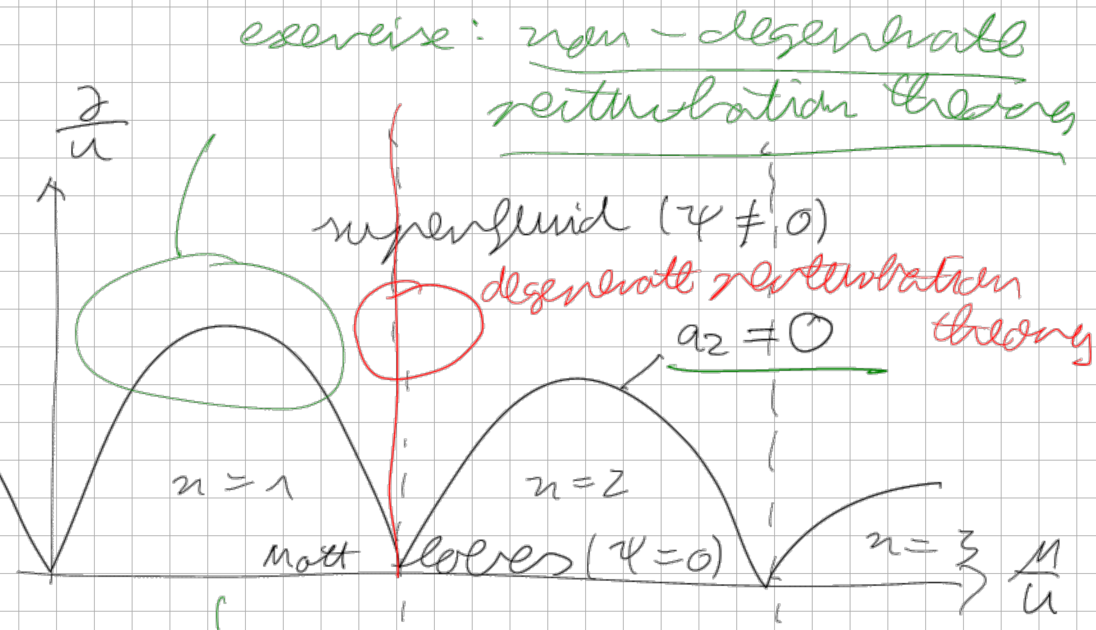
Chapter 4 Brillouin – Wigner Perturbation Theory

