

Title: PSI 2018/2019 - Condensed Matter - Lecture 6

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Abstract:

Hartree-Fock theory

$$H = H_0 + V_{int}$$

$$H_0 = \sum_{\nu} \epsilon_{\nu} c_{\nu}^{\dagger} c_{\nu}$$

$$V_{int} = \frac{1}{2} \sum_{\substack{\nu, \mu \\ \nu', \mu'}} V_{\nu\mu}^{\nu'\mu'} c_{\nu}^{\dagger} c_{\mu}^{\dagger} c_{\mu'} c_{\nu'}$$

$$c_{\nu}^{\dagger} c_{\mu}^{\dagger} c_{\mu'} c_{\nu'} = c_{\nu}^{\dagger} \underbrace{(c_{\mu}^{\dagger} c_{\mu'} - \langle c_{\mu}^{\dagger} c_{\mu'} \rangle)}_{d_{\mu\mu'}} + \underbrace{\langle c_{\mu}^{\dagger} c_{\mu'} \rangle}_{d_{\mu\mu'}} c_{\nu'}$$

$$= (d_{\mu\mu'} + \langle c_{\mu}^{\dagger} c_{\mu'} \rangle) \underbrace{(c_{\nu}^{\dagger} c_{\nu'} - \langle c_{\nu}^{\dagger} c_{\nu'} \rangle)}_{d_{\nu\nu'}} + \underbrace{\langle c_{\nu}^{\dagger} c_{\nu'} \rangle}_{d_{\nu\nu'}} = d_{\mu\mu'} d_{\nu\nu'} + d_{\mu\mu'} \langle c_{\nu}^{\dagger} c_{\nu'} \rangle + d_{\nu\nu'} \langle c_{\mu}^{\dagger} c_{\mu'} \rangle$$

$$\langle c_\nu^\dagger c_\mu^\dagger c_{\mu'} c_{\nu'} \rangle = \langle c_\nu^\dagger c_{\nu'} \rangle \langle c_\mu^\dagger c_{\mu'} \rangle - \langle c_\nu^\dagger c_{\mu'} \rangle \langle c_\mu^\dagger c_{\nu'} \rangle$$

$$\begin{aligned} c_\nu^\dagger c_\mu^\dagger c_{\mu'} c_{\nu'} &= -c_\nu^\dagger c_{\mu'} c_\mu^\dagger c_{\nu'} \\ &= -c_\mu^\dagger c_{\nu'} \langle c_\nu^\dagger c_{\mu'} \rangle - c_\nu^\dagger c_{\mu'} \langle c_\mu^\dagger c_{\nu'} \rangle + \langle c_\mu^\dagger c_{\nu'} \rangle \langle c_\nu^\dagger c_{\mu'} \rangle \end{aligned}$$

$$V_{\text{int}} = V_{\text{Hartree}} + V_{\text{Fock}}; \quad V_{\text{Hartree}} = \frac{1}{2} \sum_i$$

$$\langle c_\mu^\dagger c_{\mu'} \rangle + \langle c_\mu^\dagger c_{\mu'} \rangle \rangle c_\nu$$

$$\rangle \left(\overbrace{c_\nu^\dagger c_{\nu'} - \langle c_\nu^\dagger c_{\nu'} \rangle}^{d_{\nu\nu'}} + \langle c_\nu^\dagger c_{\nu'} \rangle \right) = \overbrace{d_{\mu\mu'} d_{\nu\nu'}}^{d_{\mu\mu'} d_{\nu\nu'}} + d_{\mu\mu'} \langle c_\nu^\dagger c_{\nu'} \rangle + d_{\nu\nu'} \langle c_\mu^\dagger c_{\mu'} \rangle + \langle c_\mu^\dagger c_{\mu'} \rangle \langle c_\nu^\dagger c_{\nu'} \rangle = c_\mu^\dagger c_{\mu'} \langle c_\nu^\dagger c_{\nu'} \rangle$$

$$\langle C_\nu^\dagger C_\mu^\dagger C_{\mu'} C_{\nu'} \rangle = \langle C_\nu^\dagger C_{\nu'} \rangle \langle C_\mu^\dagger C_{\mu'} \rangle - \langle C_\nu^\dagger C_{\mu'} \rangle \langle C_\mu^\dagger C_{\nu'} \rangle$$

