Formalism for quantum many-body systems : second quantization

identical = indistinguishable quantum particles

$\Rightarrow$ occupation of single-particle states

$\boxed{|\alpha\rangle} \longrightarrow$ ex. $\boxed{\phi_a(\vec{x})\ |\ m\rangle}$

$\alpha = 1, \ldots, M$

motional state — spin state

Fock states: states of definite occupation of single-particle states $|\alpha\rangle$

$$|n_1, n_2, \ldots, n_\alpha, \ldots, n_M\rangle$$

M states / modes

N particles

created from the vacuum $|0, 0, \ldots, 0, \ldots 0\rangle$

creation

$$\hat{c}^\dagger_\alpha |0, 0, \ldots, \underset{\alpha}{\overset{n_\alpha}{0}}, \ldots 0\rangle = |0, 0, \ldots, \underset{\alpha}{\overset{n_\alpha+1}{1}}, \ldots, 0\rangle$$

destruction

$$\hat{c}_\alpha |n_1, n_2, \ldots, n_\alpha, \ldots, 0\rangle \sim |n_1, n_2, \ldots, n_\alpha - 1, \ldots, 0\rangle$$

BOSONS

$n_\alpha = 0, \ldots, \infty$

$$[\hat{c}_\alpha, \hat{c}^\dagger_\beta] = \hat{c}_\alpha \hat{c}^\dagger_\beta - \hat{c}^\dagger_\beta \hat{c}_\alpha = \delta_{\alpha\beta}$$

$$[c_\alpha, c_\beta] = [c^\dagger_\alpha, c^\dagger_\beta] = 0$$

FERMIONS

$n_\alpha = 0, 1$

$$\{\hat{c}_\alpha, \hat{c}^\dagger_\beta\} = \hat{c}_\alpha \hat{c}^\dagger_\beta + c^\dagger_\beta c_\alpha = \delta_{\alpha\beta}$$

$$\{\hat{c}_\alpha, \hat{c}_\beta\} = \{\hat{c}^\dagger_\alpha, \hat{c}^\dagger_\beta\} = 0$$

$$\hookrightarrow c_\alpha^2 = \{c_\alpha, c_\alpha\} = 0$$

$$(c^\dagger_\alpha)^2 = 0$$

ordering is fundamental for fermions

Fock states

$$|n_1, n_2, \ldots, n_\alpha, \ldots, n_M\rangle = \frac{(c^\dagger_1)^{n_1}}{\sqrt{n_1!}} \frac{(c^\dagger_2)^{n_2}}{\sqrt{n_2!}} \cdots \frac{(c^\dagger_M)^{n_M}}{\sqrt{n_M!}} |0\rangle$$

Generic state in Hilbert space for N particles

$$|\Psi\rangle = \sum_{n_1, n_2 \dots n_M : \sum_\alpha n_\alpha = N} \psi(n_1, n_2, \dots, n_M) \; |n_1, n_2, \dots, n_M\rangle$$

$\sim O(\exp(N, M))$ complex coefficients

"Hartree-Fock" state → special

$$|\Psi_{HF}\rangle = \prod_{i=1}^{N} \left(\sum_\alpha \Phi_\alpha^{(i)} c_\alpha^\dagger \right) |0\rangle$$

$\Phi_\alpha^{(i)} \in \mathbb{C}$ $N \times M$ numbers single-particle

$c^\dagger_{\Phi^{(i)}}$ creates a particle in V state $|\Phi^{(i)}\rangle = \sum_\alpha \Phi_\alpha^{(i)} |\alpha\rangle$

$$\neq \sum_{n_1 n_2 \dots n_M} \psi_1(n_1)\,\psi_2(n_2) \dots \psi_M(n_M) \; |n_1\, n_2 \dots n_M\rangle$$

special ("coherent state" "Gutzwiller state")