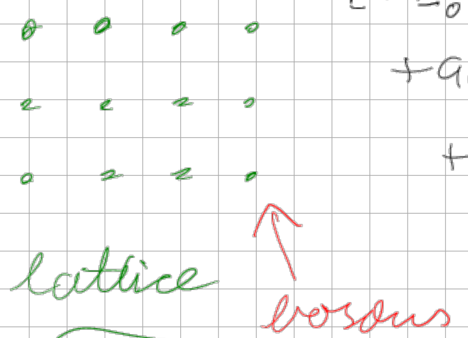
Motivation: Problem set 3

Bose-Hubbard model: mean field description $-\mu n + \frac{U}{2} n(n-1)$

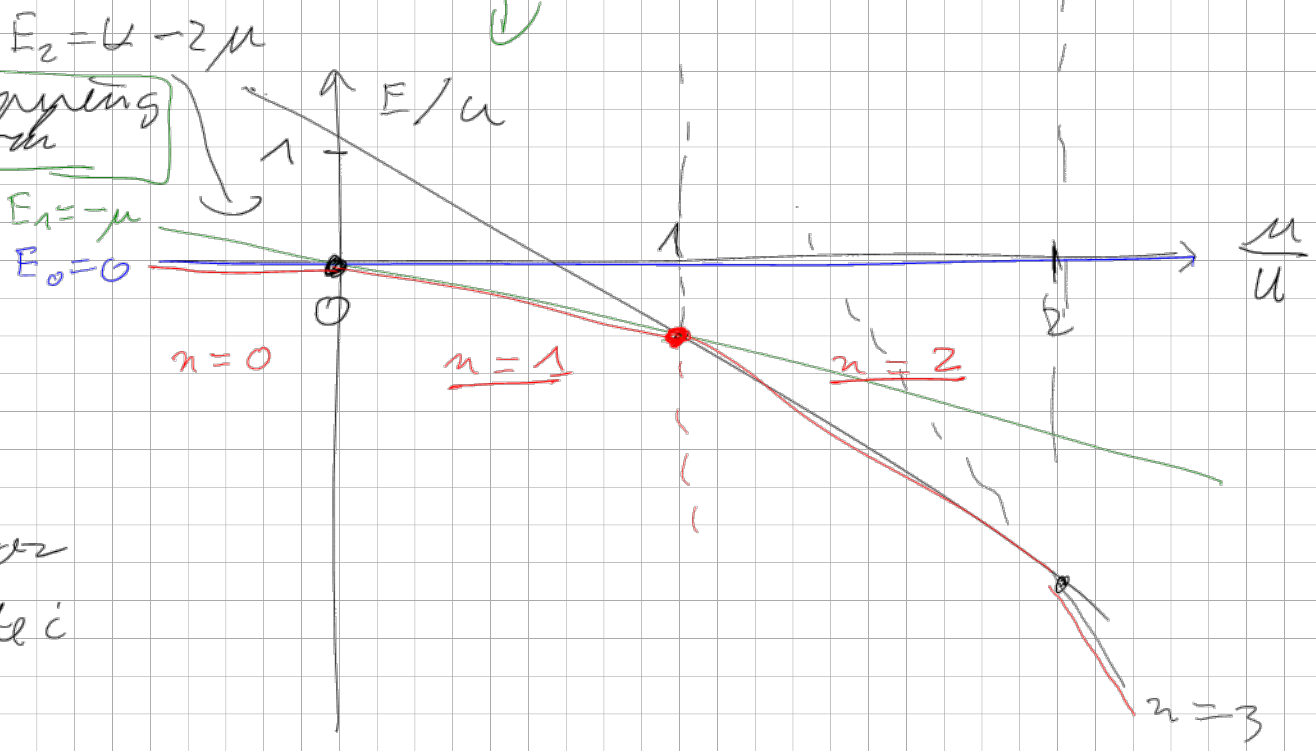
$E = E_0 + a_2 |\psi|^2 + a_4 |\psi|^4 + \dots$

vacuum $n=0$





$$\hat H = \underbrace{\sum_i \left\{ + \frac{U}{2} \hat n_i (\hat n_i - 1) - \mu \hat n_i \right\}}_{\text{local part}} + \text{hopping term}$$

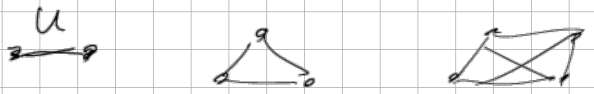


μ: chemical potential

U: on-site interaction

($U > 0$: repulsive)

$\hat n_i = \hat a_i^{+} \hat a_i$: number operator for finding a particle at site i



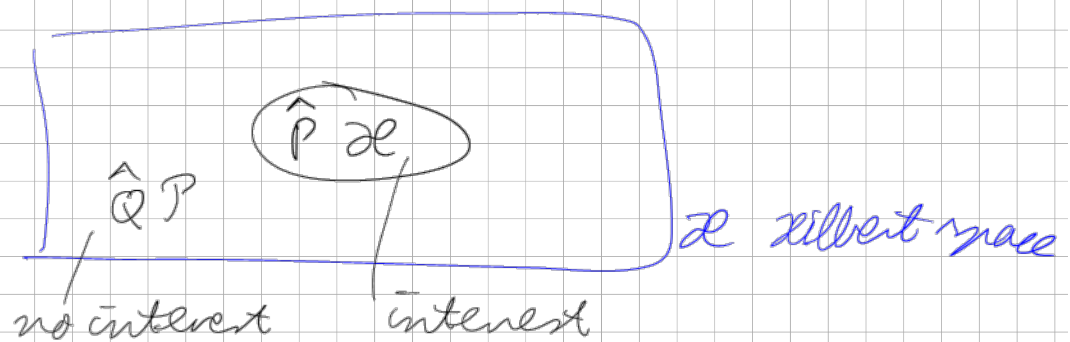
3U   6U   - - - $\frac{1}{2}n(n-1)U$

n = 2 , 3 , 4   n

$E_n = \frac{U}{2} n(n-1) - \mu n$

- unify non-degenerate and degenerate perturbation theory.
- higher perturbative order easier accessible

