2021-2022(1) 量子力学作业

秦涛　　物理与光电工程学院

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1　第一次作业: 2021．09.07

1. 证明: 普朗克黑体辐射公式在高频和低频极限下分别给出维恩公式和瑞利 -金斯公式.

证: Planck 黑体辐射公式为:

$$u_\nu\left(T\right)=\frac{8\pi\nu^2}{c^3}\frac{h\nu}{\exp\left(\frac{h\nu}{k_BT}\right)-1} \tag{1}$$

在高频极限下, $\frac{h\nu}{k_BT}\gg 1$, 即 $\exp\left(\frac{h\nu}{k_BT}\right)\gg 1$, 所以

$$u_\nu\left(T\right)\approx\frac{8\pi h\nu^3}{c^3}\exp\left(-\frac{h\nu}{k_BT}\right) \tag{2}$$

即 Wien 公式;

在低频极限下, $\frac{h\nu}{k_BT}\ll 1$, 则 $\exp\left(\frac{h\nu}{k_BT}\right)\approx 1+\frac{h\nu}{k_BT}$, 所以

$$u_\nu\left(T\right)\approx\frac{8\pi\nu^2}{c^3}\frac{h\nu}{1+\frac{h\nu}{k_BT}-1}=\frac{8\pi\nu^2}{c^3}k_BT \tag{3}$$

2. 由普朗克黑体辐射公式推导出维恩位移定律: 即黑体辐射的峰值波长 λ_{max} 与辐射温度 T 之间的关系 $\lambda_{max}T=$ 常数. (提示: 根据 $u_\nu\left(T\right)$ 得到 $u_\lambda\left(T\right)$).

解: 由黑体辐射能量密度的定义:

$$dU_\nu\left(T\right)=u_\nu\left(T\right)d\nu \tag{4}$$

由于 $\lambda=\frac{c}{\nu}$, 则

$$dU_\nu\left(T\right)=\frac{8\pi h}{\lambda^3}\frac{1}{\exp\left(\frac{hc}{k_BT\lambda}\right)-1}d\frac{c}{\lambda} \tag{5}$$

$$=-\frac{8\pi hc}{\lambda^5}\frac{1}{\exp\left(\frac{hc}{k_BT\lambda}\right)-1}d\lambda \tag{6}$$

则 $u_\lambda(T)=\frac{8\pi hc}{\lambda^5}\frac{1}{\exp\left(\frac{hc}{k_BT\lambda}\right)-1}$. 这里没有取负号, 可以如下理解: 区间 $[\nu_1,\nu_2]$ ($\nu_1<\nu_2$) 上的能量:

$$U_\nu(T)=\int_{\nu_1}^{\nu_2}u_\nu(T)\,d\nu \tag{7}$$

$$=\int_{\frac{c}{\lambda_1}}^{\frac{c}{\lambda_2}}u_\nu(T)\,d\frac{c}{\lambda} \tag{8}$$

$$=\int_{\lambda_1}^{\lambda_2}u_\nu(T)\,\frac{-c}{\lambda^2}d\lambda \tag{9}$$

由于 $\lambda_1>\lambda_2$, $U_\nu(T)=\int_{\lambda_2}^{\lambda_1}u_\nu(T)\,\frac{c}{\lambda^2}d\lambda$, 即 $u_\lambda(T)=u_\nu(T)\,\frac{c}{\lambda^2}=\frac{8\pi hc}{\lambda^5}\frac{1}{\exp\left(\frac{hc}{k_BT\lambda}\right)-1}$.

令 $\frac{du_\lambda(T)}{d\lambda}=0$, 则

$$\frac{du_\lambda(T)}{d\lambda}=-\frac{40\pi hc}{\lambda^6}\frac{1}{\exp\left(\frac{hc}{k_BT\lambda}\right)-1}-\frac{8\pi hc}{\lambda^5}\frac{\exp\left(\frac{hc}{k_BT\lambda}\right)\frac{-hc}{k_BT\lambda^2}}{\left(\exp\left(\frac{hc}{k_BT\lambda}\right)-1\right)^2}=0 \tag{10}$$

化简得辐射的峰值波长 λ_{max} 满足

$$\frac{\frac{hc}{k_BT\lambda_{max}}}{1-\exp\left(-\frac{hc}{k_BT\lambda_{max}}\right)}=5 \tag{11}$$

令 $x=\frac{hc}{k_BT\lambda_{max}}$, 则

$$\frac{x}{5}=1-e^{-x} \tag{12}$$

由图可知方程有解 $x\approx 4.96$, 于是 $T\lambda_{max}\approx\frac{hc}{4.96k_B}=2.897\times10^{-3}$mK.

../Going_on/wien.png

Figure 1: 方程的解

讨论: 不能利用 ν_{max} 求 λ_{max}, 因为 $\lambda=\frac{c}{\nu}$, λ 和 ν 不可能同时达到最大.

3. 根据普朗克给出的单个振子的平均能量, 假设固体处于温度 T, 所有原子以同一频率 ν 振动, 每个原子有三个自由度.

(1) 求 N 个原子的平均能量 E;

(2) 计算固体的比热 $C=\frac{\partial E}{\partial T}$;

(3) 确定比热在高温和低温极限下的取值.

解: (1) 每个振子的平均能量为 $\langle\epsilon\rangle=\frac{h\nu}{\exp\left(\frac{h\nu}{k_BT}\right)-1}$, 于是 N 个原子的平均能量 E 为:

$$E=\frac{3Nh\nu}{\exp\left(\frac{h\nu}{k_BT}\right)-1} \tag{13}$$

(2) 固体的比热:

$$C=\frac{\partial E}{\partial T}=\frac{1}{k_BT^2}\frac{3N\left(h\nu\right)^2\exp\left(\frac{h\nu}{k_BT}\right)}{\left(\exp\left(\frac{h\nu}{k_BT}\right)-1\right)^2} \tag{14}$$

(3) 令 $\frac{h\nu}{k_BT}=x$, 则

$$C=\frac{3Nk_Bx^2e^x}{\left(e^x-1\right)^2}=3Nk_B\frac{x^2}{\left(e^{\frac{x}{2}}-e^{-\frac{x}{2}}\right)^2} \tag{15}$$

在低温极限下, $x\to\infty$, $\frac{x^2}{\left(e^{\frac{x}{2}}-e^{-\frac{x}{2}}\right)^2}\approx\frac{x^2}{e^x}\to 0$, 则 $C\to 0$. 在高温极限下 $x\to 0$, $\frac{x^2}{\left(e^{\frac{x}{2}}-e^{-\frac{x}{2}}\right)^2}\approx\frac{x^2}{\left(1+\frac{x}{2}-\left(1-\frac{x}{2}\right)\right)^2}\to 1$, 则 $C\to 3Nk_B$.

讨论:

(1) 这里的比热为定容比热.

(2) 高温极限下给出的是经典结论.

2　第二次作业: 2021.09.14

1. (经典概率) 在一次集体活动中, 参加活动的成员的年龄分布如下:

年龄/岁	14	15	16	17	23	24	30
人数/个	10	6	7	8	2	2	1

Table 1: 参加活动成员的年龄和相应的人数

(1) 随机抽出一人, 求其年龄为 24 岁的概率;

(2) 求参加该集体活动的成员的平均年龄.

解: (1) 总人数为 36, 24 岁的成员有 2 个, 故随机抽出一人, 其年龄为 24 岁概率为:

$$\frac{2}{36}\approx 0.056 \tag{16}$$

(2) 平均年龄

$$\frac{14\times 10+15\times 6+16\times 7+17\times 8+23\times 2+24\times 2+30\times 1}{36}\approx 16.722 \tag{17}$$

2. (经典概率) 设想一个物体从 h 处自由下落, 在它落地之前, 在足够多的随机的时刻测量物体已经下落的高度.

(1) 求物体下落的高度为 x $(0<x<h)$ 的概率密度; 提示: 设下落的总时间为 T, 则物体处于 x 到 $x+dx$ 的概率等于相应的处于时刻 t 到 $t+dt$ 的概率 $\frac{dt}{T}$.

(2) 求物体已经下落的高度 $x(0<x<h)$ 的平均值.

