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

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Today's class: *Many-particle quantum systems in 1st quantization.*

- N-particle quantum systems ("1st quantization")
- *Examples: Two particles in an harmonic oscillator*
- *Assignment: Helium atom.*

N-particle systems ("First quantization")

- Example of an N-particle Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N} \left(\frac{|\vec{p}_i|^2}{2m_i} + U(\vec{r}_i) \right) + \frac{1}{2} \sum_{i,j(i\neq j)=1}^{N} V(\vec{r}_i, \vec{r}_j)$$

Single-particle operators

Two-particle operators (e.g., interactions)

- Schrödinger's equation (Dirac's notation):

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = \hat{H} |\Psi(t)\rangle$$

"ket"

$$(|\Psi(t)\rangle)^\dagger = \langle \Psi(t)|$$ "bra"

$$\langle \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N | \Psi(t) \rangle = \Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, t)$$

$$\langle \Phi | \Psi \rangle = ?$$

$$\langle \Phi | \Psi \rangle = \int d^3\vec{r}_1 \; d^3\vec{r}_2 \; \ldots \; d^3\vec{r}_N \; \Phi^*(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$$

N-particle systems: Basis set

- Basis out of single-particle states:

$$\{|\Phi_\alpha\rangle\} = \{|\varphi_{\alpha_1}\rangle\} \otimes \{|\varphi_{\alpha_2}\rangle\} \otimes \cdots \otimes \{|\varphi_{\alpha_N}\rangle\}$$

orthonormal basis (complete set) of the *N*-particle Hilbert's space

$$\langle\Phi_\alpha|\Phi_\beta\rangle = \delta_{\alpha\beta} \qquad \text{and} \qquad \sum_\alpha |\Phi_\alpha\rangle\langle\Phi_\alpha| = \mathbb{1}$$

- Any N-particle state can be written in this basis:

$$|\Psi(t)\rangle = \sum_\alpha C_\alpha(t)|\Phi_\alpha\rangle \qquad \text{with} \qquad C_\alpha(t) = \langle\Phi_\alpha|\Psi(t)\rangle$$

- We can also use the full spectrum from a N-particle operator as a basis (much harder though!). Example:

$$\{|\Psi_n\rangle\} : \hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

Systems of identical particles

- System of N *distinguishable* particles: you can differentiate the particles by performing measurements.

  Examples: “classical” particles, quantum particles with different mass (electrons and muons) or charge (electrons and protons).

- In a system of N quantum *identical* particles, they become *indistinguishable* if the have the same (observable) quantum numbers (mass, charge, spin, etc.).

- In this case, one cannot perform measurements to tell which particle is which.

  Examples: system of N electrons with the same spin (spin-polarized or “spinless”).

Systems of identical particles

- Thus, the “exchange” of two identical particles *cannot* be experimentally detected: it should have the *same probability density* (experimental fact):

$$|\Psi(\vec{r}_1,\ldots,\vec{r}_{\mathbf{k}},\ldots\vec{r}_{\mathbf{m}},\ldots\vec{r}_N)|^2 = |\Psi(\vec{r}_1,\ldots,\vec{r}_{\mathbf{m}},\ldots,\vec{r}_{\mathbf{k}},\ldots\vec{r}_N)|^2$$

$$\Psi(\vec{r}_1,\ldots,\vec{r}_{\mathbf{k}},\ldots,\vec{r}_{\mathbf{m}},\ldots\vec{r}_N) = e^{i\theta}\Psi(\vec{r}_1,\ldots,\vec{r}_{\mathbf{m}},\ldots,\vec{r}_{\mathbf{k}},\ldots\vec{r}_N)$$

States are the *same* up to a global phase

- In 3D, it is an *experimental fact* that a second exchange of the same particles brings the state back to the initial one. Thus:

$$e^{2i\theta} = 1 \Rightarrow \begin{cases} \theta = 0 & \text{(Bosons)} \quad \Psi(\ldots,\vec{r}_{\mathrm{k}},\ldots,\vec{r}_{\mathrm{m}},\ldots) = +\Psi(\ldots,\vec{r}_{\mathrm{m}},\ldots,\vec{r}_{\mathrm{k}},\ldots) \\ \theta = \pi & \text{(Fermions)} \quad \Psi(\ldots,\vec{r}_{\mathrm{k}},\ldots,\vec{r}_{\mathrm{m}},\ldots) = -\Psi(\ldots,\vec{r}_{\mathrm{m}},\ldots,\vec{r}_{\mathrm{k}},\ldots) \end{cases}$$

