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

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Today’s class: *Review of Quantum Mechanics*

- Single-particle quantum systems
- *Example: Harmonic oscillator*
- *Assigments: Ladder operators.*

Single-particle systems
("First quantization")

- Single-particle Hamiltonian:

$$\hat{H} = \frac{\left(\vec{p} - q\vec{A}\right)^2}{2m^*} + U(\vec{r})$$

Non-relativistic particle under a pontential $U(\vec{r})$ and magnetic field $\vec{B} = \nabla \times \vec{A}$

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

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

"ket"

$$\left\{ \begin{array}{l} \left(|\psi(t)\rangle\right)^\dagger = \langle\psi(t)| \\ \langle\vec{r}|\psi(t)\rangle = \psi(\vec{r},t) \\ \langle\phi|\psi\rangle = \int d^3\vec{r}\,\phi^*(\vec{r})\psi(\vec{r}) \end{array} \right.$$

"bra"

Basis in the Hilbert space

$\{|\varphi_\alpha\rangle\} \rightarrow$ orthonormal basis (complete set) of the single-particle Hilbert's space.

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

We can write: $|\psi(t)\rangle = \sum_\alpha C_\alpha(t)|\varphi_\alpha\rangle$ with $C_\alpha(t) = \langle\varphi_\alpha|\psi(t)\rangle$

Operators!
$$\left\{\begin{array}{l} \hat{A}|\psi\rangle = |\phi\rangle \\ \langle\psi|\hat{A}^\dagger = \langle\phi| \end{array}\right.$$

Representation in the $\{|\varphi_\alpha\rangle\}$ basis:

$$\left\{\begin{array}{l} A_{\alpha\beta} = \langle\varphi_\alpha|\hat{A}|\varphi_\beta\rangle = \langle\varphi_\alpha|\left(\hat{A}|\varphi_\beta\rangle\right) \\ A^*_{\beta\alpha} = \langle\varphi_\beta|\hat{A}^\dagger|\varphi_\alpha\rangle = \left(\langle\varphi_\beta|\hat{A}^\dagger\right)|\varphi_\alpha\rangle \end{array}\right.$$

Observables (Hermitian operators)

$$\left\{\begin{array}{ll} \hat{A} = \hat{A}^\dagger \rightarrow & \text{Hermitian operator.} \\ \hat{A}|\varphi_a\rangle = a|\varphi_a\rangle \rightarrow a \in \mathbb{R} & \text{Real eigenvalues (Physical observable).} \\ P_\psi(a) \equiv |\langle\varphi_a|\psi\rangle|^2 \rightarrow & \text{Probability of measuring the value } a \text{ for the observable } \hat{A} \text{ if the particle is in state } |\psi\rangle \end{array}\right.$$

Obs: if the spectrum is continuous, this becomes a *probability density*.

Example: position operator:

$$dP_\psi(\vec{r}) \equiv |\langle\vec{r}|\psi(t)\rangle|^2 d^3\vec{r} = |\psi(\vec{r},t)|^2 d^3\vec{r}$$

Probability of the particle in state $|\psi(t)\rangle$ being in a volume $d^3\vec{r}$ around position $\vec{r}$ at a time *t*.

Example: 1D Harmonic oscillator

Hamiltonian: $$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$$ with $$[\hat{x}, \hat{p}] = i\hbar$$

Position rep. $$\langle \vec{r} | \hat{p} | \psi(t) \rangle = \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x, t)$$

Let us define:

$$\left\{ \begin{aligned} \hat{X} &= \sqrt{\frac{m\omega}{\hbar}} \hat{x} \\ \hat{P} &= \frac{1}{\sqrt{m\hbar\omega}} \hat{p} \end{aligned} \right. \Longrightarrow \hat{H} = \frac{\hbar\omega}{2} \left(\hat{P}^2 + \hat{X}^2 \right)$$

and

$$\left\{ \begin{aligned} \hat{a} &= \frac{1}{\sqrt{2}} \left(\hat{X} + i\hat{P} \right) \\ \hat{a}^\dagger &= \frac{1}{\sqrt{2}} \left(\hat{X} - i\hat{P} \right) \end{aligned} \right. \Longleftrightarrow \left\{ \begin{aligned} \hat{X} &= \frac{1}{\sqrt{2}} \left(\hat{a}^\dagger + \hat{a} \right) \\ \hat{P} &= \frac{i}{\sqrt{2}} \left(\hat{a}^\dagger - \hat{a} \right) \end{aligned} \right.$$

Example: 1D Harmonic oscillator

Let us show that: $$\left[\hat{X}, \hat{P}\right] = i$$ and $$\left[\hat{a}, \hat{a}^\dagger\right] = 1$$

Also: $$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

You will show (Assignment) that:

$$[\hat{a}, \hat{a}] = \left[\hat{a}^\dagger, \hat{a}^\dagger\right] = 0$$

Defining: $$\hat{N} \equiv \hat{a}^\dagger\hat{a}$$ (Show it commutes with *H* (Assignment))

and its eigenstates : $$\hat{N}|n\rangle = n|n\rangle$$ where *n* is an integer (Show).

