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

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Today's class: *Second quantization (Part 2)*

- One-body and two-body operators in terms of creation and destruction operators.
- Density operator.
- Fermi-Dirac and Bose-Einstein distributions.

One-body operators

One-body operator written in a single-particle basis:

$$T_{kj} = \langle \varphi_k | \hat{T} | \varphi_j \rangle \Leftrightarrow \hat{T} = \sum_{kj} T_{kj} | \varphi_k \rangle \langle \varphi_j |$$

Matrix element:

$$T_{kj} = \int d^3\vec{r}\, \varphi_k^*(\vec{r})\; T(\vec{r}) \varphi_j(\vec{r})$$

Example: kinetic energy

$$K_{kj} = \left(\frac{-\hbar^2}{2m} \right) \int d^3\vec{r}\, \varphi_k^*(\vec{r})\; \nabla_{\vec{r}}^2 \varphi_j(\vec{r})$$

Two-body operators

Two-body operator written in a two-particle basis:

$$|\Phi_\alpha\rangle = S_\pm |\varphi_i\rangle \otimes |\varphi_j\rangle = \text{``}|\varphi_i\rangle|\varphi_j\rangle\text{''}$$

$$V_{\alpha\beta} = \langle\Phi_\alpha|\hat{V}|\Phi_\beta\rangle \Leftrightarrow \hat{V} = \sum_{\alpha\beta} V_{\alpha\beta}|\Phi_\alpha\rangle\langle\Phi_\beta|$$

Two-body operator written in a single-particle basis:

$$\Rightarrow \hat{V} = \sum_{ijkm} V_{ijkm}|\varphi_i\rangle|\varphi_j\rangle\langle\varphi_k|\langle\varphi_m| + \ldots$$

Matrix elements:

$$V_{ijkm} = \int d^3\vec{r}_1 d^3\vec{r}_2 \; \varphi_i^*(\vec{r}_1)\varphi_j^*(\vec{r}_2) \; V(\vec{r}_1,\vec{r}_2) \; \varphi_k(\vec{r}_1)\varphi_m(\vec{r}_2)$$

Operators in the N-body basis

One-body operator written in an N-particle basis:

$$\hat{T}^{(n)}|\varphi_{k_1}\rangle \dots |\varphi_{k_n}\rangle \dots |\varphi_{k_N}\rangle = \sum_{ij} T^{(n)}_{kj}\,\delta_{jk_n}|\varphi_{k_1}\rangle \dots |\varphi_{k}\rangle \dots |\varphi_{k_N}\rangle$$

Sum of N one-body operators written in a N-particle basis:

$$\hat{T}_{\rm tot} = \sum_{n=1}^{N} \hat{T}^{(n)}$$

$$\hat{T}_{\rm tot}|\varphi_{k_1}\rangle \dots |\varphi_{k_N}\rangle = \sum_{n=1}^{N}\sum_{kj} T^{(n)}_{kj}\,\delta_{jk_n}|\varphi_{k_1}\rangle \dots |\varphi_{k}\rangle \dots |\varphi_{k_N}\rangle$$

Position n !

Operators in the N-body bosonic basis

Orbitals: $|\varphi_k\rangle = \hat{b}_k^\dagger|0\rangle \qquad \langle\varphi_k| = \langle 0|\hat{b}_k$

One-body operator: $$\hat{T} = \sum_{kj} T_{kj}|\varphi_k\rangle\langle\varphi_j|$$

Two-body operator: $$\hat{V} = \sum_{ijkm} V_{ijkm}|\varphi_i\rangle|\varphi_j\rangle\langle\varphi_k|\langle\varphi_m|$$

N-body operators (sum): $$\hat{T}_{\text{tot}} = \sum_{n=1}^{N} \hat{T}^{(n)}$$

$$\hat{V}_{\text{tot}} = \frac{1}{2} \sum_{n,n'=1(n\neq n')}^{N} \hat{V}^{(n,n')}$$

Operators in the N-body bosonic basis

Number occupation representation:

$$\sum_j n_j = N$$

$$|n_1, n_2, \ldots n_k \ldots n_N\rangle \propto (\hat{b}_1^\dagger)^{n_1} (\hat{b}_2^\dagger)^{n_2} \ldots (\hat{b}_k^\dagger)^{n_k} \ldots (\hat{b}_N^\dagger)^{n_N} |0\rangle$$

Let's show that:

$$\hat{T}_{\text{tot}} |n_1, n_2, \ldots n_k \ldots n_N\rangle = \sum_{kj} T_{kj} \hat{b}_k^\dagger \hat{b}_j |n_1, n_2, \ldots n_k \ldots n_j \ldots n_N\rangle$$

Now you show that (Assignment):

Notice the order!

$$\hat{V}_{\text{tot}} |n_1, n_2, \ldots n_N\rangle = \sum_{ijkm} V_{ijkm} \hat{b}_i^\dagger \hat{b}_j^\dagger \hat{b}_m \hat{b}_k |n_1, n_2, \ldots n_N\rangle$$