解: (1) 设物体下落的高度为 x $(0<x<h)$ 的概率密度为 $P\left(x\right)$, 则

$$P\left(x\right)dx=\frac{dt}{T} \tag{18}$$

这里下落高度 h 的总时间为 T,

$$h=\frac{1}{2}gT^2 \tag{19}$$

所以 $T=\sqrt{\frac{2h}{g}}$. 于是

$$P\left(x\right)=\frac{1}{T}\frac{dt}{dx} \tag{20}$$

由于 $x(t)=\frac{1}{2}gt^2$, 所以 $\frac{dx}{dt}=gt=\sqrt{2gx}$,

$$P(x)=\frac{1}{T\sqrt{2gx}}=\frac{1}{2\sqrt{hx}} \tag{21}$$

可以验证, $\int_0^h P(x)\,dx=\int_0^h \frac{1}{2\sqrt{hx}}dx=1$, 可见 $P(x)$ 确实是概率密度.

(2) 高度的平均值为:

$$\begin{aligned}\langle x\rangle &= \int_0^h xP(x)\,dx \qquad (22)\\ &= \int_0^h x\frac{1}{2\sqrt{hx}}dx \qquad (23)\\ &= \frac{1}{\sqrt{h}}\frac{1}{3}x^{\frac{3}{2}}\Big|_0^h \qquad (24)\\ &= \frac{1}{3}h \qquad (25)\end{aligned}$$

讨论: 不管 x 是离散变量, 还是连续变量, 其平均值均为的 x 的可能取值乘以相应的概率再求和(或积分).

3. (波函数归一化与量子力学概率) 教材第 8 页练习 1, 练习 5.

练习 1: 由 $\int|\psi(x)|^2dx=1$ 得:

$$\begin{aligned}\int_{-\infty}^{\infty}|\psi(x)|^2dx =& A^2\int_{-\infty}^{\infty}e^{-\alpha^2x^2}dx \qquad (26)\\ =& A^2\sqrt{\int_{-\infty}^{\infty}e^{-\alpha^2x^2}dx\int_{-\infty}^{\infty}e^{-\alpha^2y^2}dy} \qquad (27)\\ =& A^2\sqrt{\int_0^{\infty}rdr\int_0^{2\pi}d\theta e^{-\alpha^2r^2}} \qquad (28)\\ =& A^2\sqrt{2\pi\int_0^{\infty}rdre^{-\alpha^2r^2}} \qquad (29)\\ =& A^2\sqrt{2\pi\,\frac{e^{-\alpha^2r^2}}{-2\alpha^2}\Big|_0^{\infty}} \qquad (30)\\ =& A^2\sqrt{\frac{\pi}{\alpha^2}}=1 \qquad (31)\end{aligned}$$

所以, $A=(\frac{\alpha^2}{\pi})^{\frac{1}{4}}$.

讨论: 希望大家牢记本题结果.

练习 5:

(1) 在球壳 $(r,r+dr)$ 中被观测到的概率, 对角度无限制, 所以它可表示为

$$r^2dr\int_0^{\pi}\sin\theta d\theta\int_0^{2\pi}d\varphi\,|\psi(r,\theta,\varphi)|^2 \tag{32}$$

(2) 在 (θ,φ) 方向立体角元中找到粒子的概率为

$$d\Omega\int_0^{\infty}r^2dr\,|\psi(r,\theta,\varphi)|^2 \tag{33}$$

讨论: 立体角 $d\Omega=\sin\theta d\theta d\varphi$, $\int d\Omega=\int_0^\pi \sin\theta d\theta\int_0^{2\pi}d\varphi=4\pi$.

4. (波函数归一化与导数) 考虑波函数 $\Psi(x,t)=Ae^{-\lambda|x|}e^{-i\omega t}$. 这里, A, λ, ω 均为实的.

(1) 求归一化常数 A.

(2) 计算 $\frac{\partial\Psi(x,t)}{\partial t}$, $\frac{\partial\Psi(x,t)}{\partial x}$, $\frac{\partial^2\Psi(x,t)}{\partial x^2}$.

解: (1) 由 $\int dx|\psi(x,t)|^2=1$ 得,

$$\begin{aligned}\int dx|\psi(x,t)|^2 &= A^2\int_{-\infty}^{\infty}dxe^{-2\lambda|x|}=A^2\left(\int_{-\infty}^{0}dxe^{2\lambda x}+\int_0^{\infty}dxe^{-2\lambda x}\right) && (34)\\ &= A^2\left(\left.\frac{e^{2\lambda x}}{2\lambda}\right|_{-\infty}^{0}+\left.\frac{e^{-2\lambda x}}{-2\lambda}\right|_0^{\infty}\right) && (35)\\ &= \frac{A^2}{\lambda}=1 && (36)\end{aligned}$$

所以可取 $A=\sqrt{\lambda}$.

(2) 已经得到: $\Psi(x,t)=\sqrt{\lambda}e^{-\lambda|x|}e^{-i\omega t}$, 故

$$\frac{\partial\Psi(x,t)}{\partial t}=-i\omega\sqrt{\lambda}e^{-\lambda|x|}e^{-i\omega t} \tag{37}$$

对于 $\frac{\partial\Psi(x,t)}{\partial x}$,

$$\frac{\partial\Psi(x,t)}{\partial x}=\begin{cases}\lambda\sqrt{\lambda}e^{\lambda x}e^{-i\omega t}, & x<0\\ -\lambda\sqrt{\lambda}e^{-\lambda x}e^{-i\omega t}, & x>0\end{cases} \tag{38}$$

所以

$$\frac{\partial\Psi(x,t)}{\partial x}=[\theta(-x)-\theta(x)]\lambda\Psi(x,t) \tag{39}$$

这里阶跃函数 $\theta(x)=\begin{cases}1, & x>0\\ 0, & x<0\end{cases}$. 并注意到 $\left.\frac{\partial\Psi(x,t)}{\partial x}\right|_{x=0^-}=\lambda\Psi(0,t)$, $\left.\frac{\partial\Psi(x,t)}{\partial x}\right|_{x=0^+}=-\lambda\Psi(0,t)$, 即 $x=0$ 处, 一阶导数不连续. 这里, 我们不认为 $\Psi(x,t)$ 在 $x=0$ 不可导, 而把 $x=0$ 处视为其一阶导数的第一类间断点.

(3) 由 (2) 得:

$$\begin{aligned}\frac{\partial^2\Psi(x,t)}{\partial x^2} &= \frac{\partial[\theta(-x)-\theta(x)]}{\partial x}\lambda\Psi(x,t)+[\theta(-x)-\theta(x)]^2\lambda^2\Psi(x,t) && (40)\\ &= (\lambda-2\delta(x))\lambda\Psi(x,t) && (41)\end{aligned}$$

讨论:

(a) $\delta(x)$ 与 $\theta(x)$ 的联系 $\delta(x)=\frac{d\theta(x)}{dx}$.

(b) $\delta(x)$ 不是普通的函数, 它是函数序列的极限, 例: $\lim_{\alpha\to\infty}\frac{\sin(\alpha x)}{\pi x}=\delta(x)$.

3 第三次作业: 2021.09.28

1. 设某时刻一维自由粒子的波函数为一个高斯波包 $\psi(x)=Ae^{ikx-\frac{x^2}{2\alpha^2}}$. 对于该量子态,

(1) 确定归一化常数 A.

(2) 计算坐标的平均值 $\langle\hat{x}\rangle$, 动量算符的平均值 $\langle\hat{p}\rangle$, 坐标算符的不确定度 $\Delta x=\sqrt{\langle(\hat{x}-\langle\hat{x}\rangle)^2\rangle}$, 以及动量算符的不确定度 $\Delta p=\sqrt{\langle(\hat{p}-\langle\hat{p}\rangle)^2\rangle}$.

提示: 对任意算符 $\hat{A}$, $\left\langle\left(\hat{A}-\left\langle\hat{A}\right\rangle\right)^2\right\rangle=\left\langle\hat{A}^2\right\rangle-\left\langle\hat{A}\right\rangle^2$.

解:

(1) 由归一化要求:

$$\int_{-\infty}^{\infty}dx\left|\psi\left(x\right)\right|^2=1 \tag{42}$$

$$\left|A\right|^2\int_{-\infty}^{\infty}dxe^{-\frac{x^2}{\alpha^2}}=1 \tag{43}$$

即 $\left|A\right|^2\sqrt{\pi\alpha^2}=1$, 于是可以取 $A=\frac{1}{(\pi\alpha^2)^{\frac{1}{4}}}$.