4.1 General Formalism:



projection operator $\hat P$

idempotent property $\hat P^2 = \hat P$

complementary projection operator $\hat Q = 1 - \hat P$

$$\hat Q^2 = (1-\hat P)^2 = 1 - 2\hat P + \underbrace{\hat P^2}_{=\hat P} = 1 - \hat P = \hat Q \; ✓$$ also a projection operator

$$\hat P \hat Q = \hat P(1-\hat P) = \hat P - \hat P^2 = \hat P - \hat P = 0 = \hat Q \hat P \Rightarrow [\hat P, \hat Q]_- = 0$$

$\Rightarrow \hat P$ and $\hat Q$ project into independent subspaces of $\mathcal{H}$

eigenvalue problem: $\hat H |\Psi_n\rangle = E_n |\Psi_n\rangle$

$\hat 1 = \hat P + \hat Q$ $\hat 1 = \hat P + \hat Q$

$$\hat H \left(\hat P |\Psi_n\rangle\right) + \hat H \left(\hat Q |\Psi_n\rangle\right) = E_n \left(\hat P |\Psi_n\rangle\right) + E_n \left(\hat Q |\Psi_n\rangle\right) \quad \Big| \hat P \cdot \quad \hat Q \cdot$$

$$\hat{P}\hat{H}\left(\hat{P}|\Psi_n\rangle\right) + \hat{P}\hat{H}\left(\hat{Q}|\Psi_n\rangle\right) = E_n \underbrace{\hat{P}^2}_{=\hat{P}}|\Psi_n\rangle + E_n \cancel{\underbrace{\hat{P}\hat{Q}}_{=0}|\Psi_n\rangle} \qquad (1)$$

$$\hat{Q}\hat{H}\hat{P}|\Psi_n\rangle + \hat{Q}\hat{H}\left(\underbrace{\hat{Q}}_{=\hat{Q}\cdot\hat{Q}}|\Psi_n\rangle\right) = E_n \underbrace{\hat{Q}\hat{P}}_{=0}|\Psi_n\rangle + E_n\left(\underbrace{\hat{Q}^2}_{=\hat{Q}}|\Psi_n\rangle\right) \qquad (2)$$

two intertwined equations defining $\hat{P}|\Psi_n\rangle$ and $\hat{Q}|\Psi_n\rangle$

Aim: Find one equation for $\hat{P}|\Psi_n\rangle$ by eliminating $\hat{Q}|\Psi_n\rangle$

$$\hat{Q}\hat{H}\hat{P}|\Psi_n\rangle = \underbrace{(E_n - \hat{Q}\hat{H}\hat{Q})}_{\text{invert this}}\left(\hat{Q}|\Psi_n\rangle\right)$$

$$\hat{Q}|\Psi_n\rangle = (E_n - \hat{Q}\hat{H}\hat{Q})^{-1}\hat{Q}\hat{H}\hat{P}|\Psi_n\rangle \quad \Big|\ \hat{Q}\cdot$$

$$\boxed{\hat{Q}|\Psi_n\rangle} = \hat{Q}(E_n - \hat{Q}\hat{H}\hat{Q})^{-1}\hat{Q}\hat{H}\hat{P}|\Psi_n\rangle \qquad (2')$$

(2') in (1):

$$\left\{\hat{P}\hat{H}\hat{P} + \hat{P}\hat{H}\hat{Q}\boxed{(E_n - \hat{Q}\hat{H}\hat{Q})^{-1}}\hat{Q}\hat{H}\hat{P}\right\}|\Psi_n\rangle = E_n\hat{P}|\Psi_n\rangle$$

one equation for $\hat{P}|\Psi_n\rangle$

resolvent

$$\hat{H} = \cancel{\hat{H}_0} + \lambda\hat{V}$$

implement this for perturbation theory

4.2 Specialization:

$\hat{P}$ was considered to be independent of $\hat{H}$

Now: $[\hat{P}, \hat{H}_0]_- \underset{\text{assumption}}{=} 0$

$$\hat{H}_0 |\psi_n^{(0)}\rangle = E_n^{(0)} |\psi_n^{(0)}\rangle \quad , \quad \langle \psi_n^{(0)} | \psi_m^{(0)} \rangle = \delta_{nm}$$

$$\hat{P} = \sum_{n \in N} \underbrace{|\psi_n^{(0)}\rangle \langle \psi_n^{(0)}|}_{\text{dyadic product}}$$