$$\begin{aligned} C_\nu^\dagger C_\mu^\dagger C_{\mu'} C_{\nu'} &= -C_\nu^\dagger C_{\mu'} C_\mu^\dagger C_{\nu'} \\ &= -C_\mu^\dagger C_{\nu'} \langle C_\nu^\dagger C_{\mu'} \rangle - C_\nu^\dagger C_{\mu'} \langle C_\mu^\dagger C_{\nu'} \rangle + \langle C_\mu^\dagger C_{\nu'} \rangle \langle C_\nu^\dagger C_{\mu'} \rangle \end{aligned}$$

$$V_{\text{int}} = V_{\text{Hartree}} + V_{\text{Fock}}; \quad V_{\text{Hartree}} = \frac{1}{2} \sum_{\mu\mu', \nu\nu'} V_{\nu\mu}^{\nu'\mu'} (C_\mu^\dagger C_{\mu'} n_{\nu\nu'} + C_\nu^\dagger C_{\nu'} n_{\mu\mu'} - n_{\mu\mu'} n_{\nu\nu'})$$

$$V_{\text{Fock}} = -\frac{1}{2} \sum_{\mu\mu', \nu\nu'} V_{\nu\mu}^{\nu'\mu'} (C_\mu^\dagger C_{\nu'} n_{\nu\mu'} + C_\nu^\dagger C_{\mu'} n_{\mu\nu'} - n_{\mu\nu'} n_{\nu\mu'})$$

$$\langle C_\mu^\dagger C_{\mu'} \rangle + \langle C_\mu^\dagger C_{\mu'} \rangle C_\nu$$

$$\underbrace{\langle C_\nu^\dagger C_{\nu'} - \langle C_\nu^\dagger C_{\nu'} \rangle + \langle C_\nu^\dagger C_{\nu'} \rangle}_{d_{\nu\nu'}} = \underbrace{d_{\mu\mu'}}_0 + d_{\mu\mu'} \langle C_\nu^\dagger C_{\nu'} \rangle + d_{\nu\nu'} \langle C_\mu^\dagger C_{\mu'} \rangle + \langle C_\mu^\dagger C_{\mu'} \rangle \langle C_\nu^\dagger C_{\nu'} \rangle = C_\mu^\dagger C_{\mu'} \langle C_\nu^\dagger C_{\nu'} \rangle$$

$$\langle c_{\nu}^{\dagger} c_{\mu'} \rangle - \langle c_{\nu}^{\dagger} c_{\mu'} \rangle \langle c_{\mu}^{\dagger} c_{\nu'} \rangle$$

$$\langle c_{\nu}^{\dagger} c_{\mu'} \rangle - c_{\nu}^{\dagger} c_{\mu'} \langle c_{\mu}^{\dagger} c_{\nu'} \rangle + \langle c_{\mu}^{\dagger} c_{\nu'} \rangle \langle c_{\nu}^{\dagger} c_{\mu'} \rangle$$

$$\frac{1}{2} \sum_{\mu, \mu', \nu, \nu'} V_{\nu\mu}^{\nu'\mu'} (c_{\mu}^{\dagger} c_{\mu'} n_{\nu\nu'} + c_{\nu}^{\dagger} c_{\nu'} n_{\mu\mu'} - n_{\mu\mu'} n_{\nu\nu'})$$

$$\frac{1}{2} \sum_{\mu, \mu', \nu, \nu'} V_{\nu\mu}^{\nu'\mu'} (c_{\mu}^{\dagger} c_{\nu'} n_{\nu\mu'} + c_{\nu}^{\dagger} c_{\mu'} n_{\mu\nu'} - n_{\mu\nu'} n_{\nu\mu'})$$