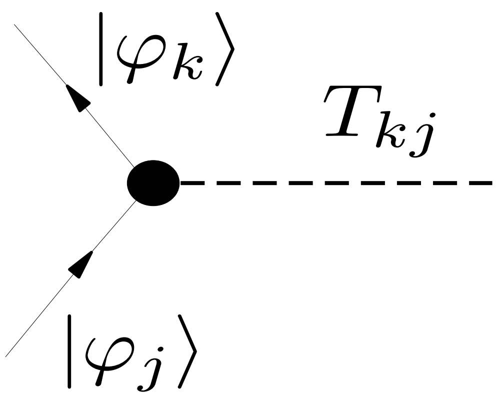
Operators in second quantized form

We then write (Bosons):

$$\hat{T}_{\mathrm{tot}} = \sum_{kj} T_{kj} \hat{b}_k^\dagger \hat{b}_j$$

$$\hat{V}_{\mathrm{tot}} = \sum_{ijkm} V_{ijkm} \hat{b}_i^\dagger \hat{b}_j^\dagger \hat{b}_m \hat{b}_k$$

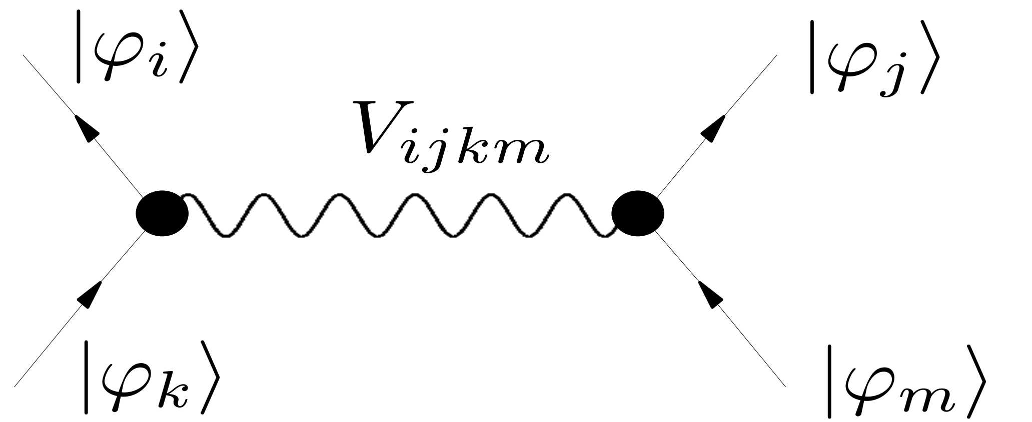
"Diagrams":



It turns out that, for Fermions, they take the *same form* (Assignment):

$$\hat{T}_{\mathrm{tot}} = \sum_{kj} T_{kj} \hat{c}_k^\dagger \hat{c}_j$$

$$\hat{V}_{\mathrm{tot}} = \sum_{ijkm} V_{ijkm} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_m \hat{c}_k$$



Example: non-interacting system

Hamiltonian:

$$\hat{H}_{\mathrm{tot}} = \sum_{n=1}^{N} \hat{h}^{(n)}$$

Single-particle basis:

$$\hat{h}|\varphi_i\rangle = \epsilon_i|\varphi_i\rangle$$

In this basis:

$$\hat{H}_{\mathrm{tot}} = \sum_{k} \epsilon_k \hat{n}_k$$

$\hat{n}_k = \hat{c}_k^\dagger \hat{c}_k$ (Fermions)

$\hat{n}_k = \hat{b}_k^\dagger \hat{b}_k$ (Bosons)

Many-body spectrum:

$$\hat{H}_{\mathrm{tot}}|n_1, \ldots, n_N\rangle = \left(\sum_k \epsilon_k n_k\right)|n_1, \ldots, n_N\rangle$$

$$E_{n_1,\ldots,n_N} = \sum_{k=1}^{N} \epsilon_k n_k$$

Density operator

Canonical :

$$\hat{\rho} \equiv e^{-\beta \hat{H}_{\mathrm{tot}}} \qquad \beta = \frac{1}{k_B T}$$

Grand-canonical:

$$\hat{\rho}_G \equiv e^{-\beta\left(\hat{H}_{\mathrm{tot}} - \mu \hat{N}\right)} \qquad \hat{N} = \sum_{k=1}^{N} \hat{n}_k$$

Many-particle spectrum:

$$\hat{H}_{\mathrm{tot}} |\alpha\rangle = E_\alpha |\alpha\rangle$$

Partition function:

$$\mathcal{Z} = \sum_\alpha e^{-\beta E_\alpha} = \mathrm{Tr}(\hat{\rho})$$

Thermal average:

$$\langle \hat{A} \rangle = \frac{\mathrm{Tr}\left(\hat{\rho}\hat{A}\right)}{\mathrm{Tr}\left(\hat{\rho}\right)} = \frac{1}{\mathcal{Z}} \sum_\alpha A_\alpha e^{-\beta E_\alpha}$$

Assignment

Given the non-interacting Hamiltonian

$$\hat{H}_{\mathrm{tot}} = \sum_k \epsilon_k \hat{n}_k$$

calculate the grand-canonical thermal average of $\hat{n}_k$

$$\langle \hat{n}_k \rangle = \frac{\mathrm{Tr}\left(\hat{\rho}_G \hat{n}_k\right)}{\mathrm{Tr}\left(\hat{\rho}_G\right)}$$

for both Bosons and for Fermions.