Quantum Theory of Many-Body systems in Condensed Matter (4302112) 2020

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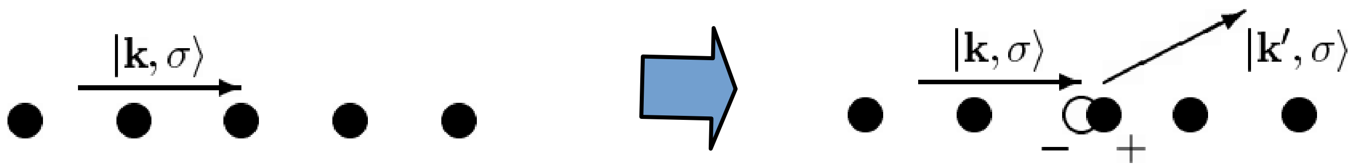
Today’s class: *Phonon Green’s functions*

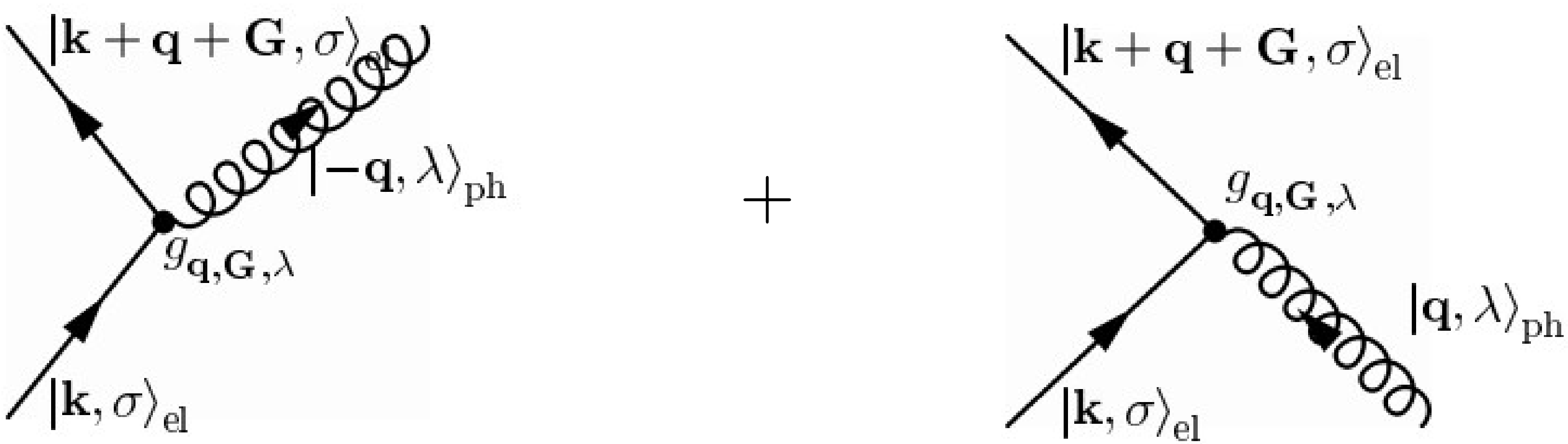
- Free phonon propagator.
- Electron-phonon vertex.
- Phonon-mediated electron-electron interaction.

Review: Electron-phonon interaction



Electron-phonon vertex:

$$\hat{H}_{\mathrm{el-ph}} = \frac{1}{V_{\mathbf{r}}} \sum_{\mathbf{k},\sigma,\mathbf{q}} g_{\mathbf{q}} \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma} \hat{c}_{\mathbf{k},\sigma} \left(\hat{b}^{\dagger}_{-\mathbf{q}} + \hat{b}_{\mathbf{q}} \right) \qquad g_{\mathbf{q}} = ie\sqrt{\frac{N\hbar}{2M\omega_q}} qV(\mathbf{q})$$



Free phonon propagator

$$\hat{H}_{\rm ph} = \sum_{\mathbf{q}} \Omega_{\mathbf{q}} \left(\hat{b}^\dagger_{\mathbf{q}} \hat{b}_{\mathbf{q}} + 1/2 \right)$$