(2) 首先

$$\begin{aligned}\bar{x}&=\int_{-\infty}^{\infty}dx\psi^*\left(x,0\right)x\psi\left(x,0\right) &(44)\\ &=\int_{-\infty}^{\infty}dxx\frac{1}{\left(\pi\alpha^2\right)^{1/2}}e^{-\frac{x^2}{\alpha^2}} &(45)\end{aligned}$$

由于被积函数是 x 的奇函数，所以 $\bar{x}=0$.

$$\begin{aligned}\bar{p}&=\int_{-\infty}^{\infty}dx\psi^*\left(x,0\right)\hat{p}\psi\left(x,0\right) &(46)\\ &=\int_{-\infty}^{\infty}dx\psi^*\left(x,0\right)\frac{\hbar}{i}\frac{d}{dx}\psi\left(x,0\right) &(47)\\ &=\int_{-\infty}^{\infty}dx\psi^*\left(x,0\right)\left(\hbar k-\frac{\hbar x}{i\alpha^2}\right)\psi\left(x,0\right) &(48)\\ &=\int_{-\infty}^{\infty}dx\left(\hbar k-\frac{\hbar x}{i\alpha^2}\right)\frac{1}{\left(\pi\alpha^2\right)^{1/2}}e^{-\frac{x^2}{\alpha^2}} &(49)\\ &=\hbar k\int_{-\infty}^{\infty}dx\frac{1}{\left(\pi\alpha^2\right)^{1/2}}e^{-\frac{x^2}{\alpha^2}}-\int_{-\infty}^{\infty}dx\frac{\hbar x}{i\alpha^2}\frac{1}{\left(\pi\alpha^2\right)^{1/2}}e^{-\frac{x^2}{\alpha^2}} &(50)\end{aligned}$$

上式中第二项是 x 的奇函数，所以 $\bar{p}=\hbar k$.

$$\begin{aligned}\overline{x^2}&=\int_{-\infty}^{\infty}dx\psi^*\left(x,0\right)x^2\psi\left(x,0\right) &(51)\\ &=\frac{1}{\left(\pi\alpha^2\right)^{1/2}}\int_{-\infty}^{\infty}dxx^2e^{-\frac{x^2}{\alpha^2}} &(52)\\ &=\frac{1}{\left(\pi\alpha^2\right)^{1/2}}\int_{-\infty}^{\infty}dx\left(-\frac{d}{du}\right)e^{-ux^2} &(53)\\ &=-\frac{1}{\left(\pi\alpha^2\right)^{1/2}}\frac{d}{du}\int_{-\infty}^{\infty}dxe^{-ux^2} &(54)\end{aligned}$$

这里令 $u=\frac{1}{\alpha^2}$, $\overline{x^2}=-\frac{1}{(\pi\alpha^2)^{1/2}}\frac{d}{du}\sqrt{\frac{\pi}{u}}=\frac{\alpha^2}{2}$.

$$\begin{aligned}\overline{p^2}&=\int_{-\infty}^{\infty}dx\psi^*\left(x,0\right)\hat{p}^2\psi\left(x,0\right) &(55)\\ &=\int_{-\infty}^{\infty}dx\psi^*\left(x,0\right)\left(-\hbar^2\frac{d^2}{dx^2}\right)\psi\left(x,0\right) &(56)\end{aligned}$$

$$\frac{\hbar}{i}\frac{d}{dx}\psi(x,0)=\left(\hbar k-\frac{\hbar x}{i\alpha^2}\right)\psi(x,0) \tag{57}$$

$$\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2\psi(x,0)=\frac{\hbar^2}{\alpha^2}\psi(x,0)+\left(\hbar k-\frac{\hbar x}{i\alpha^2}\right)^2\psi(x,0) \tag{58}$$

$$=\left(\frac{\hbar^2}{\alpha^2}+\hbar^2k^2-\frac{2\hbar^2kx}{i\alpha^2}-\frac{\hbar^2x^2}{\alpha^4}\right)\psi(x,0) \tag{59}$$

所以

$$\overline{p^2}=\frac{1}{(\pi\alpha^2)^{1/2}}\int_{-\infty}^{\infty}dx\left(\frac{\hbar^2}{\alpha^2}+\hbar^2k^2-\frac{2\hbar^2kx}{i\alpha^2}-\frac{\hbar^2x^2}{\alpha^4}\right)e^{-\frac{x^2}{\alpha^2}} \tag{60}$$

$$=\frac{\hbar^2}{\alpha^2}+\hbar^2k^2-\frac{\hbar^2}{\alpha^4}\frac{\alpha^2}{2}=\hbar^2k^2+\frac{\hbar^2}{2\alpha^2} \tag{61}$$

我们最终得到

$$\overline{(x-\bar{x})^2}=\overline{x^2}-(\bar{x})^2=\frac{\alpha^2}{2} \tag{62}$$

$$\overline{(\hat{p}-\bar{p})^2}=\overline{\hat{p}^2}-(\bar{p})^2=\frac{\hbar^2}{2\alpha^2} \tag{63}$$

即 $\Delta x=\frac{\alpha}{\sqrt{2}}$，$\Delta p=\frac{\hbar}{\sqrt{2}\alpha}$. 注意到: $\Delta x\Delta p=\frac{\hbar}{2}$.

2. 对于第 2 次作业第 4 题中的 $\Psi(x,t)$, 计算下列物理量:

(1) 计算 $\langle\hat{x}\rangle$ 和 $\left\langle(\hat{x}-\langle\hat{x}\rangle)^2\right\rangle$;

(2) 计算动能的平均值 $\left\langle\hat{T}\right\rangle$, 这里 $\hat{T}=\frac{\hat{p}^2}{2m}$.

解:

(1) 由于 $\Psi(x,t)=\sqrt{\lambda}e^{-\lambda|x|}e^{-i\omega t}$,

$$\langle\hat{x}\rangle=\int_{-\infty}^{\infty}\hat{x}\left|\Psi(x,t)\right|^2dx \tag{64}$$

$$=\lambda\int_{-\infty}^{\infty}xe^{-2\lambda|x|}dx=0 \tag{65}$$

这里, 被积函数是奇函数.

$$\left\langle\hat{x}^2\right\rangle=\int_{-\infty}^{\infty}\hat{x}^2\left|\Psi(x,t)\right|^2dx \tag{66}$$

$$=\lambda\int_{-\infty}^{\infty}x^2e^{-2\lambda|x|}dx \tag{67}$$

$$=2\lambda\int_0^{\infty}x^2e^{-2\lambda x}dx \tag{68}$$

$$=2\lambda\left(\left.\frac{x^2e^{-2\lambda x}}{-2\lambda}\right|_0^{\infty}+\frac{1}{\lambda}\int_0^{\infty}xe^{-2\lambda x}dx\right) \tag{69}$$

$$=2\left(\left.\frac{xe^{-2\lambda x}}{-2\lambda}\right|_0^{\infty}+\frac{1}{2\lambda}\int_0^{\infty}e^{-2\lambda x}dx\right) \tag{70}$$

$$=\frac{1}{2\lambda^2} \tag{71}$$

所以 $\left\langle(\hat{x}-\langle\hat{x}\rangle)^2\right\rangle=\left\langle\hat{x}^2\right\rangle-\langle\hat{x}\rangle^2=\frac{1}{2\lambda^2}$. **(注意: 原来题目的写法有个错误, 平方应在内部.)**

(2) 由于 $\frac{\partial^2\Psi(x,t)}{\partial x^2}=(\lambda-2\delta(x))\lambda\Psi(x,t)$, 所以

$$\left\langle\hat{T}\right\rangle=\int_{-\infty}^{\infty}\Psi^*(x,t)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\Psi(x,t)\,dx \tag{72}$$
$$=-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\Psi^*(x,t)(\lambda-2\delta(x))\lambda\Psi(x,t)\,dx \tag{73}$$
$$=-\frac{\hbar^2}{2m}\left(\lambda^2\int_{-\infty}^{\infty}|\Psi(x,t)|^2\,dx-2\lambda\int_{-\infty}^{\infty}|\Psi(x,t)|^2\delta(x)\,dx\right) \tag{74}$$
$$=\frac{\hbar^2\lambda^2}{2m} \tag{75}$$