$$\langle c_{\nu}^{\dagger} c_{\mu'} \rangle + \delta_{\nu\nu'} \langle c_{\mu}^{\dagger} c_{\mu'} \rangle + \langle c_{\mu}^{\dagger} c_{\mu'} \rangle \langle c_{\nu}^{\dagger} c_{\nu'} \rangle = c_{\mu}^{\dagger} c_{\mu'} \langle c_{\nu}^{\dagger} c_{\nu'} \rangle + c_{\nu}^{\dagger} c_{\nu'} \langle c_{\mu}^{\dagger} c_{\mu'} \rangle - \langle c_{\mu}^{\dagger} c_{\mu'} \rangle \langle c_{\nu}^{\dagger} c_{\nu'} \rangle$$

$$\sum_{k_1, k_2, k_3, k_4} V_{k_1 k_2}^{k_3 k_4} c_{k_3}^{\dagger} c_{k_4}^{\dagger} c_{k_2} c_{k_1} = \sum_{k_1, k_2, q} \tilde{V}(q) c_{k_1+q}^{\dagger} c_{k_2+q}^{\dagger} c_{k_2} c_{k_1}$$

Tutorial 2.

$$V_{\text{Hartree}} = \frac{1}{2} \sum_{p, p', q} \tilde{V}(q) (c_{p'+q}^{\dagger} c_p n_{p-q, p} + c_{p-q}^{\dagger} c_{p'} n_{p+q, p} - n_{p+q, p} n_{p-q, p})$$

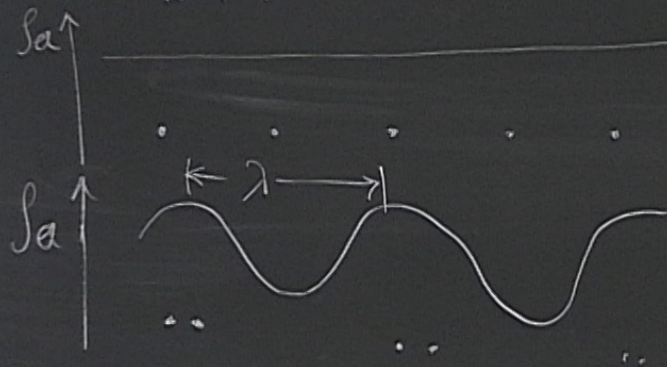
$$V_{\text{Fock}} = -\frac{1}{2} \sum_{p, p', q} \tilde{V}(q) (c_{p'+q}^{\dagger} c_p n_{p-q, p} + c_{p-q}^{\dagger} c_{p'} n_{p+q, p} - n_{p-q, p} n_{p+q, p})$$

$$= (d_{\mu\mu'} + \langle c_{\mu}^{\dagger} c_{\mu'} \rangle) (\langle c_{\nu}^{\dagger} c_{\nu'} \rangle - \langle c_{\nu}^{\dagger} c_{\nu'} \rangle + \langle c_{\nu}^{\dagger} c_{\nu'} \rangle) = \overline{d_{\mu\mu'} d_{\nu\nu'}} + d_{\mu\mu'} \langle c_{\nu}^{\dagger} c_{\nu'} \rangle$$

$$\langle c_k^{\dagger} c_{k'} \rangle = ?$$

$$\langle c_k^{\dagger} c_{k'} \rangle = n_{kk'} = \delta_{kk'} n_k$$

$$n_{p,q} = \delta_{p,q} n_p$$



$$Q = \frac{2\pi}{\lambda}$$

$$n_{kk'} = \delta_{k,k+Q} n_{k,k+Q}$$

$$\langle c_{\mu}^{\dagger} c_{\mu'} \rangle \left(c_{\nu}^{\dagger} c_{\nu'} - \langle c_{\nu}^{\dagger} c_{\nu'} \rangle + \langle c_{\nu}^{\dagger} c_{\nu'} \rangle \right) = \overbrace{d_{\mu\mu'} d_{\nu\nu'}} + d_{\mu\mu'} \langle c_{\nu}^{\dagger} c_{\nu'} \rangle + d_{\nu\nu'} \langle c_{\mu}^{\dagger} c_{\mu'} \rangle + \langle c_{\mu}^{\dagger} c_{\mu'} \rangle \langle c_{\nu}^{\dagger} c_{\nu'} \rangle = c_{\mu}^{\dagger} c_{\mu'} c_{\nu}^{\dagger} c_{\nu'}$$

