第三课：Schrodinger方程

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1. 哥本哈根解释：
   a. 概率波$|\psi|^2$；
   b. 不确定原理($p\times q \neq q\times p$)；
   c. 互补原理(粒子/波⇒量子态)
2. 波函数假设：S方程⇒ ψ；
3. 算符：$\hat{F}\cdot\psi = f\cdot\psi$；
4. 薛定谔方程：$-\frac{\hbar^2}{2m}\nabla^2\psi + \mu\psi = \frac{i\hbar\partial\psi}{\partial t}$
   a. 记作：$\hat{H}\psi = \mathrm{E}\psi = \frac{\mathrm{i}\hbar\,\partial\psi}{\partial \mathrm{t}}$ (其中$\hat{\mathrm{H}}$为哈密顿算符);
5. 定态薛定谔方程：
   a. 当势能μ与时间t无关时，势能记作$\mu(\vec{r})$，波函数为$\psi(\vec{r},t) = \psi(r)\cdot\psi(t)$；
   b. $\Rightarrow \psi(t)\left[-\frac{\hbar^2}{2m}\nabla^2\psi(r)\right] + \mu(r)\cdot\psi(r)\psi(t) = \psi(r)\cdot\frac{i\hbar\psi(t)}{\partial(t)}$;
   c. 两边同除以$\psi(\mathrm{r})\cdot\psi(\mathrm{t})$ $\Rightarrow \frac{1}{\psi(\mathrm{r})}\cdot\left(-\frac{\hbar^2}{2\mathrm{m}}\nabla^2\psi(\mathrm{r})\right) + \mu(\mathrm{r}) = \frac{1}{\psi(\mathrm{t})}\cdot\frac{\mathrm{i}\hbar^2\,\partial\psi(\mathrm{t})}{\partial \mathrm{t}} = \mathrm{E}$;
   d. 得到方程组：
      i. $\frac{i\hbar\partial\psi(t)}{\partial t} = E\cdot\psi(t)$;
      ii. $-\frac{\hbar^2}{2m}\nabla^2\psi(r) + \mu(r)\cdot\psi(r) = E\psi(r)$ (定态薛定谔方程，E确定);
   e. $\because \psi(t) = e^{\frac{E}{i\hbar}t} = e^{-\frac{iE}{\hbar}t}$;
   f. 求解得：$\psi(r,t) = \psi(r)\cdot e^{-\frac{iE}{\hbar}t}$
6. 定态的性质：
   a. 粒子在空间的几率密度($|\psi|^2 = \psi_n * \psi_n = \omega_n(\vec{r},t)$)与时间无关；
   b. 几率流密度($\vec{J_n}(\vec{r},t) = \vec{J}_n(\vec{r})$)与时间按无关；
   c. 任何不显含t的力学量平均值与t无关；
7. 一维无限深势阱：
   a. 薛定谔方程的一维形式：$-\frac{\hbar^2}{2m}\nabla^2\psi(x) + \mu(x)\cdot\psi(x) = E\psi(x)$；
   b. 一维无限深势阱：
      i. $V(x) = \begin{cases} 0, & |x| \le a, \\ \infty, & |\mathrm{x}| > \mathrm{a} \end{cases}$;
   c. $\because -\frac{\hbar^2}{2\mu}\cdot\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \Rightarrow \frac{d^2}{dx^2}\psi(x) - \frac{2\mu}{\hbar^2}[V(x)-E]\psi(x) = 0$;
   d. 各势区的S方程：
      i. $\frac{d^2}{dx^2}\psi^I(x) - \frac{2\mu}{\hbar^2}(V-E)\psi^I(x) = 0,\ x \le -a$;
      ii. $\frac{d^2}{dx^2}\psi^{II}(x) + \frac{2\mu}{\hbar^2}E\psi^{II}(x) = 0,\ -a < x < a$ (记$\frac{2\mu}{\hbar^2}E = \alpha^2$);
      iii. $\frac{d^2}{dx^2}\psi^{III}(x) - \frac{2\mu}{\hbar^2}(V-E)\psi^{III}(x) = 0,\ x \le -a$ (记$\frac{2\mu}{\hbar^2}(V-E) = \beta^2$);
   e. 简记作：
      $\frac{d^2}{dx^2}\psi^I - \beta^2\psi^I = 0$
      $\frac{d^2}{dx^2}\psi^{II} + \alpha^2\psi^{II} = 0$;
      $\frac{d^2}{dx^2}\psi^{III} - \beta^2\psi^{III} = 0$
   f. 因为波函数具有周期性；
   g. $\alpha^2 = \left(\frac{n\pi}{a}\right)^2 = \frac{2\mu}{\hbar^2}E \Rightarrow E = \frac{\hbar^2}{2\mu}\cdot\left(\frac{n\pi}{a}\right)^2 = \frac{\hbar^2 n^2\pi^2}{2\mu a^2}$;
   h. $\begin{vmatrix} A\cdot\sin(-\alpha a+\delta) = 0 & \Rightarrow & A\cdot\sin(-\alpha a)\cos\delta + A\cdot\cos(\alpha a)\sin\delta = 0 \\ A\cdot\sin(\alpha a+\delta) = 0 & \Rightarrow & A\cdot\sin(\alpha a)\cos\delta + A\cdot\cos(\alpha a)\sin\delta = 0 \end{vmatrix}$;
   i. $\Rightarrow \begin{vmatrix} \cos(\alpha a)\sin\delta = 0 & \Rightarrow & \sin\delta = 0\ or\ \cos\alpha a = 0 \\ \sin(\alpha a)\cos\delta = 0 & \Rightarrow & \cos\delta = 0\ or\ \sin\alpha a = 0 \end{vmatrix}$;
   j. 分析其中两种情况：
      i. $\sin\delta = 0 \Rightarrow \delta = 0$;
         1) $\cos\delta = 1 \Rightarrow \sin\alpha a = 0$;
         2) $\because \alpha^2 = \frac{2\mu}{\hbar^2}E$;
         3) $\alpha a = n\pi \Rightarrow \alpha = \frac{n\pi}{a}\ (n = 0, \pm1, \pm2, \dots)$;
         4) $\Rightarrow E = \frac{\hbar^2}{2\mu}\alpha^2 = \frac{\hbar^2}{2\mu}\left(\frac{n\pi}{a}\right)^2 = \frac{n^2\pi^2\hbar^2}{2\mu a^2} = E_n$;
         5) $\psi_n^{II} = A\cdot\sin\alpha x = A\cdot\sin(\frac{n\pi}{a}x)$;
      ii. $\cos\delta = 0 \Rightarrow \delta = \frac{\pi}{?}$;