讨论: 在第 (2) 问中, 如果**忽视**了 $\delta(x)$ 项, 将会得到 $\left\langle\hat{T}\right\rangle=-\frac{\hbar^2\lambda^2}{2m}$, 即负的动能, 这显然是**荒谬**的结果. 另外一种解法是先求 $\varphi(p)$:

$$\varphi(p,t)=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}dp\sqrt{\lambda}e^{-\lambda|x|}e^{-\frac{ipx}{\hbar}}e^{-i\omega t} \tag{76}$$
$$=\frac{1}{\sqrt{2\pi\hbar}}\left(\int_{-\infty}^{0}dp\sqrt{\lambda}e^{\left(\lambda-i\frac{p}{\hbar}\right)x}+\int_{0}^{\infty}dp\sqrt{\lambda}e^{\left(-i\frac{p}{\hbar}-\lambda\right)x}\right)e^{-i\omega t} \tag{77}$$
$$=\sqrt{\frac{\lambda}{2\pi\hbar}}\frac{2\lambda e^{-i\omega t}}{\lambda^2+\frac{p^2}{\hbar^2}} \tag{78}$$

于是:

$$\left\langle\hat{T}\right\rangle=\int_{-\infty}^{\infty}\frac{p^2}{2m}\varphi^*(p,t)\varphi(p,t)\,dp \tag{79}$$
$$=\frac{\lambda}{2\pi\hbar}4\lambda^2\frac{1}{2m}\int_{-\infty}^{\infty}dp\frac{p^2}{\left(\lambda^2+\frac{p^2}{\hbar^2}\right)^2} \tag{80}$$
$$=\frac{\hbar^2\lambda^3}{m\pi}\int_{-\infty}^{\infty}dk\frac{k^2}{(\lambda^2+k^2)^2} \tag{81}$$
$$=\frac{\hbar^2\lambda^2}{2m} \tag{82}$$

这里, $\int_{-\infty}^{\infty}dk\frac{k^2}{(\lambda^2+k^2)^2}=2\pi i\,\mathrm{Res}\left(\frac{k^2}{(\lambda^2+k^2)^2}\right)\Big|_{k=i\lambda}=\frac{\pi}{2\lambda}$.

3. 已知三维量子体系氢原子的基态波函数为 $\psi(r)=A\exp\left(-\frac{r}{a}\right)$, 这里 A 为归一化常数, a 为玻尔半径, $r=\sqrt{x^2+y^2+z^2}$,

(1) 证明: 动能算符 $\hat{T}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$;

(2) (选做) 证明: 球坐标系下动能算符 $\hat{T}=-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2}\frac{1}{\sin\theta^2}\frac{\partial^2}{\partial\varphi^2}\right)$;

(3) 计算动能的平均值;

(4) 计算势能的平均值 $\left\langle\hat{V}\right\rangle$, 这里 $\hat{V}=-\frac{e^2}{4\pi\epsilon_0 r}$.

解: 首先确定归一化常数, 由于

$$1=\int_0^{\infty}r^2dr\int_0^{\pi}d\theta\int_0^{2\pi}d\varphi\,|\psi(r)|^2 \tag{83}$$
$$=4\pi|A|^2\int_0^{\infty}r^2\exp\left(-\frac{2r}{a}\right)dr \tag{84}$$

这里 $(n>1)$,

$$\int_0^\infty r^n \exp\left(-\frac{2r}{a}\right)dr = r^n\frac{\exp\left(-\frac{2r}{a}\right)}{-\frac{2}{a}}\Bigg|_0^\infty - n\left(-\frac{a}{2}\right)\int_0^\infty r^{n-1}\exp\left(-\frac{2r}{a}\right)dr \tag{85}$$

即

$$\int_0^\infty r^n \exp\left(-\frac{2r}{a}\right)dr = \frac{an}{2}\int_0^\infty r^{n-1}\exp\left(-\frac{2r}{a}\right)dr \tag{86}$$

而

$$\int_0^\infty \exp\left(-\frac{2r}{a}\right)dr = \frac{a}{2} \tag{87}$$

所以

$$\int_0^\infty r^n \exp\left(-\frac{2r}{a}\right)dr = n!\left(\frac{a}{2}\right)^{n+1} \tag{88}$$

于是

$$\int_0^\infty r^2 \exp\left(-\frac{2r}{a}\right)dr = 2\left(\frac{a}{2}\right)^3 = \frac{a^3}{4} \tag{89}$$

可取 $A=\frac{1}{\sqrt{\pi a^3}}$.

(1) 动能算符

$$\bar{T} = \int_{-\infty}^{\infty} d^3p\left|\varphi(\boldsymbol{p})\right|^2\frac{p^2}{2m} \tag{90}$$

$$= \int_{-\infty}^{\infty} d^3p\varphi^*(\boldsymbol{p})\frac{p^2}{2m}\varphi(\boldsymbol{p}) \tag{91}$$

$$= \int_{-\infty}^{\infty} d^3p\frac{1}{(2\pi\hbar)^{3/2}}\int_{-\infty}^{\infty} d^3re^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}\psi^*(\boldsymbol{r})\frac{p^2}{2m}\varphi(\boldsymbol{p}) \tag{92}$$

由于 $\boldsymbol{p}e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}=\frac{\hbar}{i}\nabla e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}$，则 $p^2e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}=\boldsymbol{p}\cdot\boldsymbol{p}e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}=-\hbar^2\nabla\cdot\nabla e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}=-\hbar^2\nabla^2e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}$,

$$\bar{T} = \int_{-\infty}^{\infty} d^3p\frac{1}{(2\pi\hbar)^{3/2}}\int_{-\infty}^{\infty} d^3r\psi^*(\boldsymbol{r})\frac{p^2}{2m}e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}\varphi(\boldsymbol{p}) \tag{93}$$

$$= \int_{-\infty}^{\infty} d^3p\frac{1}{(2\pi\hbar)^{3/2}}\int_{-\infty}^{\infty} d^3r\psi^*(\boldsymbol{r})\left(-\frac{\hbar^2}{2m}\nabla^2\right)e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}\varphi(\boldsymbol{p}) \tag{94}$$

$$\text{注意：}\left(-\frac{\hbar^2}{2m}\nabla^2\right)\text{与}e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}\text{ 的顺序不能换} \tag{95}$$

$$= \int_{-\infty}^{\infty} d^3r\psi^*(\boldsymbol{r})\left(-\frac{\hbar^2}{2m}\nabla^2\right)\frac{1}{(2\pi\hbar)^{3/2}}\int_{-\infty}^{\infty} d^3pe^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}\varphi(\boldsymbol{p}) \tag{96}$$

$$= \int_{-\infty}^{\infty} d^3r\psi^*(\boldsymbol{r})\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi(\boldsymbol{r}) \tag{97}$$

即动能的算符形式为:

$$\hat{T} = \frac{\hbar^2}{2m}\nabla\cdot\nabla \tag{98}$$

$$= -\frac{\hbar^2}{2m}\left(\boldsymbol{e}_x\frac{\partial}{\partial x}+\boldsymbol{e}_y\frac{\partial}{\partial y}+\boldsymbol{e}_z\frac{\partial}{\partial z}\right)\cdot\left(\boldsymbol{e}_x\frac{\partial}{\partial x}+\boldsymbol{e}_y\frac{\partial}{\partial y}+\boldsymbol{e}_z\frac{\partial}{\partial z}\right) \tag{99}$$

$$= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) \tag{100}$$

(2) 在直角坐标和球坐标下, 对任意连续可微函数 $\psi(\boldsymbol{r})$ 分别有:

$$d\psi(\boldsymbol{r}) = \frac{\partial\psi}{\partial x}dx + \frac{\partial\psi}{\partial y}dy + \frac{\partial\psi}{\partial z}dz \tag{101}$$

$$= \frac{\partial\psi}{\partial r}dr + \frac{\partial\psi}{\partial\theta}d\theta + \frac{\partial\psi}{\partial\varphi}d\varphi \tag{102}$$

另一方面,

$$d\psi(\boldsymbol{r}) = \nabla\psi\cdot d\boldsymbol{r} \tag{103}$$

这里令 $\nabla\psi = u\boldsymbol{e}_r + v\boldsymbol{e}_\theta + w\boldsymbol{e}_\varphi$, 并且 $\boldsymbol{r} = r(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$,

$$d\boldsymbol{r} = \frac{\partial\boldsymbol{r}}{\partial r}dr + \frac{\partial\boldsymbol{r}}{\partial\theta}d\theta + \frac{\partial\boldsymbol{r}}{\partial\varphi}d\varphi \tag{104}$$

$$\frac{\partial\boldsymbol{r}}{\partial r} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) = \boldsymbol{e}_r \tag{105}$$

$$\frac{\partial\boldsymbol{r}}{\partial\theta} = r(\cos\theta\cos\varphi, \cos\theta\sin\varphi, -\sin\theta) = r\boldsymbol{e}_\theta \tag{106}$$

$$\frac{\partial\boldsymbol{r}}{\partial\varphi} = r\sin\theta(-\sin\varphi, \cos\varphi, 0) = r\sin\theta\boldsymbol{e}_\varphi \tag{107}$$

