

量子物理第三章习题答案

1. 电子的动量为

$$p = \frac{h}{\lambda} = \frac{6.63 \times 10^{-34} \text{ J} \cdot \text{s}}{550 \times 10^{-9} \text{ m}} = 1.21 \times 10^{-27} \text{ kg} \cdot \text{m/s},$$

电子的动能为

$$K = \frac{p^2}{2m_e} = \frac{(1.21 \times 10^{-27} \text{ kg} \cdot \text{m/s})^2}{2 \times 9.11 \times 10^{-31} \text{ kg}} = 7.98 \times 10^{-25} \text{ J} = 4.98 \times 10^{-6} \text{ eV}.$$

2. 电子的动量为

$$p = \sqrt{2m_e K} = \sqrt{2 \times 9.11 \times 10^{-31} \text{ kg} \times 50,000 \times 1.60 \times 10^{-19} \text{ J}} = 1.21 \times 10^{-22} \text{ kg} \cdot \text{m/s},$$

对应物质波的波长 (分辨本领) 为

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34} \text{ J} \cdot \text{s}}{1.21 \times 10^{-22} \text{ kg} \cdot \text{m/s}} = 5.48 \times 10^{-12} \text{ m} = 5.48 \times 10^{-3} \text{ nm}.$$

3. 因为

$$\int_{-\infty}^{\infty} |\psi(x, y, t = 0)|^2 dx dy = \int_{-\infty}^{\infty} (x^2 + y^2) e^{-2(x^2 + y^2)} dx dy,$$

转换为极坐标 $(x, y) = (r \cos \theta, r \sin \theta)$, 其 Jacobi 矩阵为

$$DF = \begin{pmatrix} \cos \theta & -r \sin \theta \\ \sin \theta & r \cos \theta \end{pmatrix},$$

因此

$$\begin{aligned} \int_{-\infty}^{\infty} (x^2 + y^2) e^{-2(x^2 + y^2)} dx dy &= \int_0^{2\pi} \int_0^{\infty} r^2 e^{-2r^2} |\det(DF)| dr d\theta \\ &= \int_0^{2\pi} \int_0^{\infty} r^3 e^{-2r^2} dr d\theta \\ &= 2\pi \int_0^{\infty} \frac{1}{2} t e^{-2t} dt \quad (t = r^2) \\ &= \frac{\pi}{4}, \end{aligned}$$

因此归一化的波函数为

$$\psi(x, y, t = 0) = \frac{2}{\sqrt{\pi}} (x + iy) e^{-(x^2 + y^2)},$$

几率密度为

$$|\psi(x, y, t = 0)|^2 = \frac{4}{\pi} (x^2 + y^2) e^{-2(x^2 + y^2)}.$$

4. 因为

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} e^{-2|x|} dx = 2 \int_0^{\infty} e^{-2x} dx = 1,$$

因此归一化的波函数就是 $\psi(x) = e^{-|x|}$ 本身。

动量表象的波函数为

$$\begin{aligned} \phi(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-\frac{ipx}{\hbar}} dx \\ &= \frac{1}{\sqrt{2\pi\hbar}} \left(\int_{-\infty}^0 e^{\left(1 - \frac{ip}{\hbar}\right)x} dx + \int_0^{\infty} e^{\left(-1 - \frac{ip}{\hbar}\right)x} dx \right) \\ &= \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{1}{1 - \frac{ip}{\hbar}} + \frac{1}{1 + \frac{ip}{\hbar}} \right) \\ &= \frac{1}{\sqrt{2\pi\hbar}} \frac{2}{1 + \frac{p^2}{\hbar^2}}. \end{aligned}$$

5. 因为

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} e^{-2x^2/\sigma^2} dx = \frac{\sigma}{2} \int_{-\infty}^{\infty} e^{-t^2/2} dt,$$

而标准正态分布 $N(0,1)$ 的几率密度函数满足

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/2} dx = 1,$$

因此

$$\frac{\sigma}{2} \int_{-\infty}^{\infty} e^{-t^2/2} dt = \sigma \sqrt{\frac{\pi}{2}},$$

因此归一化的波函数为

$$\psi(x) = \left(\frac{2}{\sqrt{2\pi}\sigma} \right)^{1/2} e^{-x^2/\sigma^2}.$$

动量表象的波函数为

$$\begin{aligned} \phi(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-\frac{ipx}{\hbar}} dx \\ &= \left(\frac{1}{\sqrt{2\pi}^{3/2} \hbar \sigma} \right)^{1/2} \int_{-\infty}^{\infty} e^{-\frac{ipx}{\hbar} - \frac{x^2}{\sigma^2}} dx \\ &= \left(\frac{1}{\sqrt{2\pi}^{3/2} \hbar \sigma} \right)^{1/2} e^{-\frac{\sigma^2 p^2}{4\hbar^2}} \int_{-\infty}^{\infty} e^{-\frac{1}{\sigma^2} \left(x + i \frac{\sigma^2 p}{2\hbar} \right)^2} dx \\ &= \left(\frac{\sigma}{\sqrt{2\pi}^{3/2} \hbar} \right)^{1/2} e^{-\frac{\sigma^2 p^2}{4\hbar^2}} \int_{-\infty}^{\infty} e^{-\left(x + i \frac{\sigma^2 p}{2\hbar} \right)^2} dx, \end{aligned}$$

令 $a \in \mathbb{R}$,

$$I(a) = \int_{-\infty}^{\infty} e^{-(x+ia)^2} dx,$$

因此

$$\begin{aligned} I'(a) &= \int_{-\infty}^{\infty} \frac{\partial}{\partial a} e^{-(x+ia)^2} dx \\ &= \int_{-\infty}^{\infty} -2i(x+ia) e^{-(x+ia)^2} dx \\ &= i \int_{-\infty}^{\infty} \frac{\partial}{\partial x} e^{-(x+ia)^2} dx \\ &= i \left[e^{-(x+ia)^2} \right]_{x \rightarrow -\infty}^{x \rightarrow \infty} \\ &= 0, \end{aligned}$$

