Homework2 答案

1. 粒子一维势场中运动. $\psi_n(x), \psi_m(x)$是属于E_m, E_n的束缚态本征函数. $E_n \neq E_m$.证明它们正交, 即$\int_{-\infty}^{\infty} \psi_n(x)\psi_m(x)dx = 0$

证: $\psi_n(x), \psi_m(x)$均满足定态Schrödinger方程,即

$$\psi''_n(x) = \frac{2m}{\hbar^2}[V(x) - E_n]\psi_n(x) \tag{1}$$

$$\psi''_m(x) = \frac{2m}{\hbar^2}[V(x) - E_m]\psi_m(x) \tag{2}$$

以$\psi_m(x)$左乘式(1),以$\psi_n(x)$左乘式(2), 再相减得

$$\begin{aligned}\frac{2m}{\hbar^2}(E_m - E_n)\psi_n(x)\psi_m(x) &= \psi_m(x)\psi''_n(x) - \psi_n(x)\psi''_m(x) \\ &= \frac{d}{dx}(\psi_m(x)\psi'_n(x) - \psi_n(x)\psi'_m(x))\end{aligned}$$

对全空间积分,得到(束缚态波函数在无穷远处必须趋于0)

$$\begin{aligned}\frac{2m}{\hbar^2}(E_m - E_n)\int_{-\infty}^{\infty} dx\ \psi_n(x)\psi_m(x) &= \int_{-\infty}^{\infty} dx\ \frac{d}{dx}(\psi_m(x)\psi'_n(x) - \psi_n(x)\psi'_m(x)) \\ &= (\psi_m(x)\psi'_n(x) - \psi_n(x)\psi'_m(x))\ |_{-\infty}^{\infty} = 0\end{aligned}$$

因此,当$E_n \neq E_m$,就有

$$\int_{-\infty}^{\infty} \psi_n(x)\psi_m(x)dx = 0$$

2. 假设一个粒子的初始态是两个能量本征态(E_2, E_1)的叠加$\psi(x, 0) = c_1\psi_1(x) + c_2\psi_2(x)$, 设$c_1, c_2, \psi_1, \psi_2$为实数. 计算$t > 0$时刻$< x(t) >$.

解: 易得$\Psi(x, t) = c_1\psi_1(x)e^{-\frac{i}{\hbar}E_1 t} + c_2\psi_2(x)e^{-\frac{i}{\hbar}E_2 t}$, 假设$\psi_1(x), \psi_2(x)$是归一化波函数, 且$c_1^2 + c_2^2 = 1$, 即$\psi(x, 0)$也是归一化函数:

$$\int dx\ \psi(x, t)\psi^*(x, t) = |c_1|^2 + |c_2|^2 = 1, \tag{3}$$

利用了ψ_1, ψ_2正交.

$$
\begin{aligned}
<x(t)> &= \int dx\ \Psi^*(x,t) x \Psi(x,t) \qquad (4)\\
&= \int dx\ [c_1\psi_1(x)e^{\frac{i}{\hbar}E_1 t} + c_2\psi_2(x)e^{\frac{i}{\hbar}E_2 t}]\cdot x\cdot[c_1\psi_1(x)e^{-\frac{i}{\hbar}E_1 t} + c_2\psi_2(x)e^{\frac{-i}{\hbar}E_2 t}]\\
&= \int dx\ x[c_1^2\psi_1^2(x) + c_2^2\psi_2^2(x) + c_1c_2\psi_1(x)\psi_2(x)(e^{\frac{i}{\hbar}(E_1-E_2)t} + e^{\frac{i}{\hbar}(E_2-E_1)t})]\\
&= \int dx\ x[c_1^2\psi_1^2(x) + c_2^2\psi_2^2(x) + 2c_1c_2\psi_1(x)\psi_2(x)\cos(\frac{E_2-E_1}{\hbar}t)]
\end{aligned}
$$

$$
<x(t)> \;=\; c_1^2 <x>_1 + c_2^2 <x>_2 + 2c_1c_2 <x>_{12}\cos\omega t
$$

其中

$$
\begin{aligned}
<x>_1 &= \int dx\ x\psi_1^2(x)\\
<x>_2 &= \int dx\ x\psi_2^2(x)\\
<x>_{12} &= \int dx\ x\psi_1(x)\psi_2(x)\\
\omega &= \frac{E_2-E_1}{\hbar}
\end{aligned}
$$

可以看到：当$\langle x\rangle_{12}\neq 0$时候粒子位置的期望值是周期振动.