于是,

$$d\psi(\boldsymbol{r}) = (u\boldsymbol{e}_r + v\boldsymbol{e}_\theta + w\boldsymbol{e}_\varphi)\cdot(\boldsymbol{e}_r dr + r\boldsymbol{e}_\theta d\theta + r\sin\theta\boldsymbol{e}_\varphi d\varphi) \tag{108}$$

$$= udr + vrd\theta + wr\sin\theta d\varphi \tag{109}$$

与方程 (102) 比较得:

$$u = \frac{\partial\psi}{\partial r} \tag{110}$$

$$v = \frac{1}{r}\frac{\partial\psi}{\partial\theta} \tag{111}$$

$$w = \frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\varphi} \tag{112}$$

即在球坐标系下, 任意函数 $\psi(\boldsymbol{r})$ 的梯度为:

$$\nabla\psi = \boldsymbol{e}_r\frac{\partial\psi}{\partial r} + \boldsymbol{e}_\theta\frac{1}{r}\frac{\partial\psi}{\partial\theta} + \boldsymbol{e}_\varphi\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\varphi} \tag{113}$$

特别的,

$$\nabla r = \boldsymbol{e}_r \tag{114}$$

$$\nabla\theta = \frac{1}{r}\boldsymbol{e}_\theta \tag{115}$$

$$\nabla\varphi = \frac{1}{r\sin\theta}\boldsymbol{e}_\varphi \tag{116}$$

(这里要注意到 $\nabla\times\nabla r = 0$, $\nabla\times\nabla\theta = 0$, $\nabla\times\nabla\varphi = 0$) 下面计算:

$$\nabla\cdot\nabla\psi = \nabla\cdot\left(\boldsymbol{e}_r\frac{\partial\psi}{\partial r} + \boldsymbol{e}_\theta\frac{1}{r}\frac{\partial\psi}{\partial\theta} + \boldsymbol{e}_\varphi\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\varphi}\right) \tag{117}$$

$$\begin{aligned}
\nabla\cdot\left(\boldsymbol{e}_r\frac{\partial\psi}{\partial r}\right) =&\nabla\cdot\left(\frac{\boldsymbol{e}_r}{r^2\sin\theta}r^2\sin\theta\frac{\partial\psi}{\partial r}\right) && (118)\\
=&\nabla\cdot\left(\frac{\boldsymbol{e}_r}{r^2\sin\theta}\right)r^2\sin\theta\frac{\partial\psi}{\partial r}+\frac{\boldsymbol{e}_r}{r^2\sin\theta}\cdot\nabla\left(r^2\sin\theta\frac{\partial\psi}{\partial r}\right) && (119)\\
=&\nabla\cdot\left(\frac{\boldsymbol{e}_\theta\times\boldsymbol{e}_\varphi}{r^2\sin\theta}\right)r^2\sin\theta\frac{\partial\psi}{\partial r}+\frac{\boldsymbol{e}_r}{r^2\sin\theta}\cdot\nabla\left(r^2\sin\theta\frac{\partial\psi}{\partial r}\right) && (120)\\
=&\nabla\cdot\left(\nabla\theta\times\nabla\varphi\right)r^2\sin\theta\frac{\partial\psi}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial r}\left(r^2\sin\theta\frac{\partial\psi}{\partial r}\right) && (121)\\
=&\frac{1}{r^2\sin\theta}\frac{\partial}{\partial r}\left(r^2\sin\theta\frac{\partial\psi}{\partial r}\right) && (122)\\
=&\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) && (123)
\end{aligned}$$

这里利用了 $\nabla\cdot(\nabla\theta\times\nabla\varphi)=\nabla\times\nabla\theta\cdot\nabla\varphi-\nabla\theta\cdot(\nabla\times\nabla\varphi)=0$. 类似的,

$$\nabla\cdot\left(\boldsymbol{e}_\theta\frac{1}{r}\frac{\partial\psi}{\partial\theta}\right)=\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) \tag{124}$$

$$\nabla\cdot\left(\boldsymbol{e}_\varphi\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\varphi}\right)=\frac{1}{r^2}\frac{\partial}{\partial\varphi}\left(\frac{1}{\sin\theta}\frac{\partial\psi}{\partial\varphi}\right)=\frac{1}{r^2\sin\theta}\frac{\partial^2\psi}{\partial\varphi^2} \tag{125}$$

因此,

$$\nabla\cdot\nabla\psi=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin\theta}\frac{\partial^2\psi}{\partial\varphi^2} \tag{126}$$

故动能算符

$$\hat{T}=-\frac{\hbar^2}{2m}\nabla\cdot\nabla=-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2}\frac{1}{\sin\theta^2}\frac{\partial^2}{\partial\varphi^2}\right) \tag{127}$$

讨论: 上述方法可以推广到计算柱坐标:

$$\boldsymbol{r}=(r\cos\theta,r\sin\theta,z) \tag{128}$$

中的动能算符.

(3) 由于

$$\hat{T}\psi\left(r\right)=-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\psi\left(r\right)=\frac{A}{a}\frac{\hbar^2}{2m}\left(\frac{2}{r}e^{-\frac{r}{a}}-\frac{1}{a}e^{-\frac{r}{a}}\right) \tag{129}$$

所以

$$\begin{aligned}
\left\langle\hat{T}\right\rangle=&\int d^3\boldsymbol{r}\psi^*\left(r\right)\hat{T}\psi\left(r\right) && (130)\\
=&\frac{|A|^2}{a}\frac{\hbar^2}{2m}4\pi\int_0^\infty r^2dr\left(\frac{2}{r}e^{-\frac{2r}{a}}-\frac{1}{a}e^{-\frac{2r}{a}}\right) && (131)\\
=&\frac{\hbar^2}{2ma^2} && (132)
\end{aligned}$$

讨论: 这个结果与玻尔的氢原子理论一致. 由角动量量子化可得, 基态的角动量为 $\hbar=amv$, 故 $v=\frac{\hbar}{ma}$, 动能 $T=\frac{1}{2}mv^2=\frac{\hbar^2}{2ma^2}$.

(4)

$$\left\langle \hat{V} \right\rangle = \int d^3\boldsymbol{r}\psi^*(r)\hat{V}\psi(r) \tag{133}$$

$$= |A|^2\left(-\frac{e^2}{4\pi\epsilon_0}\right)4\pi\int_0^\infty r^2 dr\frac{1}{r}e^{-\frac{2r}{a}} \tag{134}$$

$$= -\frac{e^2}{4\pi\epsilon_0 a} \tag{135}$$

讨论: 符合预期, a 即为氢原子基态的半径.

4 第四次作业: 2021.10.12

1. 证明概率密度 $\rho(\boldsymbol{r})$ 和概率流密度 $\boldsymbol{j}(\boldsymbol{r})$ 可以分别表示为下列算符的平均值: $\hat{\rho}(\boldsymbol{r}_0) = \delta(\boldsymbol{r}-\boldsymbol{r}_0)$, $\hat{\boldsymbol{j}}(\boldsymbol{r}_0) = \frac{1}{2m}(\hat{\boldsymbol{p}}\delta(\boldsymbol{r}-\boldsymbol{r}_0)+\delta(\boldsymbol{r}-\boldsymbol{r}_0)\hat{\boldsymbol{p}})$.