因此

$$I(a) \equiv I(0) = \int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi},$$

$$\phi(p) = \left(\frac{\sigma}{\sqrt{2\pi}\hbar} \right)^{1/2} e^{-\frac{\sigma^2 p^2}{4\hbar^2}}.$$

坐标算符 \hat{x} 的期望值为

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx = \frac{2}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\infty} x e^{-2x^2/\sigma^2} dx = 0,$$

动量算符 \hat{p} 的期望值为

$$\langle p \rangle = \int_{-\infty}^{\infty} p |\phi(p)|^2 dp = \frac{\sigma}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} p e^{-\frac{\sigma^2 p^2}{4\hbar^2}} dp = 0,$$

动能算符 $\hat{K} = \frac{1}{2m} \hat{p}^2$ 的期望值为

$$\langle K \rangle = \frac{1}{2m} \int_{-\infty}^{\infty} p^2 |\phi(p)|^2 dp = \frac{\sigma}{2\sqrt{2\pi\hbar}m} \int_{-\infty}^{\infty} p^2 e^{-\frac{\sigma^2 p^2}{2\hbar^2}} dp = \frac{\hbar^2}{2\sqrt{2\pi}\sigma^2 m} \int_{-\infty}^{\infty} t^2 e^{-\frac{t^2}{2}} dt,$$

而

$$\sqrt{2\pi} = \int_{-\infty}^{\infty} e^{-\frac{t^2}{2}} dt = \left[t e^{-\frac{t^2}{2}} \right]_{t \rightarrow -\infty}^{t \rightarrow \infty} + \int_{-\infty}^{\infty} t^2 e^{-\frac{t^2}{2}} dt = \int_{-\infty}^{\infty} t^2 e^{-\frac{t^2}{2}} dt,$$

因此

$$\langle K \rangle = \frac{\hbar^2}{2\sigma^2 m}.$$

6. 因为

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-1}^1 1 dx = 2,$$

因此归一化的波函数为

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{2}}, & |x| < 1, \\ 0, & |x| \geq 1. \end{cases}$$

动量表象的波函数为

$$\begin{aligned} \phi(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-\frac{ipx}{\hbar}} dx \\ &= \frac{1}{2\sqrt{\pi\hbar}} \int_{-1}^1 e^{-\frac{ipx}{\hbar}} dx \\ &= \sqrt{\frac{\hbar}{\pi}} \frac{1}{p} \sin \frac{p}{\hbar}. \end{aligned}$$

坐标算符 \hat{x} 的期望值为

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx = \frac{1}{2} \int_{-\infty}^{\infty} x dx = 0,$$

算符 \hat{x}^2 的期望值为

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx = \frac{1}{2} \int_{-\infty}^{\infty} x^2 dx = \frac{1}{3},$$

动量算符 \hat{p} 的期望值为

$$\langle p \rangle = \int_{-\infty}^{\infty} p |\phi(p)|^2 dp = \frac{\hbar}{\pi} \int_{-\infty}^{\infty} \frac{1}{p} \sin^2 \frac{p}{\hbar} dp = \frac{\hbar}{\pi} \int_{-\infty}^{\infty} \frac{1}{t} \sin^2 t dt,$$

因为

$$\lim_{t \rightarrow 0} \frac{1}{t} \sin^2 t = 0,$$

所以积分 $\int_{-\infty}^{\infty} \frac{1}{t} \sin^2 t dt$ 是收敛的。根据 $f(t) = \frac{1}{t} \sin^2 t$ 是奇函数的性质可以得出

$$\langle p \rangle = 0,$$

算符 \hat{p}^2 的期望值为

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} p^2 |\phi(p)|^2 dp = \frac{\hbar}{\pi} \int_{-\infty}^{\infty} \sin^2 \frac{p}{\hbar} dp = \frac{1}{\pi} \int_{-\infty}^{\infty} \sin^2 t dt,$$

积分 $\int_{-\infty}^{\infty} \sin^2 t dt$ 是不收敛的。所以

$$\langle p^2 \rangle = \infty,$$

因此

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{1}{\sqrt{3}},$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \infty,$$

满足不确定关系 $\Delta x \Delta p \geq \frac{\hbar}{2}$ 。

7. 根据题意可得

$$\Delta x = L,$$

根据不确定关系可得

$$\Delta p \geq \frac{\hbar}{2L},$$

而盒子是对称的, 因此 $\langle p \rangle = 0$,

$$\langle p^2 \rangle = (\Delta p)^2 + \langle p \rangle^2 = (\Delta p)^2 \geq \frac{\hbar^2}{8L^2},$$

最小动能为

$$K = \frac{\langle p^2 \rangle_{\min}}{2m} = \frac{\hbar^2}{8mL^2}.$$

代入数据可得

(a) 0.95 eV,

(b) 0.05 MeV,

(c) 9.5×10^{-36} MeV.