$$n_{p,q} = \delta_{p,q} n_p$$

$$\delta_{kk'} n_{kk}$$

$$V_{\text{Hartree}} = \frac{1}{2} \sum_{pp'} \tilde{V}(0) \left(c_{p'}^{\dagger} c_{p'} n_{pp} + c_p^{\dagger} c_p n_{p'p'} \right)$$

$$V_{\text{Hartree}} = \sum_{pp'} \tilde{V}(0) n_{pp} c_p^{\dagger} c_{p'}$$

$$n_{kk'} = \delta_{k,k+Q} n_{k,k+Q}$$

$$Q = \frac{2\pi}{\lambda}$$

$$\tilde{V}(q) = \frac{1}{\Omega} \int e^{iq \cdot r} V(r) d^3 r$$

$$= \frac{1}{\Omega} \int e^{i|q|r \cos \theta} \frac{e^2}{4\pi\epsilon_0 r} r^2 \sin \theta d\theta d\phi$$

$$+ d_{\mu\mu'} \langle c_{\nu}^{\dagger} c_{\nu'} \rangle + d_{\nu\nu'} \langle c_{\mu}^{\dagger} c_{\mu'} \rangle + \langle c_{\mu}^{\dagger} c_{\mu'} \rangle \langle c_{\nu}^{\dagger} c_{\nu'} \rangle = c_{\mu}^{\dagger} c_{\mu'} \langle c_{\nu}^{\dagger} c_{\nu'} \rangle + c_{\nu}^{\dagger} c_{\nu'} \langle c_{\mu}^{\dagger} c_{\mu'} \rangle - \langle c_{\mu}^{\dagger} c_{\mu'} \rangle \langle c_{\nu}^{\dagger} c_{\nu'} \rangle$$

$$+ c_p^{\dagger} c_p n_{p'p'}$$

$$= \dots n_{pp} c_{p'}^{\dagger} c_{p'}$$

$$q) = \dots \frac{1}{r}$$

$$V_{\text{Fock}} = -\frac{1}{2} \sum_{\mathbf{p}\mathbf{p}'} \tilde{V}(\mathbf{p}-\mathbf{p}') c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}} n_{\mathbf{p}'\mathbf{p}'} - \frac{1}{2} \sum_{\mathbf{p}\mathbf{p}'} \tilde{V}(\mathbf{p}-\mathbf{p}') c_{\mathbf{p}'}^{\dagger} c_{\mathbf{p}'} n_{\mathbf{p}\mathbf{p}}$$

$$\tilde{V}(\mathbf{p}-\mathbf{p}') = \tilde{V}(\mathbf{p}'-\mathbf{p}) = \tilde{V}(|\mathbf{p}-\mathbf{p}'|)$$

$$V_{\text{Fock}} = - \sum_{\mathbf{q}\mathbf{v}} \tilde{V}(\mathbf{q}-\mathbf{p}) n_{\mathbf{q}\mathbf{q}\mathbf{v}} c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}}$$

$$H = \sum_{\mathbf{p}} \left(\epsilon(\mathbf{p}) + \underbrace{\sum_{\mathbf{q}} \left(\tilde{V}(\mathbf{0}) - \tilde{V}(\mathbf{q}-\mathbf{p}) n_{\mathbf{q}\mathbf{q}\mathbf{v}} \right)}_{\text{Self Energy}} \right) c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}}$$

Self Energy

$$\frac{e^2}{4\pi\epsilon_0 r} \int \sin\theta d\theta d\phi dr \propto \frac{1}{|q|^2}$$

$$+ d_{\mu\mu'} \langle c_{\nu}^{\dagger} c_{\nu'} \rangle + d_{\nu\nu'} \langle c_{\mu}^{\dagger} c_{\mu'} \rangle + \langle c_{\mu}^{\dagger} c_{\mu'} \rangle \langle c_{\nu}^{\dagger} c_{\nu'} \rangle = c_{\mu}^{\dagger} c_{\mu'} \langle c_{\nu}^{\dagger} c_{\nu'} \rangle + c_{\nu}^{\dagger} c_{\nu'} \langle c_{\mu}^{\dagger} c_{\mu'} \rangle - \langle c_{\mu}^{\dagger} c_{\mu'} \rangle \langle c_{\nu}^{\dagger} c_{\nu'} \rangle$$