解: 取所给算符的平均值

$$\int d^3r\psi^*(\boldsymbol{r})\hat{\rho}(\boldsymbol{r}_0)\psi(\boldsymbol{r}) = \int d^3r\psi^*(\boldsymbol{r})\delta(\boldsymbol{r}-\boldsymbol{r}_0)\psi(\boldsymbol{r}) \tag{136}$$

$$=\psi^*(\boldsymbol{r}_0)\psi(\boldsymbol{r}_0) \tag{137}$$

$$=\rho(\boldsymbol{r}_0) \tag{138}$$

$$\int d^3r\psi^*(\boldsymbol{r})\hat{\boldsymbol{j}}(\boldsymbol{r}_0)\psi(\boldsymbol{r}) = \int d^3r\psi^*(\boldsymbol{r})\frac{1}{2m}(\hat{\boldsymbol{p}}\delta(\boldsymbol{r}-\boldsymbol{r}_0)+\delta(\boldsymbol{r}-\boldsymbol{r}_0)\hat{\boldsymbol{p}})\psi(\boldsymbol{r}) \tag{139}$$

$$=\frac{1}{2m}\left(\int d^3r\psi^*(\boldsymbol{r})\hat{\boldsymbol{p}}\delta(\boldsymbol{r}-\boldsymbol{r}_0)\psi(\boldsymbol{r}) + \int d^3r\psi^*(\boldsymbol{r})\delta(\boldsymbol{r}-\boldsymbol{r}_0)\hat{\boldsymbol{p}}\psi(\boldsymbol{r})\right) \tag{140}$$

$$=\frac{1}{2m}\left(\int d^3r\psi^*(\boldsymbol{r})(-i\hbar\nabla)\delta(\boldsymbol{r}-\boldsymbol{r}_0)\psi(\boldsymbol{r}) + \int d^3r\psi^*(\boldsymbol{r})\delta(\boldsymbol{r}-\boldsymbol{r}_0)(-i\hbar\nabla)\psi(\boldsymbol{r})\right) \tag{141}$$

$$=\frac{1}{2m}\left(\int d^3r(i\hbar\nabla\psi^*(\boldsymbol{r}))\delta(\boldsymbol{r}-\boldsymbol{r}_0)\psi(\boldsymbol{r}) - i\hbar\psi^*(\boldsymbol{r})\nabla\psi(\boldsymbol{r})|_{\boldsymbol{r}=\boldsymbol{r}_0}\right) \tag{142}$$

$$=\frac{1}{2m}((i\hbar\nabla\psi^*(\boldsymbol{r}))\psi(\boldsymbol{r}) - i\hbar\psi^*(\boldsymbol{r})\nabla\psi(\boldsymbol{r}))|_{\boldsymbol{r}=\boldsymbol{r}_0} \tag{143}$$

$$=\frac{i\hbar}{2m}((\nabla\psi^*(\boldsymbol{r}))\psi(\boldsymbol{r}) - \psi^*(\boldsymbol{r})\nabla\psi(\boldsymbol{r}))|_{\boldsymbol{r}=\boldsymbol{r}_0} \tag{144}$$

$$=\boldsymbol{j}(\boldsymbol{r}_0) \tag{145}$$

讨论: (1) 这里利用 δ 函数的性质: $\int_{-\infty}^{\infty} dx f(x)\delta'(x-x_0) = -\left.\frac{\partial f}{\partial x}\right|_{x=x_0}$. 证明需要用到分部积分.

(2) 概率密度和概率流密度是物理量. 可通过计算相应算符的平均值得到.

2. 考虑一维情形, 粒子状态由波函数 $\psi(x,t)$ 描述, 设 P_{ab} 是在 t 时刻发现粒子处于区间 $(a<x<b)$ 内的概率.

(1) 证明 $\frac{dP_{ab}}{dt} = J(a,t) - J(b,t)$. 这里概率流密度 $J(x,t) = \frac{i\hbar}{2m}(\psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x} - \psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x})$.

(2) 分别确定 $\psi(x,t)$ 和 $J(x,t)$ 的量纲.

(3) 若 $\psi(x,t) = Ae^{-\lambda(x-x_0)^2-i\omega t}$, 这里 A, λ, x_0, ω 均为实数. 利用 $J(x,t)$ 的公式确定其概率流密度.

解 (1) 对处于状态 $\psi(x,t)$ 的波函数, 它处于区间 ($a<x<b$) 的概率为

$$P_{ab}=\int_a^b \psi^*(x,t)\psi(x,t)dx \tag{146}$$

则

$$i\hbar\frac{dP_{ab}}{dt}=\int_a^b i\hbar\frac{\partial\psi^*(x,t)}{\partial t}\psi(x,t)dx+\int_a^b \psi^*(x,t)i\hbar\frac{\partial\psi(x,t)}{\partial t}dx \tag{147}$$

粒子的状态满足 Schrödinger 方程

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=\hat{H}\psi(x,t)=(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x))\psi(x,t) \tag{148}$$

它的复共轭为,

$$-i\hbar\frac{\partial\psi^*(x,t)}{\partial t}=(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x))\psi^*(x,t) \tag{149}$$

所以

$$\begin{aligned}
i\hbar\frac{dP_{ab}}{dt}&=\int_a^b\left[-\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\psi^*(x,t)\right]\psi(x,t)dx &(150)\\
&+\int_a^b\psi^*(x,t)\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\psi(x,t)\right]dx &(151)\\
&=\int_a^b\frac{\hbar^2}{2m}\frac{\partial^2\psi^*(x,t)}{\partial x^2}\psi(x,t)dx-\int_a^b\psi^*(x,t)\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}dx &(152)\\
&=\frac{\hbar^2}{2m}\int_a^b\frac{\partial}{\partial x}\left(\frac{\partial\psi^*(x,t)}{\partial x}\psi(x,t)dx-\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\right)dx &(153)\\
&=\frac{\hbar^2}{2m}\left[\frac{\partial\psi^*(x,t)}{\partial x}\psi(x,t)-\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\right]\Bigg|_a^b &(154)\\
&=i\hbar\,\frac{-i\hbar}{2m}\left[\frac{\partial\psi^*(x,t)}{\partial x}\psi(x,t)-\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\right]\Bigg|_a^b &(155)\\
&=i\hbar\left(-J(x,t)\right)\big|_a^b &(156)\\
&=i\hbar\left(J(a,t)-J(b,t)\right) &(157)
\end{aligned}$$

(2) 由归一化条件得 $\int dx\,|\psi(x,t)|^2=1$: 从量纲的角度看, $L\,[\psi]^2=1$, 那么 $[\psi]=L^{-1/2}$. 由概率流密度 $J(x,t)=\frac{i\hbar}{2m}(\psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}-\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x})$ 的公式得: $[J]=\frac{[\hbar]}{[m]}[\psi]\left[\frac{\partial\psi^*}{\partial x}\right]=\frac{L^2MT^{-2}T}{M}L^{-1/2}\frac{L^{-1/2}}{L}=T^{-1}$. 利用 $\frac{dP_{ab}}{dt}$ 判断 J 的量纲也是一个好办法. 概率 P_{ab} 是无量纲的.

(3) 对于 $\psi(x,t)=Ae^{-\lambda(x-a)^2-i\omega t}$, 可得

$$\frac{\partial\psi^*(x,t)}{\partial x}=\frac{\partial}{\partial x}\left(Ae^{-\lambda(x-a)^2+i\omega t}\right)=-2A\lambda\,(x-a)\,e^{-\lambda(x-a)^2+i\omega t} \tag{158}$$

$$\frac{\partial\psi(x,t)}{\partial x}=\frac{\partial}{\partial x}\left(Ae^{-\lambda(x-a)^2-i\omega t}\right)=-2A\lambda\,(x-a)\,e^{-\lambda(x-a)^2-i\omega t} \tag{159}$$

所以概率流密度 $\frac{i\hbar}{2m}(\psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}-\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x})=0$.

讨论:

(1) 这是一个一维问题, 需要使用一维的微商符号 $\frac{\partial}{\partial x}$;

(2) 波函数的量纲和空间的维度有关: n 维空间 $[\psi] = L^{-n/2}$;

3. 自然界存在不稳定的粒子. 随着时间的推移, 它会分解成其它粒子. 可建立如下模型研究这一过程. 设粒子处于量子态 $\psi(x,t)$, 其势能 $V(x) = V_0(x) - i\Gamma$, 这里 $V_0(x)$ 是实的, 而 Γ 是正的实常数. 令 $P = \int_{-\infty}^{\infty} |\psi(x,t)|^2 dx$,

(1) 证明: $\frac{dP}{dt} = -\frac{2\Gamma}{\hbar}P$;

(2) 令 $P(0) = 1$, 求 $P(t)$.

(3) 定义发现粒子的总概率衰减为开始时的 e^{-1} 所经历的时间 t_0 定义为其寿命, 试确定不稳定粒子寿命的表达式.