8. 如果本征值不是实数, 令 $E = u + iv, v \neq 0$, 那么

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = \int_{-\infty}^{\infty} \left| \psi(x) e^{-\frac{iEt}{\hbar}} \right|^2 dx = e^{\frac{2vt}{\hbar}} \int_{-\infty}^{\infty} |\psi(x)|^2 dx = e^{\frac{2vt}{\hbar}},$$

因为 $v \neq 0$, 所以 $\Psi(x, t)$ 不是常数, 不满足归一化条件。

9. 记 $X = \left\{ \psi(x) : -\frac{\hbar^2}{2m} \psi''(x) + V(x)\psi(x) = E\psi(x), \int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty \right\}$ 为所有“平方可积, 并且满足定态薛定谔方程的函数”的集合。

现在证明 X 是复数域 \mathbb{C} 上的向量空间:

(A) $(X, +)$ 是 Abel 群:

(I) 对于任意 $\psi(x), \theta(x) \in X$, 都具有

$$-\frac{\hbar^2}{2m}(\psi(x) + \theta(x))'' + V(x)(\psi(x) + \theta(x)) = E(\psi(x) + \theta(x)),$$

$$\begin{aligned} \int_{-\infty}^{\infty} |\psi(x) + \theta(x)|^2 dx &\leq \int_{-\infty}^{\infty} (|\psi(x)| + |\theta(x)|)^2 dx \\ &\leq \int_{-\infty}^{\infty} (2 \max(|\psi(x)|, |\theta(x)|))^2 dx \\ &\leq \int_{-\infty}^{\infty} 4 (|\psi(x)|^2 + |\theta(x)|^2) dx < \infty. \end{aligned}$$

所以 $\psi(x) + \theta(x) \in X$ 。

(II) 根据加法交换律, $\psi(x) + \theta(x) = \theta(x) + \psi(x)$ 。

(B)

(I) 对于任意 $\psi(x) \in X, z \in \mathbb{C}$, 都具有

$$\begin{aligned} -\frac{\hbar^2}{2m}(z\psi(x))'' + V(x)(z\psi(x)) &= E(z\psi(x)), \\ \int_{-\infty}^{\infty} |z\psi(x)|^2 dx &= |z|^2 \int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty. \end{aligned}$$

所以 $z\psi(x) \in X$ 。

(II) 对于任意 $\psi(x), \theta(x) \in X, z, w \in \mathbb{C}$, 都具有

$$\begin{aligned} z(w\psi(x)) &= (zw)\psi(x), \\ 1\psi(x) &= \psi(x), \\ (z+w)\psi(x) &= z\psi(x) + w\psi(x), \\ z(\psi(x) + \theta(x)) &= z\psi(x) + z\theta(x). \end{aligned}$$

证明完毕。

现在证明, 当 $\psi(x) \in X$ 时, $\psi^*(x) \in X$ 。记 $\psi(x) = u(x) + iv(x)$, 可得

$$\left(-\frac{\hbar^2}{2m}u''(x) + V(x)u(x) - Eu(x) \right) + i \left(-\frac{\hbar^2}{2m}v''(x) + V(x)v(x) - Ev(x) \right) = 0,$$

因为 $\{1, i\}$ 是向量空间 \mathbb{C} 上线性无关的一组基, 所以

$$\begin{cases} -\frac{\hbar^2}{2m}u''(x) + V(x)u(x) = Eu(x), \\ -\frac{\hbar^2}{2m}v''(x) + V(x)v(x) = Ev(x), \end{cases}$$

而

$$\int_{-\infty}^{\infty} |u(x)|^2 dx \leq \int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty,$$

$$\int_{-\infty}^{\infty} |v(x)|^2 dx \leq \int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty,$$

因此 $u(x), v(x) \in X$ 。因为 $\psi^*(x) = u(x) - iv(x)$ ，所以 $\psi^*(x) \in X$ 。证明完毕。

因为 $\psi(x), \psi^*(x) \in X$ ，所以 $\psi(x) + \psi^*(x), i(\psi(x) - \psi^*(x)) \in X$ ，而这两者都是实函数，所以完成了题目的证明。

10. 令 $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$ 「如果不是，可以进行归一化」。那么

$$\begin{aligned} E &= E \int_{-\infty}^{\infty} |\psi(x)|^2 dx \\ &= \int_{-\infty}^{\infty} \psi^*(x) (E\psi(x)) dx \\ &= \int_{-\infty}^{\infty} \psi^*(x) \left(-\frac{\hbar^2}{2m} \psi''(x) + V(x)\psi(x) \right) dx \\ &= -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \psi^*(x) \psi''(x) dx + \int_{-\infty}^{\infty} V(x) |\psi(x)|^2 dx \\ &= \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} |\psi'(x)|^2 dx + \int_{-\infty}^{\infty} V(x) |\psi(x)|^2 dx \\ &\geq \int_{-\infty}^{\infty} V(x) |\psi(x)|^2 dx \\ &\geq \inf V(x) \int_{-\infty}^{\infty} |\psi(x)|^2 dx \\ &= \inf V(x). \end{aligned}$$

其中第 4 行到第 5 行利用了以下等式，对于 $f(x), g(x)$ 满足

$$\lim_{|x| \rightarrow \infty} f(x) = 0, \lim_{|x| \rightarrow \infty} g(x) = 0, \sup |g'(x)| < \infty,$$

都具有

$$\int_{-\infty}^{\infty} f(x)g''(x)dx = [f(x)g'(x)]_{x \rightarrow -\infty}^{x \rightarrow \infty} - \int_{-\infty}^{\infty} f'(x)g'(x)dx = - \int_{-\infty}^{\infty} f'(x)g'(x)dx.$$

11. 第 n 个定态的波函数为

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, & \text{for } n \text{ even,} \\ \sqrt{\frac{2}{L}} \cos \frac{n\pi x}{L}, & \text{for } n \text{ odd,} \end{cases}$$

(这题利用动量表象计算动量期望值是会死人的，所以换了另一个办法)

(A) n 是偶数 (even) :

坐标算符 \hat{x} 的期望值为

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx = \frac{2}{L} \int_{-L/2}^{L/2} x \sin^2 \frac{n\pi x}{L} dx = 0,$$

算符 \hat{x}^2 的期望值为

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx = \frac{2}{L} \int_{-L/2}^{L/2} x^2 \sin^2 \frac{n\pi x}{L} dx = \frac{2L^2}{n^3\pi^3} \int_{-n\pi/2}^{n\pi/2} t^2 \sin^2 t dt = \frac{1}{12} L^2 \left(1 - \frac{6}{n^2\pi^2} \right),$$

