第二章 波函数和 Schroedinger 方程

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1. 态叠加原理

如果 Ψ_1 和 Ψ_2 是体系的可能状态,则它们的线性叠加

$$\Psi = c_1\Psi_1 + c_2\Psi_2 \quad (c_1, c_2 \text{是复数})$$

也是这个体系的一个可能状态.

$$\Psi(\vec{r},t) \leftrightarrow C(\vec{p},t)$$

$$\begin{cases} C(\vec{p},t) = \dfrac{1}{(2\pi\hbar)^{3/2}} \displaystyle\iiint_{-\infty}^{\infty} \Psi(\vec{r},t)\, e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}}\, dx\,dy\,dz \\ \Psi(\vec{r},t) = \dfrac{1}{(2\pi\hbar)^{3/2}} \displaystyle\iiint_{-\infty}^{\infty} C(\vec{p},t)\, e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}\, dp_x\,dp_y\,dp_z \end{cases}$$

2. Schrödinger方程 (量子力学的一个基本假设)

Time-dependent Schrödinger Equation:

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + U(\vec{r})\Psi$$

算符: $E \to i\hbar\frac{\partial}{\partial t}$; $\vec{p} \to -i\hbar\nabla$

3. 几率流密度

$$\vec{J} = \frac{i\hbar}{2m}(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi)$$

几率连续性方程:

$$\frac{\partial}{\partial t}w + \nabla\cdot\vec{J} = 0$$

↳ $w(\vec{r},t) = \Psi^*(\vec{r},t)\Psi(\vec{r},t)$

4. 定态 Schrödinger方程

Time-independent Schrödinger Equation:

$$\hat{H}\Psi = E\Psi$$

↳ $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})$

定态波函数: $\Psi(\vec{r},t) = \psi(\vec{r})\, e^{-\frac{i}{\hbar}Et}$

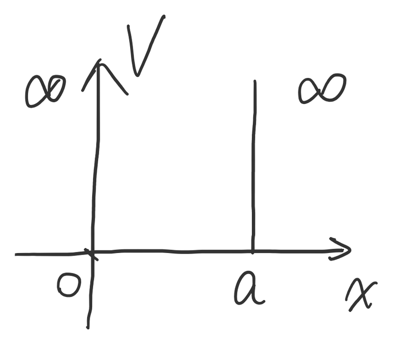
定态的性质:
- ① 粒子在空间几率和时间无关: $w(\vec{r},t) = |\Psi(\vec{r},t)|^2 = |\psi(\vec{r})|^2$
- ② 几率流密度与时间无关
- ③ 能量和时间无关

含时Schrödinger方程的一般解可以写成定态波函数的线性叠加:

$$\Psi(\vec{r},t) = \sum_n C_n\psi_n(\vec{r})\, e^{-\frac{i}{\hbar}E_n t}$$

5. 一维无限深方势阱

①

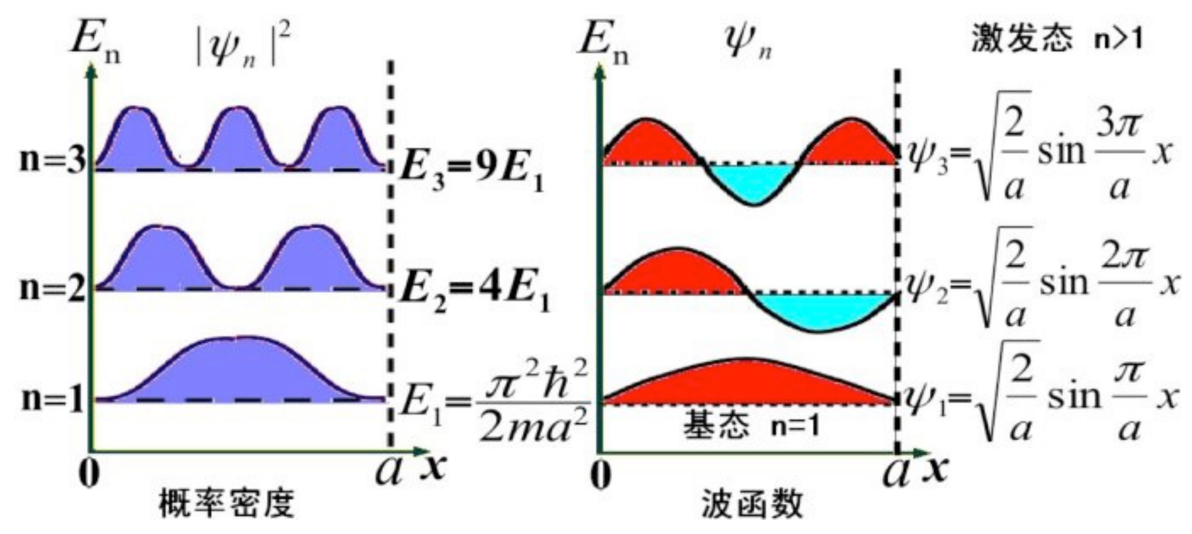


$$V(x) = \begin{cases} 0 & 0<x<a \\ \infty & x<0,\ x>a \end{cases}$$

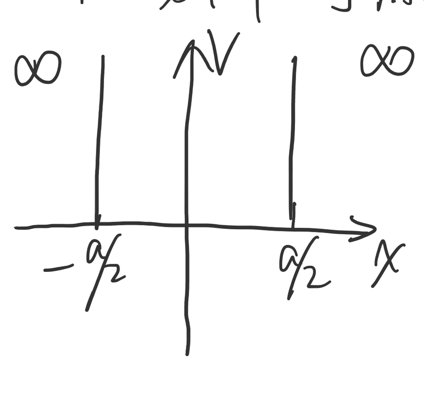
$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) & 0<x<a \\ 0 & x<0,\ x>a \end{cases}$$

⇒ 基态无节点, 第k个激发态有k个节点 (n=1) (n=k+1) (除 $x=0$ 和 $x=a$)

$$E_n = \frac{\hbar^2\pi^2n^2}{2ma^2} \qquad n=1,2,\cdots$$



② 如果方势阱关于原点对称:



$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}}\cos\left(\frac{n\pi x}{a}\right) & n=1,3,5,\cdots \quad |x|<\frac{a}{2} \\ \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) & n=2,4,6,\cdots \quad |x|<\frac{a}{2} \\ 0 & |x|>\frac{a}{2} \end{cases}$$

$$E_n = \frac{\hbar^2\pi^2n^2}{2ma^2} \qquad n=1,2,\cdots$$

6. 宇称

空间反射: $\vec{r} \to -\vec{r}$; $\Psi(\vec{r},t) \to \Psi(-\vec{r},t)$

空间反射下,如果有 $\Psi(-\vec{r},t) = \pm\Psi(\vec{r},t)$, 则称波函数有确定的宇称(状态具有空间对称性)

$$\begin{cases} \Psi(-\vec{r},t) = \Psi(\vec{r},t) & \text{偶宇称} \\ \Psi(-\vec{r},t) = -\Psi(\vec{r},t) & \text{奇宇称} \end{cases}$$

7. 线性谐振子 ($E_p = \frac{1}{2}m\omega^2x^2$)

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

$$\psi_n(x) = N_n e^{-\frac{\alpha^2}{2}x^2}H_n(\alpha x)$$

↳ $\alpha = \sqrt{\frac{m\omega}{\hbar}}$

↳ $N_n = \left(\frac{\alpha}{\pi^{\frac{1}{2}}2^n n!}\right)^{1/2}$