解: (1) 与第 2 题的过程类似, 首先考察一个有限区间 $[-a,a]$ 上的 $P_a = \int_{-a}^{a} |\psi(x,t)|^2 dx$,

$$i\hbar\frac{dP_a}{dt} = \int_{-a}^{a}\left[-\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0(x) + i\Gamma\right)\psi^*(x,t)\right]\psi(x,t)dx \tag{160}$$

$$+\int_{-a}^{a}\psi^*(x,t)\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0(x) - i\Gamma\right)\psi(x,t)\right]dx \tag{161}$$

与第 2 题推导类似,

$$i\hbar\frac{dP_a}{dt} = -i\hbar\int_{-a}^{a}\frac{\partial j}{\partial x}dx - 2i\Gamma\int_{-a}^{a}|\psi(x,t)|^2 dx \tag{162}$$

$$= i\hbar(j_{-a} - j_a) - 2i\Gamma\int_{-a}^{a}|\psi(x,t)|^2 dx \tag{163}$$

由于 $\psi \sim x^{-\frac{1}{2}+s}$, j_a 中的项 $\psi^*\frac{\partial}{\partial x}\psi \sim x^{-\frac{1}{2}+s}\left(-\frac{1}{2}+s\right)x^{-\frac{3}{2}+s} = \left(-\frac{1}{2}+s\right)x^{-2+2s}$, 令 $a \to \infty$, 则 $j_a \to 0$, j_{-a} 类似讨论. 利用 $\psi(|x| \to \infty) \to 0$ 也可以得到 $j_{\pm a} \to 0$. 同时, $a \to \infty$, 则 $P_a \to P$, 所以

$$\frac{dP}{dt} = -\frac{2\Gamma}{\hbar}P \tag{164}$$

(2) 由 (1) 得:

$$\frac{dP}{P} = -\frac{2\Gamma}{\hbar}dt \tag{165}$$

即

$$\ln P = C - \frac{2\Gamma}{\hbar}t \tag{166}$$

这里 C 为待定常数. 于是 $P = e^{C-\frac{2\Gamma}{\hbar}t}$. 由初始条件 $P(0) = 1$ 得 $C = 0$, 所以

$$P(t) = e^{-\frac{2\Gamma}{\hbar}t} \tag{167}$$

(3) 由题意, 令 $-\frac{2\Gamma}{\hbar}t_0 = -1$, 则 $t_0 = \frac{\hbar}{2\Gamma}$, 故粒子寿命为 $\frac{\hbar}{2\Gamma}$.

讨论: 由于势能有非零虚部, 则**能量算符不是厄米的**, 从而**定域的概率守恒不再成立**, 或者说体系的演化不再是幺正 (Unitary) 的.

4. 对由**归一化**波函数 $\psi(\boldsymbol{r}')$ 所描述的量子体系, 魏格纳 (E.P. Wigner) 分布函数定义为

$$W(\boldsymbol{r}',\boldsymbol{p}') = \frac{1}{(2\pi\hbar)^3}\int e^{-i\boldsymbol{p}'\cdot\boldsymbol{r}''/\hbar}\psi^*\left(\boldsymbol{r}' - \frac{\boldsymbol{r}''}{2}\right)\psi\left(\boldsymbol{r}' + \frac{\boldsymbol{r}''}{2}\right)d^3r''$$

(1) 证明: $W(\boldsymbol{r}',\boldsymbol{p}') = W^*(\boldsymbol{r}',\boldsymbol{p}')$;

(2) 证明: $\int W(\boldsymbol{r}',\boldsymbol{p}')\,d^3p' = |\psi(\boldsymbol{r}')|^2$;

(3) 对于某可观测量对应的算符 $C(\hat{\boldsymbol{r}})$, 证明: $\langle C(\hat{\boldsymbol{r}})\rangle = \int\int C(\boldsymbol{r}') W(\boldsymbol{r}',\boldsymbol{p}') d^3r'd^3p'$;

(4) 证明: $\int\int W(\boldsymbol{r}',\boldsymbol{p}') d^3r'd^3p' = 1$.

解:

(1)

$$\begin{aligned}
W^*(\boldsymbol{r}',\boldsymbol{p}') =& \frac{1}{(2\pi\hbar)^3}\left(\int e^{-i\boldsymbol{p}'\cdot\boldsymbol{r}''/\hbar}\psi^*\left(\boldsymbol{r}'-\frac{\boldsymbol{r}''}{2}\right)\psi\left(\boldsymbol{r}'+\frac{\boldsymbol{r}''}{2}\right)d^3r''\right)^* && (168)\\
=& \frac{1}{(2\pi\hbar)^3}\int e^{i\boldsymbol{p}'\cdot\boldsymbol{r}''/\hbar}\psi\left(\boldsymbol{r}'-\frac{\boldsymbol{r}''}{2}\right)\psi^*\left(\boldsymbol{r}'+\frac{\boldsymbol{r}''}{2}\right)d^3r'' && (169)\\
=& \frac{1}{(2\pi\hbar)^3}\int_0^\infty r''^2dr''\int_0^\pi \sin\theta d\theta\int_0^{2\pi} d\varphi e^{i\boldsymbol{p}'\cdot\boldsymbol{r}''/\hbar}\psi\left(\boldsymbol{r}'-\frac{\boldsymbol{r}''}{2}\right)\psi^*\left(\boldsymbol{r}'+\frac{\boldsymbol{r}''}{2}\right) && (170)
\end{aligned}$$

令 $\boldsymbol{r}''\to\tilde{\boldsymbol{r}}\to-\boldsymbol{r}''$, 利用球坐标考虑, $r''\to\tilde{r}=r''$, $\theta\to\tilde{\theta}=\pi-\theta$, $\varphi\to\tilde{\varphi}=\varphi+\pi$, $\int_0^\infty r''^2dr''\int_0^\pi\sin\theta d\theta\int_0^{2\pi}d\varphi = \int_0^\infty\tilde{r}^2d\tilde{r}\int_0^\pi\sin\left(\pi-\tilde{\theta}\right)d\left(\pi-\tilde{\theta}\right)\int_0^{2\pi}d(\tilde{\varphi}-\pi) = \int_0^\infty\tilde{r}^2d\tilde{r}\left(-\int_\pi^0\sin\tilde{\theta}d\tilde{\theta}\right)\int_{-\pi}^\pi d\tilde{\varphi} = \int_0^\infty\tilde{r}^2d\tilde{r}\int_0^\pi\sin\tilde{\theta}d\tilde{\theta}\int_\pi^{3\pi}d\tilde{\varphi}$, 且被积函数是 φ 的周期为 2π 的函数, 于是

$$\begin{aligned}
W^*(\boldsymbol{r}',\boldsymbol{p}') =& \frac{1}{(2\pi\hbar)^3}\int_0^\infty\tilde{r}^2d\tilde{r}\int_0^\pi\sin\tilde{\theta}d\tilde{\theta}\int_\pi^{3\pi}d\tilde{\varphi}e^{-i\boldsymbol{p}'\cdot\tilde{\boldsymbol{r}}/\hbar}\psi\left(\boldsymbol{r}'+\frac{\tilde{\boldsymbol{r}}}{2}\right)\psi^*\left(\boldsymbol{r}'-\frac{\tilde{\boldsymbol{r}}}{2}\right) && (171)\\
=& \frac{1}{(2\pi\hbar)^3}\int_0^\infty\tilde{r}^2d\tilde{r}\int_0^\pi\sin\tilde{\theta}d\tilde{\theta}\int_0^{2\pi}d\tilde{\varphi}e^{-i\boldsymbol{p}'\cdot\tilde{\boldsymbol{r}}/\hbar}\psi\left(\boldsymbol{r}'+\frac{\tilde{\boldsymbol{r}}}{2}\right)\psi^*\left(\boldsymbol{r}'-\frac{\tilde{\boldsymbol{r}}}{2}\right) && (172)\\
=& W(\boldsymbol{r}',\boldsymbol{p}') && (173)
\end{aligned}$$

方程172利用了周期函数在一个周期上的积分与区间的起点无关.

如果用直角坐标, 也可以. 令 $\boldsymbol{r}''\to\tilde{\boldsymbol{r}}\to-\boldsymbol{r}''$, 以 x 分量为例说明, $\tilde{x}=-x''$. $\int_{-\infty}^\infty dx'' = \int_{-\infty}^\infty d(-\tilde{x}) = -\int_\infty^{-\infty}d\tilde{x} = \int_{-\infty}^\infty d\tilde{x}$.