$$+ c_p^{\dagger} c_p n_{p'p'}$$

$$= \sum_{pp'} \tilde{V}(0) n_{pp} c_{p'}^{\dagger} c_{p'}$$

$$v(q) = \frac{1}{\Omega} \int e^{i\mathbf{q} \cdot \mathbf{r}} V(r) d^3 r$$

$$= \frac{1}{\Omega} \int e^{i|\mathbf{q}|r \cos \theta} \frac{e^2}{4\pi\epsilon_0 r} r^2 \sin \theta d\theta d\phi dr \propto \frac{1}{|\mathbf{q}|^2}$$

$$V_{\text{Fock}} = -\frac{1}{2} \sum_{\mathbf{p}\mathbf{p}'} \tilde{V}(\mathbf{p}-\mathbf{p}') c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}} n_{\mathbf{p}'\mathbf{p}'} - \frac{1}{2} \sum_{\mathbf{p}\mathbf{p}'} \tilde{V}(\mathbf{p}-\mathbf{p}') c_{\mathbf{p}'}^{\dagger} c_{\mathbf{p}'} n_{\mathbf{p}\mathbf{p}}$$

$$\tilde{V}(\mathbf{p}-\mathbf{p}') = \tilde{V}(\mathbf{p}'-\mathbf{p}) = \tilde{V}(|\mathbf{p}-\mathbf{p}'|)$$

$$V_{\text{Fock}} = - \sum_{\mathbf{p}\mathbf{q}} \tilde{V}(\mathbf{q}-\mathbf{p}) n_{\mathbf{q}\mathbf{q}} c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}}$$

$$H = \sum_{\mathbf{p}} \left(\epsilon(\mathbf{p}) + \underbrace{\sum_{\mathbf{q}} \left(\tilde{V}(0) - \tilde{V}(\mathbf{q}-\mathbf{p}) n_{\mathbf{q}\mathbf{q}} \right)}_{\text{Self Energy}} \right) c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}}$$

Self Energy

$$H = \sum_{\mathbf{p}} \frac{\hbar^2 \mathbf{p}^2}{2m^*} c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}}$$

$$V_{\text{Hartree}} = \frac{U}{2\Omega} \sum_{\substack{k, k', q \\ \sigma, \sigma'}} \left(c_{k+q, \sigma}^\dagger c_{k\sigma} n_{k'-q, \sigma'; k'\sigma'} + c_{k-q, \sigma'}^\dagger c_{k'\sigma'} n_{k+q, \sigma; k\sigma} - n_{k'-q, \sigma'; k'\sigma'} n_{k+q, \sigma; k\sigma} \right)$$

$$V_{\text{Fock}} = -\frac{U}{2\Omega} \sum_{\substack{k, k', q \\ \sigma, \sigma'}} \left(c_{k+q, \sigma}^\dagger c_{k'\sigma'} n_{k'-q, \sigma'; k\sigma} + c_{k'-q, \sigma'}^\dagger c_{k\sigma} n_{k+q, \sigma; k'\sigma'} - n_{k'-q, \sigma'; k\sigma} n_{k+q, \sigma; k'\sigma'} \right)$$

$$V_{\text{int}} = \frac{U}{2\Omega} \sum_{\substack{k, k' \\ \sigma, \sigma'}} \left(c_{k\sigma}^\dagger c_{k\sigma} n_{k'\sigma'} + c_{k'\sigma'}^\dagger c_{k'\sigma'} n_{k\sigma} - n_{k'\sigma'} n_{k\sigma} \right)$$

$$- \frac{U}{2\Omega} \sum_{\substack{k, k' \\ \sigma, \sigma'}} \left(c_{k'\sigma}^\dagger c_{k'\sigma'} n_{k\sigma} \delta_{\sigma\sigma'} + c_{k\sigma}^\dagger c_{k\sigma} n_{k'\sigma'} \delta_{\sigma\sigma'} - n_{k\sigma} n_{k'\sigma'} \delta_{\sigma\sigma'} \right)$$