$\sim O(M)$ coefficients

Physical observables

one-body observables $\hat{A} = \sum_{i=1}^{N} \hat{A}_i^{(1)}$

$$\left(\text{ex.} = \sum_{i=1}^{N} \frac{\hat{\vec{p}}_i^{\,2}}{2m} \right)$$

arbitrary basis for single particles $\{|\mu\rangle\}$

$$\hat{A} = \sum_{\mu\nu} \langle\mu| \hat{A}^{(1)} |\nu\rangle \; \hat{c}_\mu^\dagger \hat{c}_\nu$$

two-body observables $\hat{V} = \frac{1}{2} \sum_{i \neq j} \hat{v}^{(2)}(\hat{A}_i^{(1)}, \hat{A}_j^{(1)})$

$$\text{ex.} = \frac{1}{2} \sum_{i\neq j} v^{(2)}(\vec{r}_i, \vec{r}_j)$$

$$\hat{V} = \frac{1}{2} \sum_{\mu\nu\lambda\rho} \langle\mu\nu| \hat{v}^{(2)}(\hat{A}_1^{(1)}, \hat{A}_2^{(1)}) |\lambda\rho\rangle \; \hat{c}_\mu^\dagger \hat{c}_\nu^\dagger \hat{c}_\rho \hat{c}_\lambda$$

Hamiltonian for a many-body system of itinerant particles

$$\hat H := \sum_{i=1}^{N} \overbrace{\left(\frac{\vec p_i^{\,2}}{2m} + V_{ext}(\vec r_i) \right)}^{\hat H_i^{(1)}} + \frac{1}{2} \sum_{i \neq j} \overbrace{\hat v^{(2)}(\vec r_i, \vec r_j)}^{\hat H_{ij}^{(2)}}$$

first quantization

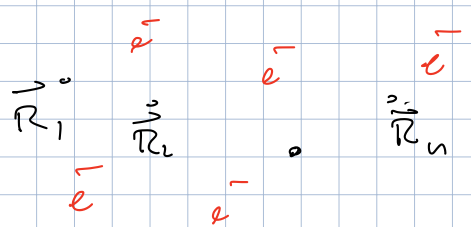
$\longrightarrow$ second quantization

$$\boxed{\hat H = \sum_{\mu\nu} \langle \mu | \hat H^{(1)} | \nu \rangle \, \hat c^+_\mu \hat c_\nu + \sum_{\mu\nu\lambda\rho} \langle \mu\nu | H^{(2)} | \lambda\rho \rangle \, \hat c^+_\mu \hat c^+_\nu \hat c_\rho \hat c_\lambda}$$

Examples 1) electrons in molecules

$$V_{ext}(\vec r_i) = - \sum_N \frac{Z_N e^2}{4\pi\epsilon_0 |\vec r_i - \vec R_N|}$$

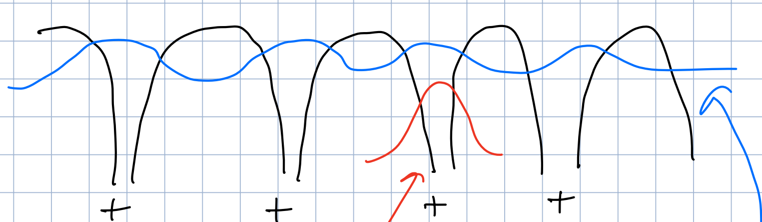
el.-nucleus interaction



$$v^{(2)}(\vec r_i, \vec r_j) = \frac{1}{4\pi\epsilon_0} \frac{e^2}{|\vec r_i - \vec r_j|}$$

$|\mu\rangle \longrightarrow$ ex. H-atom orbitals centred around the various nuclei

2) electrons in a solid



$V_{ext}(\vec r_i)$

$v^{(2)}(\vec r_i, \vec r_j)$ Coulomb interaction

$|\mu\rangle \rightarrow$ Bloch waves

Wannier states

etc ...

Quantum many-body problems that we want to solve

1) Diagonalization of $\hat{H}$ $\qquad \hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$

$\rightarrow$ ground state

$\rightarrow$ low-energy excited states

$\rightarrow$ equilibrium thermodynamics $\qquad \beta = \frac{1}{k_B T}$

$$Z = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right) = \sum_n e^{-\beta E_n}$$

$$\langle\hat{A}\rangle = \mathrm{Tr}\left(\hat{A}\,e^{-\beta\hat{H}}\right)/Z = \sum_n \langle\Psi_n|\hat{A}|\Psi_n\rangle \frac{e^{-\beta E_n}}{Z}$$

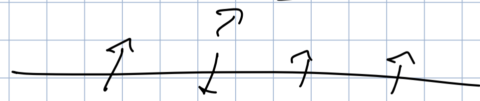
$\rightarrow$ non-equilibrium dynamics

$$|\Psi(0)\rangle \rightarrow |\Psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\Psi(0)\rangle$$