3.证明对任意两个满足薛定谔方程的归一化解$\Psi_1(x,t),\Psi_2(x,t)$ 有

$$
\frac{d}{dt}\int_{-\infty}^{\infty}\Psi_1^*\Psi_2 dx = 0
$$

解:
由 $i\hbar\partial_t\Psi_1 = \hat{H}\Psi_1,\ i\hbar\partial_t\Psi_2 = \hat{H}\Psi_2,\ \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$

$$
\begin{aligned}
\frac{d}{dt}\int_{-\infty}^{\infty}\Psi_1^*\Psi_2 dx &= \int_{-\infty}^{\infty}\partial_t\Psi_1^*\Psi_2 dx + \int_{-\infty}^{\infty}\Psi_1^*\partial_t\Psi_2 dx\\
&= \frac{-i\hbar}{2m}\int_{-\infty}^{\infty}(\Psi_2\partial_x^2\Psi_1^* - \Psi_1^*\partial_x^2\Psi_2)dx\\
&= \frac{-i\hbar}{2m}\int_{-\infty}^{\infty}\partial_x(\Psi_2\partial_x\Psi_1^* - \Psi_1^*\partial_x\Psi_2)dx\\
&= \frac{-i\hbar}{2m}(\Psi_2\partial_x\Psi_1^* - \Psi_1^*\partial_x\Psi_2)\Big|_{-\infty}^{\infty}
\end{aligned}
$$

$\because\ x\to\infty, \Psi_1(x,t), \Psi_2(x,t)\to 0$.上式为0 即：$\frac{d}{dt}\int_{-\infty}^{\infty}\Psi_1^*\Psi_2 dx = 0$

4 Schrödinger方程分离变量解中E必须是实数(提示，假设其是复数，那么波函数在任何时间归一化要求其虚部为零)
解:已知$\Psi(\vec{r},t)=\psi_E(\vec{r})\exp(^{\frac{-iEt}{\hbar}})$
假设E=Re[E]+iIm[E] 且在t=0时刻 $\Psi(\vec{r},0)$ 是归一化的.
即$\int_{-\infty}^{\infty}|\psi_E(\vec{r})|^2 d\vec{r}^3=1$
则在任意t时刻

$$
\begin{aligned}
\int_{-\infty}^{\infty}|\Psi(\vec{r},t)|^2 d\vec{r}^3 &= \int_{-\infty}^{\infty}\psi_E^*(\vec{r})\exp(\frac{iE^*t}{\hbar})\psi_E(\vec{r})\exp(-\frac{iEt}{\hbar})d\vec{r}^3 \\
&= \int_{-\infty}^{\infty}|\psi_E(\vec{r})|^2\exp(\frac{2Im[E]}{\hbar}t)d\vec{r}^3
\end{aligned}
$$

显然,如果$Im[E]\neq 0$,上述积分与时间相关,不能保持任意时刻都归一化.

5. Griffiths书，习题1.15. 描述一个自发衰变粒子，其寿命为τ.

$$P(t)=\int|\psi(x,t)|^2 dx=e^{-t/\tau}$$

要得到这个几率衰减，可以设$V(x)=V_0(x)-i\Gamma$，其中V_0是真实的势能。Γ是正实数。证明:

$$\frac{dP(t)}{dt}=-\frac{2\Gamma}{\hbar}P(t) \tag{5}$$

求出P(t)，并给出以Γ表示的粒子寿命。

解：根据含时Schrödinger方程，可知

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\psi = H\psi = (\frac{p^2}{2m}+V_0(x))\psi - i\Gamma\psi \\
-i\hbar\frac{\partial}{\partial t}\psi^* = H^*\psi^* = (\frac{p^2}{2m}+V_0(x))\psi^* + i\Gamma\psi^*
\end{aligned}
$$