N: subset of quantum numbers

$\hat{P}_n = |\psi_n^{(0)}\rangle\langle\psi_n^{(0)}|$ projection operator due to $\hat{P}_n^2 = \hat{P}_n$

$$\hat{P}_n \hat{P}_{n'} = |\psi_n^{(0)}\rangle \underbrace{\langle \psi_n^{(0)} | \psi_{n'}^{(0)} \rangle}_{= \delta_{nn'}} \langle \psi_{n'}^{(0)} | = \delta_{nn'} \hat{P}_n$$

$$\Rightarrow \hat{P}^2 = \sum_{n \in N} \sum_{n' \in N} \hat{P}_n \hat{P}_{n'} = \sum_{n \in N} \hat{P}_n = \hat{P} \checkmark$$

$$\hat{Q} = \sum_{n \in \overline{N}} \hat{P}_n \quad , \quad \hat{Q}^2 = \hat{Q} \quad , \quad \hat{Q}\hat{P} = \hat{P}\hat{Q} = 0$$

$\overline{N}$: complement of N

$$\hat{Q}\hat{H}_0\hat{P} = \sum_{n \in N} \hat{Q}\hat{H}_0 \underbrace{\hat{P}_n}_{= |\psi_n^{(0)}\rangle\langle\psi_n^{(0)}|} = \sum_{n \in N} \hat{Q} E_n^{(0)} |\psi_n^{(0)}\rangle\langle\psi_n^{(0)}| = E_n^{(0)} \hat{Q}\hat{P} = 0$$

$\hat{P}\,\hat{H}_0\,\hat{Q} = 0$ analogously

$$\hat{P}\left\{\underbrace{\hat{H}}_{=\hat{H}_0+\lambda\hat{V}} + \lambda^2\hat{V}\hat{Q}\boxed{\left(E_n - \hat{Q}\hat{H}\hat{Q}\right)^{-1}}\hat{Q}\hat{V}\right\}\hat{P}|\Psi_n\rangle = E_n\,\hat{P}|\Psi_n\rangle$$

full energy eigenvalue

$= \hat{H}_{eff}$

effective Schrödinger equation in subspace $\hat{P}\mathcal{H}$ with $\hat{H}_{eff}$

4.3 Resolvent:

$$\hat{H}_{eff} = \hat{H}_0 + \lambda\hat{V} + \lambda^2\hat{V}\hat{Q}R(E_n)\hat{Q}\hat{V}$$

$$R(E_n) = \left[\underbrace{E_n - \hat{Q}(\hat{H}_0 + \lambda\hat{V})\hat{Q}}\right]^{-1}$$

$$= \left(1 - \lambda\hat{Q}\hat{V}\hat{Q}\right)\left(E_n - \hat{Q}\hat{H}_0\hat{Q}\right)$$

$(\hat{A}\hat{B})^{-1} = \hat{B}^{-1}\hat{A}^{-1}$

$$= \left(E_n - \hat{Q}\hat{H}_0\hat{Q}\right)^{-1}\underbrace{\left[1 - \lambda\hat{Q}\hat{V}\hat{Q}\left(E_n - \hat{Q}\hat{H}_0\hat{Q}\right)^{-1}\right]^{-1}}$$

$= R^{(0)}(E_n)$ $\quad R^{(0)}(E_n)$

geometric series $= \sum_{s=0}^{\infty}\left(\lambda\hat{Q}\hat{V}\hat{Q}R^{(0)}(E_n)\right)^s$

$$\hat{H}_{eff} = \hat{H}_0 + \lambda \hat{V} + \lambda^2 \underbrace{\hat{V} \left[\hat{Q} \hat{R}^{(0)}(E_n) \hat{Q}\right] \hat{V}}_{s=0}$$

$$+ \lambda^3 \underbrace{\hat{V} \left[\hat{Q} \hat{R}^{(0)}(E_n) \hat{Q}\right] \hat{V} \left[\hat{Q} R^{(0)}(E_n) \hat{Q}\right] \hat{V}}_{s=1} + \dots$$

