi_G | u_j(t)\, u_e(0) | \psi_G \rangle}$$

(we assumed longitudinal polarization $\vec{u}_j \cdot \vec{q} = q u_j$).

The Green's function and its equation of motion

Schr. picture: $\quad i \dfrac{\partial |\Psi_s\rangle}{\partial t} = H |\Psi_s\rangle$, $\quad O_s$ - time indep.

Heisenberg picture: $\quad i \dfrac{d O_H}{dt} = [O_H, H]$

$$O_H(t) = e^{iH(t-t_0)}\, O_s\, e^{-iH(t-t_0)}$$

• Definition of the Green's function (or propagator):

$$G_{ij}(t,t') = G_{ij}(t-t') = -i \langle T[u_i(t)\, u_j(t')] \rangle_\lambda$$

Here $H = H_0 + \lambda H_1$ and $\langle \dots \rangle_\lambda = \langle \psi_G(\lambda) | \dots | \psi_G(\lambda) \rangle$

T - "time ordering operator" (invented by Dyson)

$$T[A(t)\, B(t')] = \begin{cases} A(t)\, B(t') & t > t' \\ B(t')\, A(t) & t < t' \end{cases}$$

$G_{ij}(t-t')$ is called "time ordered" or "causal" GF. It is useful for approximate analytical calculations as we shall see.

- We define two more GFs:

$$G^R_{ij}(t-t') = -i\theta(t-t')\langle [u_i(t), u_j(t')]\rangle_\lambda \qquad \text{"Retarded"}$$

$$G^A_{ij}(t-t') = i\theta(t'-t)\langle [u_i(t), u_j(t')]\rangle_\lambda \qquad \text{"Advanced"}$$

- these will be more closely related to physical observables.

$G_{ij}(t)$ can be used to find ΔE_c and $F(q,t)$:

$$\Delta E_c = \lim_{t\to 0^+} \frac{1}{2} i M \sum_{i\neq j} D_{ij} \int_0^1 d\lambda\, G_{ij}(t)$$

$$F(q,t) \simeq i q^2 \sum_{je} e^{i\vec{q}\cdot(\vec{R}_e-\vec{R}_j)} G_{je}(t)$$

Equation of motion for G:

$$\boxed{H = \sum_i \left[\frac{p_i^2}{2M} + \frac{1}{2} M \Omega^2 u_i^2 \right] + \frac{1}{2} M \sum_{i \neq j} D_{ij}\, u_i u_j}$$

$$T\left[u_i(t)\, u_j(0)\right] = \theta(t)\, u_i(t)\, u_j(0) + \theta(-t)\, u_j(0)\, u_i(t)$$

$$i \frac{d G_{ij}(t)}{dt} = \underbrace{\delta(t) \langle u_i(t)\, u_j(0) - u_j(0)\, u_i(t) \rangle}_{0 \text{ because } [u_i, u_j] = 0} + \left\langle T\left[\frac{d u_i(t)}{dt} u_j(0) \right] \right\rangle$$

Work out the last term:

$$\frac{d u_i(t)}{dt} = [u_i, H] = e^{iHt} [u_i, H] e^{-iHt} = e^{iHt} \left[u_i, \frac{1}{2M} \sum_j p_j^2 \right] e^{-iHt}$$

use $[u_i, p_j] = i \delta_{ij}$

$$\frac{d u_i(t)}{dt} = e^{iHt} \frac{i p_i}{M} e^{-iHt} = \frac{i p_i(t)}{M}$$

$$\boxed{i \frac{d G_{ij}(t)}{dt} = \frac{1}{M} \langle T[p_i(t)\, u_j(0)] \rangle}$$

- Take another derivative $\frac{d}{dt}$ and follow the same steps to finally find (book Eqs. 1.4.13-14):

$$\boxed{\left(-\frac{d^2}{dt^2} - \Omega_0^2\right) G_{ij}(t) = \frac{1}{M} \delta_{ij}\, \delta(t) + \lambda \cdot \sum_k D_{ik}\, G_{kj}(t)}$$