动量算符 \hat{p} 的期望值为

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^*(x) \psi'(x) dx = -i \frac{n\pi\hbar}{L^2} \int_{-L/2}^{L/2} \sin \frac{2n\pi x}{L} dx = 0,$$

算符 \hat{p}^2 的期望值为

$$\langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi^*(x) \psi''(x) dx = \hbar^2 \int_{-\infty}^{\infty} |\psi'(x)|^2 dx = \frac{2n^2\pi^2\hbar^2}{L^3} \int_{-L/2}^{L/2} \cos^2 \left(\frac{n\pi x}{L} \right) dx = \frac{n^2\pi^2\hbar^2}{L^2},$$

因此

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{1}{2\sqrt{3}} \sqrt{1 - \frac{6}{n^2\pi^2}} L,$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \frac{n\pi\hbar}{L},$$

$$\Delta x \Delta p = \frac{\hbar}{2} \sqrt{\frac{n^2\pi^2}{3} - 2} \geq \frac{\hbar}{2} \sqrt{\frac{4\pi^2}{3} - 2} \geq \frac{\hbar}{2}.$$

(B) n 是奇数 (odd) :

坐标算符 \hat{x} 的期望值为

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx = \frac{2}{L} \int_{-L/2}^{L/2} x \cos^2 \frac{n\pi x}{L} dx = 0,$$

算符 \hat{x}^2 的期望值为

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx = \frac{2}{L} \int_{-L/2}^{L/2} x^2 \cos^2 \frac{n\pi x}{L} dx = \frac{2L^2}{n^3\pi^3} \int_{-n\pi/2}^{n\pi/2} t^2 \cos^2 t dt = \frac{1}{12} L^2 \left(1 - \frac{6}{n^2\pi^2} \right),$$

动量算符 \hat{p} 的期望值为

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^*(x)\psi'(x) dx = i \frac{n\pi\hbar}{L^2} \int_{-L/2}^{L/2} \sin \frac{2n\pi x}{L} dx = 0,$$

算符 \hat{p}^2 的期望值为

$$\langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi^*(x)\psi''(x) dx = \hbar^2 \int_{-\infty}^{\infty} |\psi'(x)|^2 dx = \frac{2n^2\pi^2\hbar^2}{L^3} \int_{-L/2}^{L/2} \sin^2 \left(\frac{n\pi x}{L} \right) dx = \frac{n^2\pi^2\hbar^2}{L^2},$$

因此

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{1}{2\sqrt{3}} \sqrt{1 - \frac{6}{n^2\pi^2}} L,$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \frac{n\pi\hbar}{L},$$

$$\Delta x \Delta p = \frac{\hbar}{2} \sqrt{\frac{n^2\pi^2}{3} - 2} \geq \frac{\hbar}{2} \sqrt{\frac{\pi^2}{3} - 2} \geq \frac{\hbar}{2}.$$

综上所述 $n = 1$ 最接近不等式极限, 其值约为 $1.1 \frac{\hbar}{2}$ 。

12. 因为

$$|\psi(x, 0)|^2 = \int_{-\infty}^{\infty} |\phi_1(x)|^2 + |\phi_2(x)|^2 dx = 2,$$

因此归一化的波函数为

$$\psi(x, 0) = \frac{1}{\sqrt{2}} (\phi_1(x) + i\phi_2(x)).$$

记 $\phi_1(x), \phi_2(x)$ 对应的定态能量分别为 E_1, E_2 ，因此

$$\Psi(x, t) = \frac{1}{\sqrt{2}} \left(\phi_1(x) e^{-\frac{iE_1 t}{\hbar}} + i \phi_2(x) e^{-\frac{iE_2 t}{\hbar}} \right),$$

$$\begin{aligned} |\Psi(x, t)|^2 &= \Psi^*(x, t) \Psi(x, t) \\ &= \frac{1}{2} \left(\phi_1(x) e^{\frac{iE_1 t}{\hbar}} - i \phi_2(x) e^{\frac{iE_2 t}{\hbar}} \right) \left(\phi_1(x) e^{-\frac{iE_1 t}{\hbar}} + i \phi_2(x) e^{-\frac{iE_2 t}{\hbar}} \right) \\ &= \frac{1}{2} \left(\phi_1(x)^2 + \phi_2(x)^2 - 2\phi_1(x)\phi_2(x) \sin \frac{(E_1 - E_2)t}{\hbar} \right). \end{aligned}$$

根据 11 题的结论

$$\begin{cases} \phi_1(x) = \sqrt{\frac{2}{L}} \cos \frac{\pi x}{L}, \\ \phi_2(x) = \sqrt{\frac{2}{L}} \sin \frac{2\pi x}{L}, \end{cases}$$

坐标算符 \hat{x} 的期望值为

$$\begin{aligned} \langle x \rangle &= \int_{-\infty}^{\infty} x |\Psi(x, t)|^2 dx \\ &= \frac{1}{L} \int_{-L/2}^{L/2} x \left(\cos^2 \frac{\pi x}{L} + \sin^2 \frac{2\pi x}{L} - 2 \cos \frac{\pi x}{L} \sin \frac{2\pi x}{L} \sin \frac{(E_1 - E_2)t}{\hbar} \right) dx \\ &= -\frac{2}{L} \left(\int_{-L/2}^{L/2} x \cos \frac{\pi x}{L} \sin \frac{2\pi x}{L} dx \right) \sin \frac{(E_1 - E_2)t}{\hbar} \\ &= -\frac{4L}{\pi^2} \left(\int_{-\pi/2}^{\pi/2} y \cos^2 y \sin y dy \right) \sin \frac{(E_1 - E_2)t}{\hbar} \\ &= -\frac{16L}{9\pi^2} \sin \frac{(E_1 - E_2)t}{\hbar}, \end{aligned}$$