An example with N=2

- Two (indistinguishable) particles in a harmonic oscillator:

$$\hat{H} = \left(\frac{\hat{p}_1^2}{2m} + \frac{1}{2}m\omega\hat{x}_1^2\right) + \left(\frac{\hat{p}_2^2}{2m} + \frac{1}{2}m\omega\hat{x}_2^2\right) = \hat{H}^{(1)} + \hat{H}^{(2)}$$

- Spectrum (complete set): basis for single-particle states.

$$\hat{H}^{(1)}|n_1\rangle_1 = E_{n_1}|n_1\rangle_1 \qquad \hat{H}^{(2)}|n_2\rangle_2 = E_{n_2}|n_2\rangle_2$$

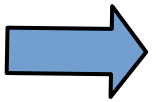
- Single-particle and two-particle basis states:

$$\begin{matrix}|0\rangle_1 \\ |1\rangle_1 \\ |2\rangle_1 \\ \vdots\end{matrix} \otimes \begin{matrix}|0\rangle_2 \\ |1\rangle_2 \\ |2\rangle_2 \\ \vdots\end{matrix} \Rightarrow \begin{matrix}|\Phi_0\rangle = |0\rangle_1 \otimes |0\rangle_2 \\ |\Phi_1\rangle = |0\rangle_1 \otimes |1\rangle_2 \\ |\Phi_2\rangle = |1\rangle_1 \otimes |0\rangle_2 \\ |\Phi_3\rangle = |1\rangle_1 \otimes |1\rangle_2 \\ |\Phi_4\rangle = |0\rangle_1 \otimes |2\rangle_2 \\ \vdots\end{matrix}$$

An example with N=2

- Position representation: $\langle x|n\rangle = \varphi_n(x)$
- Two particle states:

$$|\Phi_\alpha\rangle = |n_1\rangle_1 \otimes |n_2\rangle_2$$



$$\begin{aligned}\langle x_1 x_2|\Phi_\alpha\rangle &= \langle x_1|n_1\rangle_1 \langle x_2|n_2\rangle_2 \\ &= \varphi_{n_1}(x_1)\varphi_{n_2}(x_2) \\ &= \Phi_\alpha(x_1, x_2)\end{aligned}$$

- Is this basis appropriate for indistinguishable particles?

$$\left\{\begin{array}{lcl} |\Phi_0\rangle & = & |0\rangle_1 \otimes |0\rangle_2 \\ |\Phi_1\rangle & = & |0\rangle_1 \otimes |1\rangle_2 \\ |\Phi_2\rangle & = & |1\rangle_1 \otimes |0\rangle_2 \\ |\Phi_3\rangle & = & |1\rangle_1 \otimes |1\rangle_2 \\ |\Phi_4\rangle & = & |0\rangle_1 \otimes |2\rangle_2 \\ \vdots & & \end{array}\right.$$

For example:

$$\Phi_2(x_1, x_2) = ? \pm \Phi_2(x_2, x_1)$$

$$\varphi_1(x_1)\varphi_0(x_2) \neq \pm\varphi_1(x_2)\varphi_0(x_1)$$

No!

This basis is not appropriate for indistinguishable particles.

Symmetrizing/Antisymmetrizing Bosons and Fermions

Original basis

$$\begin{aligned}
\Phi_1(x_1,x_2) &= \varphi_0(x_1)\varphi_0(x_2)\\
\Phi_2(x_1,x_2) &= \varphi_0(x_1)\varphi_1(x_2)\\
\Phi_3(x_1,x_2) &= \varphi_1(x_1)\varphi_0(x_2)\\
\Phi_4(x_1,x_2) &= \varphi_1(x_1)\varphi_1(x_2)\\
\Phi_5(x_1,x_2) &= \varphi_0(x_1)\varphi_2(x_2)\\
&\vdots
\end{aligned}$$