"quantum quench"

EXACT DIAGONALIZATION

$\vec{S}^2 = \hbar^2 S(S+1)$



$\hat{H} \to$ quantum spins

$$D = (2S+1)^N$$

$\hat{H} \to$ N itinerant particles over M modes with maximal occupation n_{max}

$$D = \frac{(M n_{max})!}{N! \, (M n_{max} - N)! \; n_{max}!}$$

Basis for the D-dimensional Hilbert space (ex. Fock states $|n_1 n_2 .. n_M\rangle$)

$\hat{H} \to$ D x D matrix

ex. $\langle n_1 n_2 .. n_M | H | n_1' n_2' ... n_M' \rangle$

Exponential growth of D with N (M) is a fundamental limitation to exact diagonalization –

typical values $N \sim O(10)$

fundamental limit : memory storage

Tricks to reduce the size of the matrix $\hat{H}$

using symmetries ?

symmetry $\hat{U} = e^{i\vartheta \hat{A}}$ $\qquad \hat{U}^+ \hat{U} = \mathbb{1}$

unitary $\qquad \hat{A} = \hat{A}^+$

$$\hat{U}^+ \hat{H} \hat{U} = \hat{H} \quad \leftrightarrow \quad [\hat{A}, \hat{H}] = 0$$

ex. rotational invariance $\hat{A} = \hat{L}^z$ angular momentum

$\hat{A}, \hat{H}$ admit a common basis of eigenstates

$$\hat{A} \, | a_n^{(i)} \rangle = a_n \, | a_n^{(i)} \rangle$$

a_n eigenvalue

$i = 1, .., d_n \to$ degeneracy

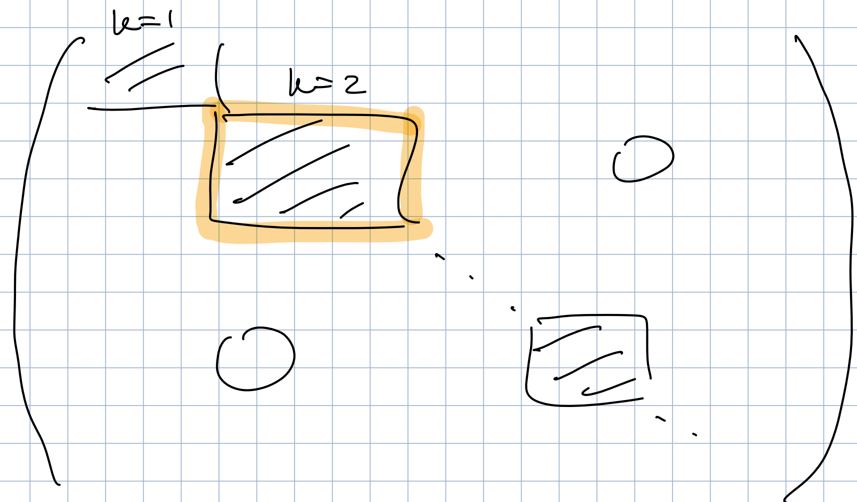
$$\hat{A} = \sum_n a_n \sum_i |a_n^{(i)}\rangle\langle a_n^{(i)}|$$

$\hat{H}$ cannot connect degenerate eigenspaces of $\hat{A}$

$$\langle a_n^{(i)}|\hat{H}|a_{n'}^{(j)}\rangle \sim \delta_{nn'}$$

→ build $\hat{H}$ matrix in the eigenbasis of $\hat{A}$

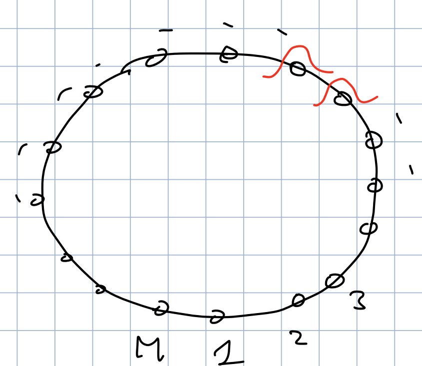
$$\{\langle a_n^{(i)}|\hat{H}|a_{n'}^{(j)}\rangle\} =$$



Block diagonal matrix

I can forget about the quantum number a_n that labels the $|\Psi_m\rangle$

Translational invariance : ex.