算符 \hat{x}^2 的期望值为

$$\begin{aligned} \langle x^2 \rangle &= \int_{-\infty}^{\infty} x^2 |\Psi(x, t)|^2 dx \\ &= \frac{1}{L} \int_{-L/2}^{L/2} x^2 \left(\cos^2 \frac{\pi x}{L} + \sin^2 \frac{2\pi x}{L} - 2 \cos \frac{\pi x}{L} \sin \frac{2\pi x}{L} \sin \frac{(E_1 - E_2)t}{\hbar} \right) dx \\ &= \frac{1}{L} \int_{-L/2}^{L/2} x^2 \left(\cos^2 \frac{\pi x}{L} + \sin^2 \frac{2\pi x}{L} \right) dx \\ &= \frac{L^2}{\pi^3} \int_{-\pi/2}^{\pi/2} y^2 (\cos^2 y + \sin^2 2y) dy \\ &= \left(\frac{1}{12} - \frac{5}{16\pi^2} \right) L^2, \end{aligned}$$

动量算符 \hat{p} 的期望值为

$$\begin{aligned}
 \langle p \rangle &= -i\hbar \int_{-\infty}^{\infty} \Psi^*(x, t) \Psi'(x, t) dx \\
 &= -\frac{i\hbar}{2} \int_{-L/2}^{L/2} \left(\phi_1(x) e^{\frac{iE_1 t}{\hbar}} - i\phi_2(x) e^{\frac{iE_2 t}{\hbar}} \right) \left(\phi_1'(x) e^{\frac{-iE_1 t}{\hbar}} + i\phi_2'(x) e^{\frac{-iE_2 t}{\hbar}} \right) dx \\
 &= -\frac{i\hbar}{2} \int_{-L/2}^{L/2} \phi_1(x) \phi_1'(x) + \phi_2(x) \phi_2'(x) + i \left(\phi_1(x) \phi_2'(x) e^{\frac{i(E_1 - E_2)t}{\hbar}} - \phi_1'(x) \phi_2(x) e^{\frac{-i(E_1 - E_2)t}{\hbar}} \right) dx \\
 &= \frac{\hbar}{2} \int_{-L/2}^{L/2} \left(\phi_1(x) \phi_2'(x) e^{\frac{i(E_1 - E_2)t}{\hbar}} - \phi_1'(x) \phi_2(x) e^{\frac{-i(E_1 - E_2)t}{\hbar}} \right) dx \\
 &= \frac{\pi\hbar}{L^2} \int_{-L/2}^{L/2} \left(2 \cos \frac{\pi x}{L} \cos \frac{2\pi x}{L} e^{\frac{i(E_1 - E_2)t}{\hbar}} + \sin \frac{\pi x}{L} \sin \frac{2\pi x}{L} e^{\frac{-i(E_1 - E_2)t}{\hbar}} \right) dx \\
 &= \frac{4\hbar}{3L} \cos \frac{(E_1 - E_2)t}{\hbar},
 \end{aligned}$$

算符 \hat{p}^2 的期望值为

$$\begin{aligned}
 \langle p^2 \rangle &= -\hbar^2 \int_{-\infty}^{\infty} \Psi^*(x, t) \Psi''(x, t) dx \\
 &= \hbar^2 \int_{-\infty}^{\infty} |\Psi'(x, t)|^2 dx \\
 &= \frac{\hbar^2}{2} \int_{-L/2}^{L/2} \left(\phi_1'(x) e^{\frac{iE_1 t}{\hbar}} - i\phi_2'(x) e^{\frac{iE_2 t}{\hbar}} \right) \left(\phi_1'(x) e^{\frac{-iE_1 t}{\hbar}} + i\phi_2'(x) e^{\frac{-iE_2 t}{\hbar}} \right) dx \\
 &= \frac{\hbar^2}{2} \int_{-L/2}^{L/2} \phi_1'(x)^2 + \phi_2'(x)^2 - 2\phi_1'(x)\phi_2'(x) \sin \frac{(E_1 - E_2)t}{\hbar} dx \\
 &= \frac{\hbar^2}{2} \int_{-L/2}^{L/2} \phi_1'(x)^2 + \phi_2'(x)^2 dx \\
 &= \frac{\pi^2 \hbar^2}{L^3} \int_{-L/2}^{L/2} 4 \cos^2 \frac{2\pi x}{L} + \sin^2 \frac{\pi x}{L} dx \\
 &= \frac{5\pi^2 \hbar^2}{2L^2}.
 \end{aligned}$$

系统能量的平均值为

$$\begin{aligned}
 \langle H \rangle &= i\hbar \int_{-\infty}^{\infty} \Psi^*(x, t) \dot{\Psi}(x, t) dx \\
 &= \frac{1}{2} \int_{-L/2}^{L/2} \left(\phi_1(x) e^{\frac{iE_1 t}{\hbar}} - i\phi_2(x) e^{\frac{iE_2 t}{\hbar}} \right) \left(E_1 \phi_1(x) e^{\frac{-iE_1 t}{\hbar}} + iE_2 \phi_2(x) e^{\frac{-iE_2 t}{\hbar}} \right) dx \\
 &= \frac{1}{2} \int_{-L/2}^{L/2} E_1 \phi_1(x)^2 + E_2 \phi_2(x)^2 + i\phi_1(x)\phi_2(x) \left(E_2 e^{\frac{i(E_1 - E_2)t}{\hbar}} - E_1 e^{\frac{-i(E_1 - E_2)t}{\hbar}} \right) dx \\
 &= \frac{1}{2} \int_{-L/2}^{L/2} E_1 \phi_1(x)^2 + E_2 \phi_2(x)^2 dx \\
 &= \frac{1}{2} (E_1 + E_2).
 \end{aligned}$$

如果测量粒子的能量，得到的结果是 E_1 或 E_2 ，几率均为 $\frac{1}{2}$ 。(哪个婊子出的题目???)