each perturbative order consists of precisely one term

$$\left[\hat{Q} R^{(0)}(E_n) \hat{Q}\right] = \sum_{l \in \overline{N}} \sum_{l' \in \overline{N}} |\psi_l^{(0)}\rangle\langle\psi_l^{(0)}| R^{(0)}(E_n) |\psi_{l'}^{(0)}\rangle \langle \psi_{l'}^{(0)}| = \sum_{l \in \overline{N}} \frac{|\psi_l^{(0)}\rangle\langle\psi_l^{(0)}|}{E_n - E_l^{(0)}}$$

side calculation

$$R^{(0)}(E_n) |\psi_{l'}^{(0)}\rangle = (E_n - \hat{Q} \hat{H}_0 \hat{Q})^{-1} |\psi_{l'}\rangle \overset{!}{=} \frac{1}{E_n - E_{l'}^{(0)}} |\psi_{l'}\rangle$$

$$= \frac{1}{E_n} \left(1 - \frac{\hat{Q} \hat{H}_0 \hat{Q}}{E_n}\right)^{-1} \qquad \hat{Q} |\psi_{l'}^{(0)}\rangle = |\psi_{l'}\rangle$$

$$\underbrace{\hat{Q}}_{=1-\cancel{\hat{P}}} \qquad l' \in \overline{N}$$

$$= \sum_{s=0}^{\infty} \left(\frac{\hat{Q} \hat{H}_0 \hat{Q}}{E_n}\right)^s$$

$$\langle \psi_l^{(0)} | R^{(0)}(E_n) | \psi_l^{(0)} \rangle = \frac{1}{E_n - E_l^{(0)}} \qquad l \in \overline{N}$$

$$\underline{\hat{H}_{eff} = \hat{H}_0 + \lambda \hat{V} + \lambda^2} \sum_{l \in \overline{N}} \frac{\hat{V} |\psi_l^{(0)}\rangle\langle\psi_l^{(0)}| \hat{V}}{E_n - E_l^{(0)}}$$

$$+\lambda^3 \underline{\sum_{l\in\bar N}\sum_{l'\in\bar N}} \frac{\hat V |\psi_l^{(0)}\rangle\langle\psi_l^{(0)}| \hat V |\psi_{l'}^{(0)}\rangle\langle\psi_{l'}^{(0)}| \hat V}{(E_n - E_l^{(0)})(E_n - E_{l'}^{(0)})} + \cdots$$

$$\underline{\hat P}\, \hat H_{eff}\, \underline{\hat P}\, |\psi_m\rangle = E_m \hat P |\psi_m\rangle \qquad \Big|\ \underline{\langle\psi_{n''}^{(0)}| \cdot}$$

$$\cancel{\sum_{n\in N}} \underline{\sum_{n^{*}\in N}} \underbrace{\langle\psi_{n''}^{(0)}|\psi_n^{(0)}\rangle}_{\delta_{nn''}} \langle\psi_{n''}^{(0)}|\hat H_{eff}|\psi_{n^*}^{(0)}\rangle \underline{\langle\psi_{n^*}^{(0)}|\psi_m\rangle}$$

$$= E_m \underline{\sum_{n\in N}} \underbrace{\langle\psi_{n''}^{(0)}|\psi_n^{(0)}\rangle}_{=\delta_{nn''}} \underline{\langle\psi_n^{(0)}|\psi_m\rangle}$$

$$\underline{\sum_{n\in N}} \left\{ \langle\psi_{n''}^{(0)}|\hat H_{eff}^{(E_m)}|\psi_n^{(0)}\rangle - \boxed{E_m}\,\delta_{nn''} \right\} \underline{\langle\psi_n^{(0)}|\psi_m\rangle} = 0$$

nontrivial solution $\quad \det\Big(\qquad \Big) = 0$

$\Rightarrow$ equation for E_m is self-consistent as E_m appears also in $\hat H_{eff}(E_m)$

Non-degenerate perturbation theory as special case:

$$\hat P = \hat P_n = |\psi_n^{(0)}\rangle\langle\psi_n^{(0)}|$$

$$E_n = \langle \Psi_n^{(0)} | \hat{H}_{eff} | \Psi_n^{(0)} \rangle$$