Fock states : $|n_1, n_2, \ldots, n_M\rangle$

Translation operator T_d

$$T_{d=1}|n_1, n_2, \dots, n_M\rangle = |n_M, n_1, n_2, \dots, n_{M-1}\rangle$$

$$T_d = |n_{M-d+1}, n_{M-d+2}, \dots, \underset{\uparrow \atop d+1}{n_1}, \dots n_{M-d}\rangle$$

$$T_d^{\dagger} \hat{H} T_d = \hat{H}$$

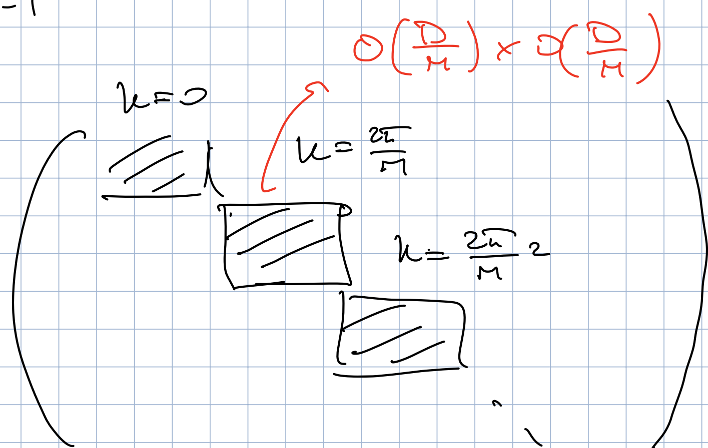
Build eigenstates of T_d: quasi-momentum eigenstates

$$|n_1 n_2 \dots n_M; \underline{k}\rangle = \frac{1}{\sqrt{M}} \sum_{r=1}^{M} e^{ikr} \hat{T}_r |n_1 n_2 \dots n_M\rangle$$

exercise: $T_d |n_1 n_2 \dots n_M; \underline{k}\rangle = e^{ikd} |n_1 n_2 \dots, n_M; k\rangle$

$$k = \frac{2\pi}{M} \underline{p} \qquad p = 0, \dots, M-1$$

$$\langle n_1 n_2 \dots n_M; k| H | n_1' n_2' \dots n_M'; k\rangle =$$



$\hat{H}$: $\underline{D \times D}$ matrix without using symmetries

$\underline{O\left(\frac{D}{M}\right) \times O\left(\frac{D}{M}\right)}$ matrices (using symmetries)

→ full diagonalization: Lapack

Krylov space and Lanczos method

(partial diagonalization of $\hat{H}$)

Power method

extract a random vector $|\phi\rangle = \sum_m c_m |\Psi_m\rangle$

$|\Psi_0\rangle$ ground state $\qquad \langle\phi|\Psi_0\rangle \neq 0$

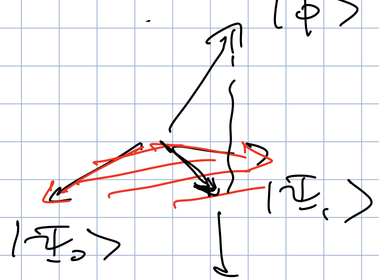
$H|\Psi_0\rangle = E_0 |\Psi_0\rangle$

$E_0 \leq E_1 \leq E_2 \leq \dots \leq E_D$

$|E_0| \geq |E_1| \geq \dots \geq |E_D| \qquad \hat{H} \to \hat{H} - \epsilon \mathbb{1}$

if degenerate ground state $\qquad \epsilon \geq E_D$

$E_0 = E_1$



$\alpha|\Psi_0\rangle + \beta|\Psi_1\rangle$

$$\hat{H}^n |\phi\rangle = \sum_m c_m E_m^n |\Psi_m\rangle$$

$$= E_0^n \left(c_0 |\Psi_0\rangle + \sum_{m\neq 0} c_m \left(\frac{E_m}{E_0}\right)^n |\Psi_m\rangle \right)$$