13. 定态薛定谔方程为

$$\begin{cases} -\frac{\hbar^2}{2m}\psi''(x) = E\psi(x), & x \in (0, a), \\ \psi(x) \equiv 0, & x \in \mathbb{R} \setminus (0, a), \end{cases}$$

因此

$$\psi(x) = \begin{cases} P \sin kx + Q \cos kx, & x \in (0, a), \\ 0, & x \in \mathbb{R} \setminus (0, a), \end{cases}$$

并且根据连续性可得

$$\lim_{x \searrow 0} \psi(x) = \lim_{x \nearrow 0} \psi(x) = 0,$$

$$\lim_{x \nearrow a} \psi(x) = \lim_{x \searrow a} \psi(x) = 0,$$

因此

$$Q = 0,$$

$$ka = n\pi,$$

$$\psi(x) = \begin{cases} P \sin \frac{n\pi x}{a}, & x \in (0, a), \\ 0, & x \in \mathbb{R} \setminus (0, a), \end{cases}$$

归一化可得

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, & x \in (0, a), \\ 0, & x \in \mathbb{R} \setminus (0, a). \end{cases}$$

而

$$\int_{-\infty}^{\infty} |\psi(x, 0)|^2 dx = A^2 \int_0^a \sin^6 \frac{\pi x}{a} dx = \frac{A^2 a}{\pi} \int_0^\pi \sin^6 t dt = \frac{5}{16} A^2 a = 1,$$

因此

$$A = \sqrt{\frac{16}{5a}},$$

$$\psi(x, 0) = \sqrt{\frac{16}{5a}} \sin^3 \frac{\pi x}{a} = \frac{1}{\sqrt{10}} (3\phi_1(x) - \phi_3(x)),$$

因此

$$\Psi(x, t) = \frac{1}{\sqrt{10}} \left(3\phi_1(x)e^{-\frac{iE_1t}{\hbar}} - \phi_3(x)e^{-\frac{iE_3t}{\hbar}} \right),$$

$$\begin{aligned} \langle x \rangle &= \int_{-\infty}^{\infty} x |\Psi(x, t)|^2 dx \\ &= \frac{1}{10} \int_0^a x \left(3\phi_1(x)e^{\frac{iE_1t}{\hbar}} - \phi_3(x)e^{\frac{iE_3t}{\hbar}} \right) \left(3\phi_1(x)e^{-\frac{iE_1t}{\hbar}} - \phi_3(x)e^{-\frac{iE_3t}{\hbar}} \right) dx \\ &= \frac{1}{10} \int_0^a x \left(9\phi_1(x)^2 + \phi_3(x)^2 - 6\phi_1(x)\phi_3(x)\cos \frac{(E_1 - E_3)t}{\hbar} \right) dx \\ &= \frac{a}{2}, \end{aligned}$$

$$\begin{aligned} \langle p \rangle &= -i\hbar \int_{-\infty}^{\infty} \Psi^*(x, t)\Psi'(x, t)dx \\ &= -\frac{i\hbar}{10} \int_0^a \left(3\phi_1(x)e^{\frac{iE_1t}{\hbar}} - \phi_3(x)e^{\frac{iE_3t}{\hbar}} \right) \left(3\phi_1'(x)e^{-\frac{iE_1t}{\hbar}} - \phi_3'(x)e^{-\frac{iE_3t}{\hbar}} \right) dx \\ &= -\frac{i\hbar}{10} \int_0^a \left(9\phi_1(x)\phi_1'(x) + \phi_3(x)\phi_3'(x) - 3 \left(\phi_1(x)\phi_3'(x)e^{\frac{i(E_1 - E_3)t}{\hbar}} + \phi_1'(x)\phi_3(x)e^{-\frac{i(E_1 - E_3)t}{\hbar}} \right) \right) dx \\ &= 0. \end{aligned}$$

14. 原来的波函数为

$$\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}, \quad 0 < x < a,$$

势阱宽度增加后，波函数的函数空间（实数域 \mathbb{R} 上的向量空间）标准正交基为

$$\phi_n(x) = \sqrt{\frac{1}{a}} \sin \frac{n\pi x}{2a}, \quad 0 < x < 2a,$$

根据傅立叶级数的性质， $\psi(x)$ 可以被表示为

$$\psi(x) = \sum_{n=1}^{\infty} c_n \phi_n(x),$$

因此

$$\begin{aligned}c_n &= \langle \psi(x), \phi_n(x) \rangle \\&= \int_0^{2a} \psi(x) \phi_n(x) dx \\&= \frac{\sqrt{2}}{a} \int_0^a \sin \frac{\pi x}{a} \sin \frac{n \pi x}{2a} dx \\&= \frac{\sqrt{2}}{\pi} \int_0^\pi \sin t \sin \frac{nt}{2} dt,\end{aligned}$$

而

$$\int_0^\pi \sin t \sin \frac{nt}{2} dt = \begin{cases} (-1)^{\frac{n+1}{2}} \frac{4}{n^2-4}, & n = 1, 3, 5, \dots, \\ \frac{\pi}{2}, & n = 2, \\ 0, & n = 4, 6, 8, \dots, \end{cases}$$

因此

$$c_n = \begin{cases} (-1)^{\frac{n+1}{2}} \frac{4\sqrt{2}}{(n^2-4)\pi}, & n = 1, 3, 5, \dots, \\ \frac{\sqrt{2}}{2}, & n = 2, \\ 0, & n = 4, 6, 8, \dots, \end{cases}$$

测量到状态 $\phi_n(x)$ 对应的能量为

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2} = \frac{n^2 \pi^2 \hbar^2}{8ma^2},$$