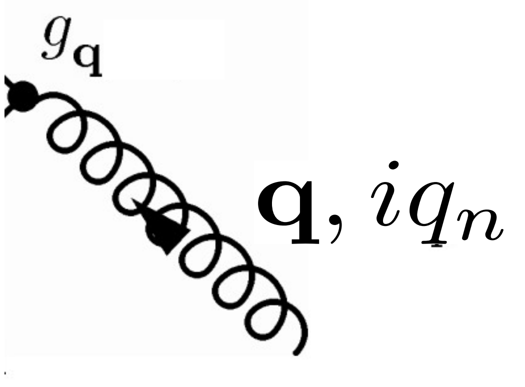
Free-phonon Hamiltonian

$$\left.\begin{aligned} \hat{A}_{\mathbf{q}} &\equiv \hat{b}^\dagger_{-\mathbf{q}} + \hat{b}_{\mathbf{q}} \\ \hat{A}^\dagger_{\mathbf{q}} &= \hat{A}_{-\mathbf{q}} \end{aligned}\right\} \Rightarrow \left\{\begin{aligned} &\hat{A}_{\mathbf{q}}(\tau) = e^{\hat{H}_{\rm ph}\tau} \hat{A}_{\mathbf{q}} e^{-\hat{H}_{\rm ph}\tau} \\ &D^{(0)}(\mathbf{q}, \tau - \tau') \equiv -\left\langle \mathcal{T}_\tau \left[\hat{A}_{\mathbf{q}}(\tau) \hat{A}_{-\mathbf{q}}(\tau') \right] \right\rangle \end{aligned}\right.$$

Free-phonon propagator

$$D^{(0)}(\mathbf{q}, iq_n) = \int_0^\beta d\tau \; D^{(0)}(\mathbf{q}, \tau) e^{iq_n \tau}$$

Bosonic Matsubara frequencies $\quad q_n = 2n\frac{\pi}{\beta}$



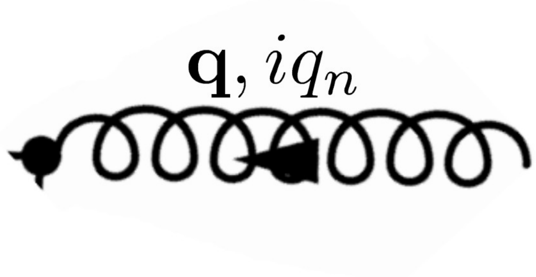
Calculation of $D^{(0)}(\mathbf{q},\tau)$ and $D^{(0)}(\mathbf{q},iq_n)$

$$\hat{H}_{\mathrm{ph}} = \sum_{\mathbf{q}} \Omega_{\mathbf{q}} \left(\hat{b}^{\dagger}_{\mathbf{q}} \hat{b}_{\mathbf{q}} + 1/2 \right) \qquad D^{(0)}(\mathbf{q},\tau) = -\left\langle \mathcal{T}_{\tau} \left[\hat{A}_{\mathbf{q}}(\tau) \hat{A}_{-\mathbf{q}}(0) \right] \right\rangle$$

$$D^{(0)}(\mathbf{q},\tau) = \begin{cases} -\left(1 + n_B(\Omega_{\mathbf{q}})\right) e^{-\Omega_{\mathbf{q}}\tau} - n_B(\Omega_{\mathbf{q}}) e^{+\Omega_{\mathbf{q}}\tau} & \tau > 0 \\ -n_B(\Omega_{\mathbf{q}}) e^{-\Omega_{\mathbf{q}}\tau} - \left(1 + n_B(\Omega_{\mathbf{q}})\right) e^{+\Omega_{\mathbf{q}}\tau} & \tau < 0 \end{cases}$$

$$D^{(0)}(\mathbf{q},iq_n) = \int_0^{\beta} d\tau \; D^{(0)}(\mathbf{q},\tau) e^{iq_n\tau} \qquad q_n = \frac{2\pi}{\beta} n$$

$$D^{(0)}(\mathbf{q},iq_n) = \frac{2\Omega_{\mathbf{q}}}{(iq_n)^2 - \Omega_{\mathbf{q}}^2}$$