< 1

$\exp\left(-n \log\left(\frac{E_0}{E_m}\right)\right)$

$$\xrightarrow[n\to\infty]{} E_0^n c_0 |\Psi_0\rangle$$

$\exp\left(-n \log\left(\frac{E_0}{E_1}\right)\right)$

$$\frac{\hat{H}^n |\phi\rangle}{\| \hat{H}^n |\phi\rangle \|} \xrightarrow[n\to\infty]{} |\Psi_0\rangle$$

$E_1 > E_0$

Lanczos method

$M \neq$ # of modes

$$|\phi\rangle, \quad \hat{H}|\phi\rangle, \quad \hat{H}^2|\phi\rangle, \ \ldots, \ \hat{H}^{M-1}|\phi\rangle$$

↪ these vectors are linearly independent if $|\phi\rangle$ is not an eigenstate of $\hat{H}$

$$K_M = \text{span}\left(|\phi\rangle, \hat{H}|\phi\rangle, \ldots, \hat{H}^{M-1}|\phi\rangle\right)$$

Krylov space — M-dimensional subspace of Hilbert space

Lanczos basis: orthonormalization of $H^m|\phi\rangle$ vectors

$|\phi_0\rangle = |\phi\rangle$ normalized

$$\beta_1|\phi_1\rangle = H|\phi_0\rangle - \langle\phi_0|H|\phi_0\rangle|\phi_0\rangle$$

$$\beta_2|\phi_2\rangle = H|\phi_1\rangle - \langle\phi_1|H|\phi_1\rangle|\phi_1\rangle - \langle\phi_0|H|\phi_1\rangle|\phi_0\rangle$$

$$\beta_3|\phi_3\rangle = H|\phi_2\rangle - \langle\phi_2|H|\phi_2\rangle|\phi_2\rangle - \langle\phi_1|H|\phi_2\rangle|\phi_1\rangle - \langle\phi_0|H|\phi_2\rangle|\phi_0\rangle$$

$\perp$ $\quad$ $\perp$ $\quad$ 0

$$H|\phi_0\rangle = \beta_1|\phi_1\rangle + \langle \quad \rangle|\phi_0\rangle$$

...

$$\beta_n|\phi_n\rangle = H|\phi_{n-1}\rangle - \langle\phi_{n-1}|H|\phi_{n-1}\rangle|\phi_{n-1}\rangle - \langle\phi_{n-2}|H|\phi_{n-2}\rangle|\phi_{n-2}\rangle$$

$$\beta_n|\phi_{n+1}\rangle = H|\phi_n\rangle - \langle\phi_n|H|\phi_n\rangle|\phi_n\rangle - \langle\phi_{n-1}|H|\phi_{n-1}\rangle|\phi_{n-1}\rangle$$

...

M vectors

Reduced Hamiltonian matrix on the Lanczos basis

$$\langle \phi_n | H | \phi_\ell \rangle = \alpha^* \delta_{\ell, n-1} + \beta^* \delta_{\ell, n} + \gamma^* \delta_{\ell, n+1}$$

$$H | \phi_\ell \rangle = \alpha | \phi_{n-1} \rangle + \beta | \phi_n \rangle + \gamma | \phi_{n+1} \rangle$$

$$\underset{H_{red}}{\{ \langle \phi_n | H | \phi_\ell \rangle \}} = \begin{pmatrix} \langle \phi_0 | H | \phi_0 \rangle & \langle \phi_0 | H | \phi_1 \rangle & 0 & \text{---} & \\ \langle \phi_1 | H | \phi_0 \rangle & \langle \phi_1 | H | \phi_1 \rangle & \langle \phi_1 | H | \phi_2 \rangle & 0 & \text{---} \\ 0 & \langle \phi_2 | H | \phi_1 \rangle & \langle \phi_2 | H | \phi_2 \rangle & \langle \phi_2 | H | \phi_3 \rangle & \text{---} \\ & & \ddots & \ddots & \ddots \end{pmatrix}$$

tridiagonal matrix

$\hookrightarrow$ M states and M eigenvalues

approximate the lowest M eigenvectors and eigenvalues of $\hat{H}$

ground state of H_{red} converge to the ground state of H as

$$\exp\left(- M \log\left(\frac{E_1}{E_0}\right)\right)$$

once you have reconstructed $|\Psi_0\rangle$

then the successive operations are equivalent to applying the power method to $|\phi\rangle - \langle \phi | \Psi_0 \rangle |\Psi_0\rangle$