对应概率为

$$\Pr \{ \phi_n(x) \} = |c_n|^2 = \begin{cases} \frac{32}{(n^2-4)^2 \pi^2}, & n = 1, 3, 5, \dots, \\ \frac{1}{2}, & n = 2, \\ 0, & n = 4, 6, 8, \dots, \end{cases}$$

因此最有可能的结果对应 $n = 2$ ，其概率为 $1/2$ ，相应的能量为 $E_2 = \frac{\pi^2 \hbar^2}{2ma^2}$ 。

粒子能量的平均值为

$$\begin{aligned}
 \langle H \rangle &= \sum_{n=1}^{\infty} |c_n|^2 E_n \\
 &= \frac{1}{2} \frac{\pi^2 \hbar^2}{2ma^2} + \sum_{k=1}^{\infty} \frac{32}{((2k-1)^2 - 4)^2 \pi^2} \frac{(2k-1)^2 \pi^2 \hbar^2}{8ma^2} \\
 &= \frac{1}{2} \frac{\pi^2 \hbar^2}{2ma^2} + \frac{4\hbar^2}{ma^2} \sum_{k=1}^{\infty} \frac{(2k-1)^2}{((2k-1)^2 - 4)^2} \\
 &= \frac{1}{2} \frac{\pi^2 \hbar^2}{2ma^2} + \frac{\hbar^2}{ma^2} \sum_{k=1}^{\infty} \frac{1}{(2k-3)^2} + \frac{1}{(2k+1)^2} + \frac{2}{4k^2 - 4k - 3},
 \end{aligned}$$

因为

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = 1 + \frac{1}{2^2} + \frac{1}{3^2} + \dots = \frac{\pi^2}{6},$$

所以

$$\sum_{n=1}^{\infty} \frac{1}{(2n)^2} = \frac{1}{2^2} + \frac{1}{4^2} + \frac{1}{6^2} + \dots = \frac{\pi^2}{24},$$

因此

$$\sum_{k=1}^{\infty} \frac{1}{(2k-3)^2} = 1 + 1 + \frac{1}{3^2} + \frac{1}{5^2} + \dots = 1 + \sum_{n=1}^{\infty} \frac{1}{n^2} - \sum_{n=1}^{\infty} \frac{1}{(2n)^2} = 1 + \frac{\pi^2}{6} - \frac{\pi^2}{24} = 1 + \frac{\pi^2}{8},$$

$$\sum_{k=1}^{\infty} \frac{1}{(2k+1)^2} = \frac{1}{3^2} + \frac{1}{5^2} + \frac{1}{7^2} + \dots = \sum_{k=1}^{\infty} \frac{1}{(2k-3)^2} - 2 = \frac{\pi^2}{8} - 1,$$

$$\begin{aligned}
 \sum_{k=1}^{\infty} \frac{2}{4k^2 - 4k - 3} &= \sum_{k=1}^{\infty} \frac{2}{(2k-3)(2k+1)} \\
 &= \frac{1}{2} \sum_{k=1}^{\infty} \frac{1}{2k-3} - \frac{1}{2k+1} \\
 &= \frac{1}{2} \left(\frac{1}{-1} - \frac{1}{3} + \frac{1}{1} - \frac{1}{5} + \frac{1}{3} - \frac{1}{7} + \dots \right) \\
 &= \frac{1}{2} \left(\frac{1}{-1} + \frac{1}{1} \right) = 0.
 \end{aligned}$$

$$\langle H \rangle = \frac{1}{2} \frac{\pi^2 \hbar^2}{2ma^2} + \frac{\hbar^2}{ma^2} \sum_{k=1}^{\infty} \frac{1}{(2k-3)^2} + \frac{1}{(2k+1)^2} + \frac{2}{4k^2 - 4k - 3} = \frac{\pi^2 \hbar^2}{2ma^2}.$$

15. 对于散射态 $E > 0$ ，定态薛定谔方程为

$$\begin{cases} -\frac{\hbar^2}{2m}\psi''(x) = E\psi(x), & x < 0, \\ -\frac{\hbar^2}{2m}\psi''(x) = (E + V_0)\psi(x), & x \geq 0, \end{cases}$$

因此

$$\psi(x) = \begin{cases} e^{iax} + Re^{-iax}, & x < 0, \\ Te^{ibx}, & x \geq 0, \end{cases}$$

其中 R, T 分别为反射率、透射率，

$$a = \frac{\sqrt{2mE}}{\hbar},$$
$$b = \frac{\sqrt{2m(E + V_0)}}{\hbar},$$

因为势能是有界的，所以波函数的零阶与一阶导数均连续，即

$$\lim_{x \nearrow 0} \psi(x) = \lim_{x \searrow 0} \psi(x),$$

$$\lim_{x \nearrow 0} \psi'(x) = \lim_{x \searrow 0} \psi'(x),$$

因此

$$\begin{cases} 1 + R = T, \\ a(1 - R) = bT, \end{cases}$$

$$\begin{cases} R = \frac{a-b}{a+b}, \\ T = \frac{2a}{a+b}, \end{cases}$$

所以粒子有可能被反射，并且被反射回来的几率为

$$|R|^2 = \left| \frac{a-b}{a+b} \right|^2 = \left(\frac{\sqrt{E+V_0} - \sqrt{E}}{\sqrt{E+V_0} + \sqrt{E}} \right)^2.$$

16. 定态薛定谔方程为

$$\begin{cases} \psi(x) \equiv 0, & x < 0 \\ -\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x), & x \geq 0, \end{cases}$$

因此

$$\psi(x) = \begin{cases} 0, & x < 0 \\ \sqrt{2}N_n e^{-\xi^2/2} H_n(\xi), & x \geq 0, \end{cases}$$