Symmetrized Basis (Bosons)

$$\begin{aligned}
\Phi_1^S(x_1,x_2) &= \varphi_0(x_1)\varphi_0(x_2)\\
\Phi_2^S(x_1,x_2) &= \tfrac{1}{\sqrt{2}}\left(\varphi_0(x_1)\varphi_1(x_2)+\varphi_1(x_1)\varphi_0(x_2)\right)\\
\Phi_3^S(x_1,x_2) &= \varphi_1(x_1)\varphi_1(x_2)\\
\Phi_4^S(x_1,x_2) &= \tfrac{1}{\sqrt{2}}\left(\varphi_0(x_1)\varphi_2(x_2)+\varphi_2(x_1)\varphi_0(x_2)\right)\\
&\vdots
\end{aligned}$$

Antisymmetrized Basis (Fermions)

$$\begin{aligned}
\Phi_1^A(x_1,x_2) &= \tfrac{1}{\sqrt{2}}\left(\varphi_0(x_1)\varphi_1(x_2)-\varphi_1(x_1)\varphi_0(x_2)\right)\\
\Phi_2^A(x_1,x_2) &= \tfrac{1}{\sqrt{2}}\left(\varphi_0(x_1)\varphi_2(x_2)-\varphi_2(x_1)\varphi_0(x_2)\right)\\
&\vdots
\end{aligned}$$

Now, particle exchange is well-defined!

$$\Phi_\alpha^{S,A}(x_1,x_2) = \pm\Phi_\alpha^{S,A}(x_2,x_1)$$

How about spin, etc.?

Sometimes, there are other “good quantum numbers” labeling the single-particle states. How to account for this?

There are a few of ways to deal with it:

1) Count each single-particle state with a given “set” of quantum numbers as “one single particle state”

Example: $|\varphi_{n\ell m\sigma}\rangle \rightarrow |\varphi_{\alpha}\rangle$ *n=0,1,2... , l=0,1,..,n-1 ; m=-l,..,+l,* $\sigma=\uparrow,\downarrow$

$$|\varphi_{000\uparrow}\rangle \rightarrow |\varphi_{0}\rangle \ , \ |\varphi_{000\downarrow}\rangle \rightarrow |\varphi_{1}\rangle \ , \ |\varphi_{100\uparrow}\rangle \rightarrow |\varphi_{2}\rangle \ \ldots$$

2) You can also build many-particle states directly from sum of angular momenta (“multiplets”). This is trickier but useful.

$$|\varphi^{(1)}_{\ell_1 m_1 \sigma_1}\rangle \otimes |\varphi^{(2)}_{\ell_2 m_2 \sigma_2}\rangle \rightarrow |\Phi_{J M_J}\rangle$$

3) …

Assignment: Helium atom

Consider the Hamiltonian:

$$\hat{H} = \hat{H}^{(1)} + \hat{H}^{(2)} + \hat{V}_{1,2}$$

$$\hat{H}^{(i)}|\phi_n^{(i)}\rangle = E_n^{(i)}|\phi_n^{(i)}\rangle$$

$\langle \vec{r}|\phi_n^{(i)}\rangle \rightarrow$ Hydrogen atom eigenstates (single particle).

$\hat{V}_{1,2} = \dfrac{(e^2/4\pi\epsilon_0)}{|\vec{r}_1 - \vec{r}_2|} \rightarrow$ Electron-electron repulsion (two-body)

Table 3.2 Hydrogenic radial wavefunctions

n	l	Orbital	$R_{nl}(r)$
1	0	$1s$	$(Z/a)^{3/2}2e^{-\rho/2}$
2	0	$2s$	$(Z/a)^{3/2}(1/8)^{1/2}(2-\rho)e^{-\rho/2}$
	1	$2p$	$(Z/a)^{3/2}(1/24)^{1/2}\rho e^{-\rho/2}$

$\rho = (2Z/na)r$ with $a = 4\pi\epsilon_0\hbar^2/\mu e^2$. For an infinitely heavy nucleus, $\mu = m_e$ and $a = a_0$, the Bohr radius.

1) Consider first the *non-interacting* case ($V_{1,2}$=0). Write the two-particle ground-state $\langle \vec{r}_1\vec{r}_2|\Phi_0^A\rangle$. What is its energy (in eV)?

2) Write the matrix element $\langle \Phi_0^A|\hat{V}_{1,2}|\Phi_0^A\rangle$ (no need to solve the integral).

This is the first correction to the ground-state energy for the He atom!

Hint: the table gives the expressions for the radial wavefunctions for the Hydrogen.