1) $\sin\delta = 1 \Rightarrow \cos\alpha a = 0$;

2) $E_n = \frac{\hbar^2}{2\mu}\alpha^2 = \frac{\hbar^2}{2\mu}\left(\frac{\left(n+\frac{1}{2}\right)\pi}{a}\right)^2 = \frac{(2n+1)^2\pi^2\hbar^2}{8\mu a^2}$;

3) $\psi_n = \begin{cases} \psi^{\mathrm{I}} = \psi^{\mathrm{III}} = 0 \\ \psi_{\mathrm{n}}^{\mathrm{II}} = \mathrm{A}\sin\left(\alpha a + \frac{\pi}{2}\right) = \mathrm{A}\cos\alpha a = \mathrm{A}\cos\frac{n+\frac{1}{2}}{a}\pi x = \mathrm{A}\cos\frac{2n+1}{2a}\pi x \end{cases} (\mathrm{n} = 0,1,2,\ldots)$;

k. 综上两种情况；

i. $E_m = \frac{m^2\pi^2\hbar^2}{8\mu a^2}$;

ii. $\psi_m = \begin{cases} \begin{cases} \psi^I = \psi^{III} = 0 \\ \psi^{II} = A\sin\frac{m\pi}{2a}x \end{cases} (m = 2n, n \in Z) \\ \begin{cases} \psi^I = \psi^{III} = 0 \\ \psi^{II} = A\cos\frac{m\pi}{2a}x \end{cases} (m = 2n+1, n \in Z) \end{cases}$;

l. 导出归一化系数A：$\int|\psi(x)|^2 dx = 1$；

m. 将定态薛定谔方程还原为薛定谔方程：$\psi(x,t) = \psi(x)\cdot\psi(t)$,其中$\psi(t) = e^{-\frac{iEnt}{\hbar}}$;