($\sqrt{2}$ 的出现是因为归一化) 因为波函数连续, 所以

$$\lim_{x \searrow 0} \psi(x) = \lim_{x \nearrow 0} \psi(x) = 0,$$

并且当 n 是奇数时

$$\lim_{\xi \rightarrow 0} H_n(\xi) = 0,$$

当 n 是偶数时

$$\lim_{\xi \rightarrow 0} H_n(\xi) \neq 0,$$

所以根据连续性, n 只能是奇数, 对应能量为

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega, \quad n = 1, 3, 5, \dots$$

17. 多维情况的定态薛定谔方程为

$$-\frac{\hbar^2}{2m}\Delta\psi + V\psi = E\psi,$$

其中 $\Delta\psi = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2}$. 令 $\psi(x, y) = F(x)G(y)$, 因此

$$-\frac{\hbar^2}{2m}(FG'' + F''G) + VFG = EFG,$$

$$-\frac{\hbar^2}{2m}\left(\frac{F''}{F} + \frac{G''}{G}\right) + V = E,$$

$$\left(-\frac{\hbar^2}{2m}\frac{F''}{F} + \frac{1}{2}m(2\omega)^2x^2\right) + \left(-\frac{\hbar^2}{2m}\frac{G''}{G} + \frac{1}{2}m\omega^2y^2\right) = E,$$

因此

$$-\frac{\hbar^2}{2m} \frac{F''}{F} + \frac{1}{2} m (2\omega)^2 x^2 = C,$$

$$-\frac{\hbar^2}{2m} \frac{G''}{G} + \frac{1}{2} m \omega^2 y^2 = D,$$

其中 $C, D > 0$ 均为常数, 并且 $C + D = E$ 。因此本征函数为

$$F_m(x) = A_m e^{-\chi^2/2} H_m(\chi),$$

$$G_n(y) = B_n e^{-\xi^2/2} H_n(\xi),$$

其中 $\chi = \sqrt{\frac{2m\omega}{\hbar}} x, \xi = \sqrt{\frac{m\omega}{\hbar}} y$, 本征能量为

$$C_m = \left(m + \frac{1}{2}\right) 2\hbar\omega,$$

$$D_n = \left(n + \frac{1}{2}\right) \hbar\omega,$$

其中 $m, n = 0, 1, 2, \dots$ 。当 $E = \left(N + \frac{1}{2}\right) \hbar\omega$ 时

$$2\left(m + \frac{1}{2}\right) + \left(n + \frac{1}{2}\right) = N + \frac{1}{2},$$

$$2m + n = N - 1,$$

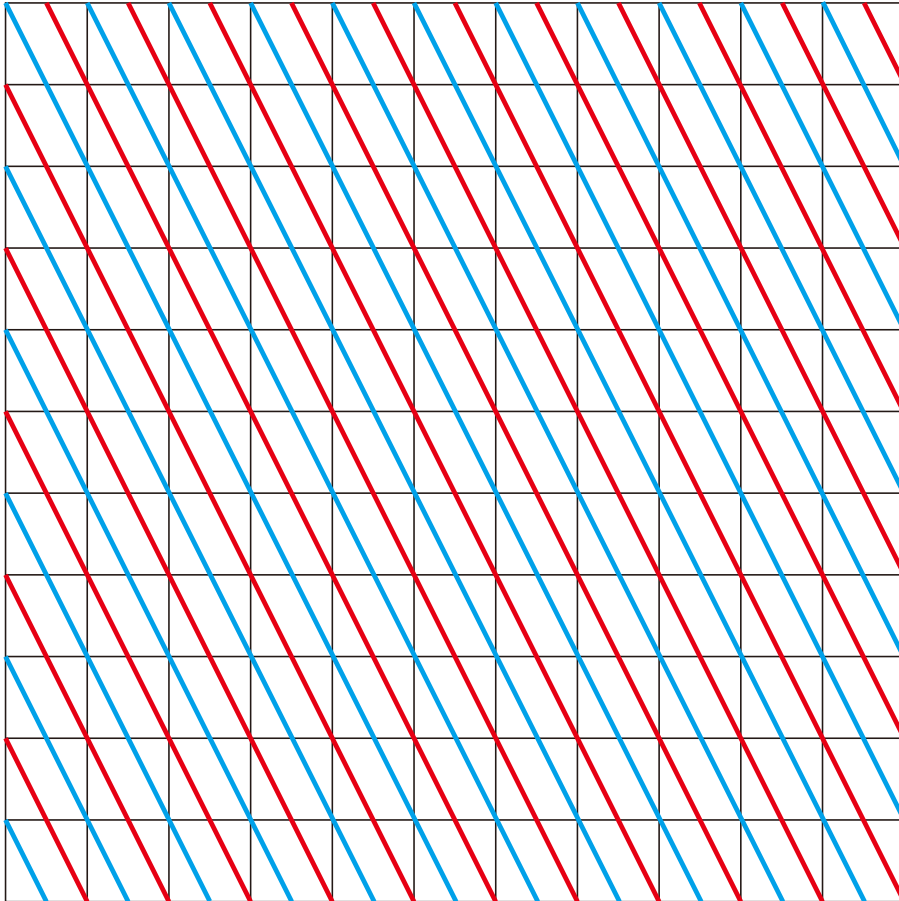
$N = 0$ 显然无解。令 $N \geq 1$, 绘制图像可以发现:

(A) 当 N 是奇数时, $2m + n$ 是偶数, 对应图像中的红线, 可以发现红线经过 $\frac{N+1}{2}$ 个格点。

(B) 当 N 是偶数时, $2m + n$ 是奇数, 对应图像中的蓝线, 可以发现蓝线经过 $\frac{N}{2}$ 个格点。

因此, 能级的简并度为 $\lceil \frac{N}{2} \rceil$, 其中 $\lceil \cdot \rceil$ 是向上取整。

n



m

N is odd

N is even