It follows that:

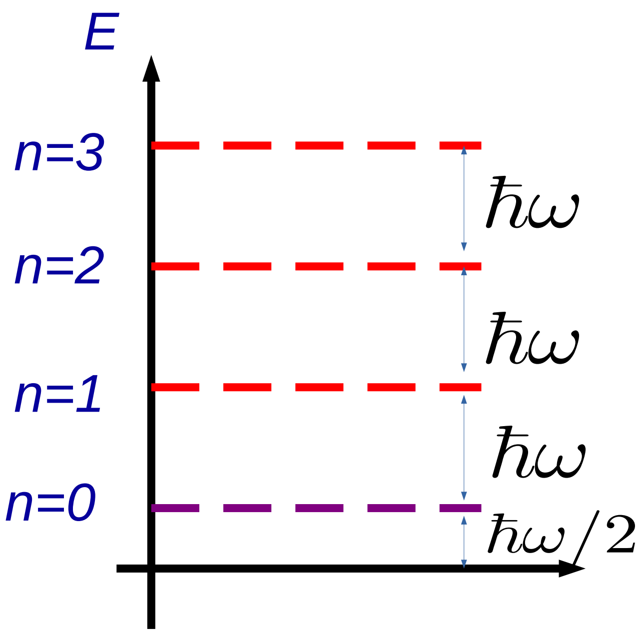
(Show)

$$\left\{\begin{aligned} &\hat{H}|n\rangle = E_n|n\rangle \\ &a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \\ &a|n\rangle = \sqrt{n}|n-1\rangle \end{aligned}\right.$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \quad n = 0, 1, \ldots$$

$$|n\rangle = \frac{\left(\hat{a}^\dagger\right)^n}{\sqrt{n!}}|0\rangle$$

Single-particle spectrum



$$\hat{H}|n\rangle = E_n|n\rangle$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \quad n = 0, 1, \ldots$$

Ground state: $E_0 = \hbar\omega$

$\{|n\rangle\} \rightarrow$ orthonormal basis of the (single-particle) Hilbert's space

$\langle n|n'\rangle = \delta_{nn'}$ and $\sum_n |n\rangle\langle n| = \mathbb{1}$

Single-particle state: $|\psi(t)\rangle = \sum_n C_n(t)|n\rangle$ with $C_n(t) = \langle n|\psi(t)\rangle$

$P_\psi(n) \equiv |\langle n|\psi\rangle|^2 \rightarrow$ Probability of measuring the value E_n for the energy if the particle is in state $|\psi\rangle$

Assignments: Ladder operators

Problem 1

Consider the 1D harmonic oscillator Hamiltonian $H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$ and the operators $\hat{a}$ e $\hat{a}^\dagger$ discussed in class.

1. Show that $[\hat{a}, \hat{a}^\dagger] = 1$ and that $[\hat{a}, \hat{a}] = [\hat{a}^\dagger, \hat{a}^\dagger] = 0$.
2. Show that $\hat{N} \equiv \hat{a}^\dagger \hat{a}$ comutes with H.
3. Show that, if $\hat{N}|\lambda\rangle = \lambda|\lambda\rangle$ then λ is a positive integer. Suggestion: show that $\hat{a}|\lambda\rangle$ is also an eigenstate of $\hat{N}$ and that $\hat{a}|0\rangle = 0$.
4. If $\hat{N}|n\rangle = n|n\rangle$, show that $|n\rangle \propto (\hat{a}^\dagger)^n|0\rangle$ where "$|0\rangle$" is such that $\hat{a}|0\rangle = 0$.
5. Show that:

   $$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$$
   $$\hat{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle\ .$$

6. Show that:

   $$\hat{a}\hat{a}^\dagger\left(\hat{a}^\dagger\right)^{p-1}|0\rangle = p\left(\hat{a}^\dagger\right)^{p-1}|0\rangle.$$

   (p is an integer)

Problem 2

Consider the single particle Hamiltonian:

$$H = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}\right) + \hbar\omega_0\left(\hat{a}^\dagger + \hat{a}\right)\ ,$$

where $\hat{a}$ and $\hat{a}^\dagger$ are (bosonic) ladder operators satisfying $[\hat{a}, \hat{a}^\dagger] = 1$ and ω and ω_0 are positive constants.

1. Discuss the physical origin of the second term in H, by comparing it with the harmonic oscillator
2. Diagonalize H and find its eigenenergies. Suggestion: introduce an operator $\hat{\alpha} = \hat{a} + \omega_0/\omega$.