Electron Matsubara Green's function

$$\hat{H} = \hat{H}_0 + \hat{H}_{\mathrm{el-ph}} \begin{cases} \hat{H}_0 = \sum_{\mathbf{k},\sigma} \epsilon_k \hat{c}^\dagger_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma} + \sum_{\mathbf{q}} \Omega_{\mathbf{q}} \left(\hat{b}^\dagger_{\mathbf{q}}\hat{b}_{\mathbf{q}} + 1/2\right) \\ \hat{H}_{\mathrm{el-ph}} = \frac{1}{V_{\mathbf{r}}} \sum_{\mathbf{k},\sigma,\mathbf{q}} g_{\mathbf{q}} \hat{c}^\dagger_{\mathbf{k}+\mathbf{q},\sigma}\hat{c}_{\mathbf{k},\sigma}\hat{A}_{\mathbf{q}} \end{cases}$$

Matsubara Green's function: $\mathcal{G}_\sigma(\mathbf{k},\tau) = -\left\langle \mathcal{T}_\tau \left[\hat{c}_{\mathbf{k},\sigma}(\tau)\hat{c}^\dagger_{\mathbf{k},\sigma}(0)\right]\right\rangle$

Perturbative expansion (Feynman diagrams):

$$\mathcal{G}_\sigma(\mathbf{k},\tau) = -\frac{\sum_{m=0}^{\infty} \frac{(-1)^m}{m!} \int_0^\beta d\tau_1 \ldots d\tau_m \left\langle \mathcal{T}_\tau \left[\hat{H}_{\mathrm{el-ph}}(\tau_1)\ \ldots \hat{H}_{\mathrm{el-ph}}(\tau_m)(\hat{c}_{\mathbf{k},\sigma})_I(\tau)(\hat{c}^\dagger_{\mathbf{k},\sigma})_I(0)\right]\right\rangle}{\sum_{m=0}^{\infty} \frac{(-1)^m}{m!} \int_0^\beta d\tau_1 \ldots d\tau_m \left\langle \mathcal{T}_\tau \left[\hat{H}_{\mathrm{el-ph}}(\tau_1)\ \ldots \hat{H}_{\mathrm{el-ph}}(\tau_m)\right]\right\rangle}$$

Effective electron-electron interaction

We can write the electron Green's functions as an effective perturbative expansion in H_1:

$$\mathcal{G}_\sigma(\mathbf{k},\tau) = -\frac{\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \dots d\tau_n \left\langle \mathcal{T}_\tau \left[\hat{H}_1(\tau_1) \ \dots \hat{H}_1(\tau_n) (\hat{c}_{\mathbf{k},\sigma})_I(\tau)(\hat{c}^\dagger_{\mathbf{k},\sigma})_I(0) \right] \right\rangle}{\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \dots d\tau_n \left\langle \mathcal{T}_\tau \left[\hat{H}_1(\tau_1) \ \dots \hat{H}_1(\tau_n) \right] \right\rangle}$$

where H_1 is quartic (two-body interaction) in electron operators:

[redacted]

$$\int_0^\beta \hat{H}_1(\tau_i) d\tau_i = \frac{1}{2} \int_0^\beta d\tau_i \int_0^\beta d\tau_j \sum_{\substack{\mathbf{k}_1\sigma_1 \\ \mathbf{k}_2\sigma_2 \\ \mathbf{q}}} V_{\text{eff}}(\mathbf{q},\tau_i-\tau_j) \hat{c}^\dagger_{\mathbf{k}_1+\mathbf{q},\sigma_1}(\tau_j) \hat{c}^\dagger_{\mathbf{k}_2-\mathbf{q},\sigma_2}(\tau_i) \hat{c}_{\mathbf{k}_2,\sigma_2}(\tau_i) \hat{c}_{\mathbf{k}_1,\sigma_1}(\tau_j)$$

Phonon-mediated electron-electron interaction:

$$\boxed{V_{\text{eff}}(\mathbf{q},\tau_i-\tau_j) \equiv \frac{1}{V_{\mathbf{r}}^2} |g_{\mathbf{q}}|^2 D^{(0)}(\mathbf{q},\tau_i-\tau_j)}$$