带入式(5)中得

$$
\begin{aligned}
\frac{dP(t)}{dt} &= \frac{d}{dt}\int|\psi(x,t)|^2 dx \\
&= \frac{d}{dt}\int\psi^*(x,t)\psi(x,t)dx \\
&= \frac{1}{i\hbar}\int[-(H^*\psi^*(x,t))\psi(x,t)+\psi(x,t)^*H\psi(x,t)]dx \\
&= \frac{1}{i\hbar}\int\psi^*(x,t)(-i2\Gamma)\psi(x,t)dx \\
&= -\frac{2\Gamma}{\hbar}P(t)
\end{aligned}
$$

上面推导利用了几率流散度的全空间积分为零。

直接求解$\frac{dP(t)}{dt}=-\frac{2\Gamma}{\hbar}P(t)$可得

$$P(t)=Ce^{-\frac{2\Gamma}{\hbar}t} \tag{6}$$

其中C为常数. 粒子寿命可定义为$P(t)$衰减为原值的$1/e$所需时间, 即得$\tau=\frac{\hbar}{2\Gamma}$. (Note: $\tau\cdot\Gamma\approx\frac{\hbar}{2}$ 实际上给出了吸收势与粒子寿命的不确定度关系。这里Γ可以理解吸收或排斥一个粒子所需的势能)

6. 计算$\frac{d\langle p\rangle}{dt}$.结果类似于牛顿定律,是后面讲到Ehrenfest定理的一个形式，它告诉我我们力学量的期望值遵循经典力学规律。

解:

$$\begin{aligned}
\frac{d\langle\hat{p}\rangle}{dt} &= \frac{d}{dt}\int dx\psi^*(x,t)\hat{p}\psi(x,t)\\
&= \int dx[(\frac{\partial}{\partial t}\psi(x,t))^*\hat{p}\psi(x,t)+\psi^*(x,t)\frac{\partial\hat{p}}{\partial t}\psi(x,t)+\psi^*(x,t)\hat{p}(\frac{\partial}{\partial t}\psi(t))]\\
&= \frac{1}{i\hbar}\int dx\ [-(\hat{p}^2/2m+V)\psi^*\hat{p}\psi+\psi^*\hat{p}(\hat{p}^2/2m+V)\psi]
\end{aligned} \tag{7}$$

利用了p不显含时间，即$\frac{\partial p}{\partial t}=0$. 对$\psi(x,t)$的时间全导数，由于我们不‘追踪’粒子，所以直接写成偏导数。

在可归一化条件下，波函数在无穷远处为零, 利用分部积分

$$\int(\hat{p}^2\psi)^*\psi dx=\int\psi^*\hat{p}^2\psi dx \tag{8}$$

注意$\hat{p}$ 向右作用，分成对V求导和对ψ求导，我们有:

$$\begin{aligned}
\frac{d\langle\hat{p}\rangle}{dt} &= \frac{1}{i\hbar}\int dx\ \psi^*(\hat{p}V-V\hat{p})\psi\\
&= \langle-\frac{dV(x)}{dx}\rangle
\end{aligned}$$

正是牛顿定律的形式。

7.考虑一个无限深势阱(阱宽a)中粒子. 如果环境温度为T, 且k_BT 远小于E_3. 根据热学知识，粒子处于E_n 的几率正比于$\exp(-E_n/(k_BT))$. 计算粒子的能量期望值$< E >$和比热c. （提示：比热的定义是$d < E > /dT$)

解:

$E_n=\frac{\hbar^2n^2\pi^2}{2ma^2}$, 由于$E_3>>k_BT$, 所以高于$E_3$的能级被占几率可以忽略.

$$\langle E\rangle=\frac{E_1\exp(-E_1/(k_BT))+E_2\exp(-E_2/(k_BT))}{Z},$$

其中$Z=\exp(-E_1/(k_BT))+\exp(-E_2/(k_BT))$
为归一化因子，也称配分函数.

定义倒温度$\beta = 1/(k_B T)$, 比热

$$c = -\frac{1}{k_B T^2}\frac{d < E >}{d(1/k_B T)} = -\frac{1}{k_B T^2}\frac{d < E >}{d\beta} = \frac{1}{k_B T^2}(\langle E^2\rangle - \langle E\rangle^2)$$

这个关系是比热与能量涨落的关系

8.计算一维无限深势井内束缚定态ψ_n的位置不确定度Δx和动量不确定度Δp。

$\psi_n = \begin{cases} Asin(\frac{n\pi x}{a}) & 0 \leq x \geq a \\ 0 & x < 0 \; or \; x > a \end{cases}$

解:

$$\begin{aligned}
\langle x\rangle &= \frac{2}{a}\int_0^a xsin^2(\frac{n\pi x}{a})dx = \frac{2}{a}\int_0^a x\frac{(1-\cos\frac{2n\pi x}{a})}{2}dx = \frac{2}{a}(\frac{x^2}{4}\Big|_0^a - \frac{a}{4n\pi}(x\sin\frac{2n\pi x}{a}\Big|_0^a \\
&\quad - \int_0^a \sin\frac{2n\pi x}{a}dx)) = \frac{a}{2} \\
\langle x^2\rangle &= \frac{2}{a}\int_0^a x^2 sin^2(\frac{n\pi x}{a})dx = \frac{2}{a}\int_0^a x^2\frac{(1-\cos\frac{2n\pi x}{a})}{2} = \frac{2}{a}(\frac{x^3}{6}\Big|_0^a - \frac{a}{4n\pi}(x^2\sin\frac{2n\pi x}{a}\Big|_0^a \\
&\quad - 2\int_0^a x\sin\frac{2n\pi x}{a}dx)) = \frac{a^2}{3} - \frac{1}{2n\pi}(\frac{a}{n\pi}(x\cos\frac{2n\pi x}{a}\Big|_0^a - \int_0^a \cos\frac{2n\pi x}{a}dx)) = \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} \\
\sigma(x) &= \sqrt{\langle x^2\rangle - \langle x\rangle^2} = a\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}} \\
\langle p\rangle &= \frac{2}{a}\int_0^a \sin\frac{n\pi x}{a}\frac{\hbar}{i}\partial_x \sin\frac{n\pi x}{a}dx = \frac{n\pi}{a^2}\frac{\hbar}{i}\int_0^a \sin\frac{2n\pi x}{a}dx = 0 \\
\langle p^2\rangle &= -\hbar^2\frac{2}{a}\int_0^a \sin\frac{n\pi x}{a}\partial_x^2 \sin\frac{n\pi x}{a}dx = \frac{2n^2\pi^2\hbar^2}{a^3}\int_0^a \sin^2\frac{n\pi x}{a}dx = \frac{n^2\pi^2\hbar^2}{a^2} \\
\sigma(p) &= \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \frac{n\pi\hbar}{a}
\end{aligned}$$

9 计算讲义Eq.(2.19)波函数下$\langle x\rangle$.你会发现它是时间震荡的.周期由什么决定。

解:

$\Psi(\vec{r},t)=\frac{1}{\sqrt{a}}\sin\frac{\pi x}{a}\exp\frac{-iE_1t}{\hbar}+\frac{1}{\sqrt{a}}\sin\frac{2\pi x}{a}\exp\frac{-iE_2t}{\hbar}\quad \text{Eq}(2.19)$

$$\langle x\rangle=\int_0^a\Psi^*\hat{x}\Psi d\vec{r}^3=\frac{1}{a}\int_0^a(x\sin^2\frac{\pi x}{a}+2xsin\frac{\pi x}{a}sin\frac{2\pi x}{a}\cos\frac{(E_1-E_2)t}{\hbar}+x\sin^2\frac{2\pi x}{a})dx$$
$$=\frac{1}{a}(\frac{a^2}{4}-\frac{1}{2}\underbrace{\int_0^a x\cos\frac{2\pi x}{a}dx}_{0}+(\int_0^a x\cos\frac{\pi x}{a}dx-\int_0^a x\cos\frac{3\pi x}{a}dx)\cos\frac{(E_1-E_2)t}{\hbar}+\frac{a^2}{4}-$$
$$\frac{1}{2}\underbrace{\int_0^a x\cos\frac{4\pi x}{a}dx)}_{0}=\frac{1}{a}(\frac{a^2}{4}+(-\frac{2a^2}{\pi^2}+\frac{2a^2}{9\pi^2})\cos\frac{(E_1-E_2)t}{\hbar}+\frac{a^2}{4})=\frac{a}{2}-\frac{16a}{9\pi^2}\cos\frac{(E_1-E_2)t}{\hbar}$$

$$T=\frac{2\pi}{\omega}=\frac{2\pi\hbar}{E_2-E_1}=\frac{4ma^2}{3\pi\hbar}$$