第三种方法是利用傅里叶变换:

$$\begin{aligned}
W^*(\boldsymbol{r}',\boldsymbol{p}') =& \frac{1}{(2\pi\hbar)^3}\int e^{i\boldsymbol{p}'\cdot\boldsymbol{r}''/\hbar}\psi\left(\boldsymbol{r}'-\frac{\boldsymbol{r}''}{2}\right)\psi^*\left(\boldsymbol{r}'+\frac{\boldsymbol{r}''}{2}\right)d^3r'' && (174)\\
=& \frac{1}{(2\pi\hbar)^3}\int d^3r''e^{\frac{i\boldsymbol{p}'\cdot\boldsymbol{r}''}{\hbar}}\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int d^3p_1\varphi(\boldsymbol{p}_1)e^{\frac{i\boldsymbol{p}_1\cdot\left(\boldsymbol{r}'-\frac{\boldsymbol{r}''}{2}\right)}{\hbar}}\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int d^3p_2\varphi^*(\boldsymbol{p}_2)e^{\frac{-i\boldsymbol{p}_2\cdot\left(\boldsymbol{r}'+\frac{\boldsymbol{r}''}{2}\right)}{\hbar}} && (175)\\
=& \frac{1}{(2\pi\hbar)^3}\int d^3p_1\varphi(\boldsymbol{p}_1)e^{\frac{i\boldsymbol{p}_1\cdot\boldsymbol{r}'}{\hbar}}\int d^3p_2\varphi^*(\boldsymbol{p}_2)e^{\frac{-i\boldsymbol{p}_2\cdot\boldsymbol{r}'}{\hbar}}\frac{1}{(2\pi\hbar)^3}\int d^3r''e^{\frac{i\left(\boldsymbol{p}'-\frac{\boldsymbol{p}_1}{2}-\frac{\boldsymbol{p}_2}{2}\right)\cdot\boldsymbol{r}''}{\hbar}} && (176)\\
=& \frac{1}{(2\pi\hbar)^3}\int d^3p_1\varphi(\boldsymbol{p}_1)e^{\frac{i\boldsymbol{p}_1\cdot\boldsymbol{r}'}{\hbar}}\int d^3p_2\varphi^*(\boldsymbol{p}_2)e^{\frac{-i\boldsymbol{p}_2\cdot\boldsymbol{r}'}{\hbar}}\delta\left(\boldsymbol{p}'-\frac{\boldsymbol{p}_1}{2}-\frac{\boldsymbol{p}_2}{2}\right) && (177)
\end{aligned}$$

另一方面,

$$W\left(\boldsymbol{r}',\boldsymbol{p}'\right)=\frac{1}{(2\pi\hbar)^3}\int e^{-i\boldsymbol{p}'\cdot\boldsymbol{r}''/\hbar}\psi^*\left(\boldsymbol{r}'-\frac{\boldsymbol{r}''}{2}\right)\psi\left(\boldsymbol{r}'+\frac{\boldsymbol{r}''}{2}\right)d^3r'' \tag{178}$$

$$=\frac{1}{(2\pi\hbar)^3}\int e^{-i\boldsymbol{p}'\cdot\boldsymbol{r}''/\hbar}\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int d^3p_1\varphi^*\left(\boldsymbol{p}_1\right)e^{\frac{-i\boldsymbol{p}_1\cdot\left(\boldsymbol{r}'-\frac{\boldsymbol{r}''}{2}\right)}{\hbar}}\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int d^3p_2\varphi\left(\boldsymbol{p}_2\right)e^{\frac{i\boldsymbol{p}_2\cdot\left(\boldsymbol{r}'+\frac{\boldsymbol{r}''}{2}\right)}{\hbar}} \tag{179}$$

$$=\frac{1}{(2\pi\hbar)^3}\int d^3p_1\varphi^*\left(\boldsymbol{p}_1\right)e^{-\frac{i\boldsymbol{p}_1\cdot\boldsymbol{r}'}{\hbar}}\int d^3p_2\varphi\left(\boldsymbol{p}_2\right)e^{\frac{i\boldsymbol{p}_2\cdot\boldsymbol{r}'}{\hbar}}\frac{1}{(2\pi\hbar)^3}\int d^3r''e^{\frac{-i\left(\boldsymbol{p}'-\frac{\boldsymbol{p}_1}{2}-\frac{\boldsymbol{p}_2}{2}\right)\cdot\boldsymbol{r}''}{\hbar}} \tag{180}$$

$$=\frac{1}{(2\pi\hbar)^3}\int d^3p_1\varphi^*\left(\boldsymbol{p}_1\right)e^{-\frac{i\boldsymbol{p}_1\cdot\boldsymbol{r}'}{\hbar}}\int d^3p_2\varphi\left(\boldsymbol{p}_2\right)e^{\frac{i\boldsymbol{p}_2\cdot\boldsymbol{r}'}{\hbar}}\delta\left(\boldsymbol{p}'-\frac{\boldsymbol{p}_1}{2}-\frac{\boldsymbol{p}_2}{2}\right) \tag{181}$$

可见方程177和181是一样的.

(2)

$$\int W\left(\boldsymbol{r}',\boldsymbol{p}'\right)d^3p'=\int d^3p'\frac{1}{(2\pi\hbar)^3}\int d^3r''e^{-i\boldsymbol{p}'\cdot\boldsymbol{r}''/\hbar}\psi^*\left(\boldsymbol{r}'-\frac{\boldsymbol{r}''}{2}\right)\psi\left(\boldsymbol{r}'+\frac{\boldsymbol{r}''}{2}\right) \tag{182}$$

由于 $\frac{1}{(2\pi\hbar)^3}\int d^3p'\int e^{-i\boldsymbol{p}'\cdot\boldsymbol{r}''/\hbar}=\delta\left(\boldsymbol{r}''-\boldsymbol{0}\right)$, 则

$$\int W\left(\boldsymbol{r}',\boldsymbol{p}'\right)d^3p'=\int d^3r''\psi^*\left(\boldsymbol{r}'-\frac{\boldsymbol{r}''}{2}\right)\psi\left(\boldsymbol{r}'+\frac{\boldsymbol{r}''}{2}\right)\delta\left(\boldsymbol{r}''-\boldsymbol{0}\right) \tag{183}$$

$$=\left|\psi\left(\boldsymbol{r}'\right)\right|^2 \tag{184}$$

(3) 利用 (2) 的结论,

$$\left\langle C\left(\hat{\boldsymbol{r}}\right)\right\rangle=\int d^3r'C\left(\boldsymbol{r}'\right)\left|\psi\left(\boldsymbol{r}'\right)\right|^2 \tag{185}$$

$$=\int d^3r'C\left(\boldsymbol{r}'\right)\left(\int d^3p'W\left(\boldsymbol{r}',\boldsymbol{p}'\right)\right) \tag{186}$$

$$=\int\int C\left(\boldsymbol{r}'\right)W\left(\boldsymbol{r}',\boldsymbol{p}'\right)d^3r'd^3p' \tag{187}$$

(4) 由于 $\psi\left(\boldsymbol{r}'\right)$ 已经归一化,

$$\int\int W\left(\boldsymbol{r}',\boldsymbol{p}'\right)d^3r'd^3p'=\int d^3r'\left(\int d^3p'W\left(\boldsymbol{r}',\boldsymbol{p}'\right)\right) \tag{188}$$

$$=\int d^3r'\left|\psi\left(\boldsymbol{r}'\right)\right|^2 \tag{189}$$

$$=1 \tag{190}$$

讨论:

(1) 魏格纳分布函数在量子光学上有重要的应用.

(2) 对算符 $C\left(\hat{\boldsymbol{p}}\right)$, 魏格纳分布函数应变换为 $W\left(\boldsymbol{r}',\boldsymbol{p}'\right)=\frac{1}{(2\pi\hbar)^3}\int\phi^*\left(\boldsymbol{p}'-\boldsymbol{p}''\right)\psi\left(\boldsymbol{p}'+\boldsymbol{p}''\right)e^{2i\boldsymbol{p}''\cdot\boldsymbol{r}'/\hbar}d^3p''$.

5 第五次作业 2021.10.19

1. 已知质量为 m 的微观粒子处于状态 $\psi(\boldsymbol{r})$, 其概率密度为 $\rho(\boldsymbol{r})$ 和概率流密度为 $\boldsymbol{j}(\boldsymbol{r})$. 设 $\xi(\boldsymbol{r})$ 为 $\psi(\boldsymbol{r})$ 的辐角, 则

(1) 证明 $\psi(\boldsymbol{r})=\sqrt{\rho(\boldsymbol{r})}e^{i\xi(\boldsymbol{r})}$

(2) 证明 $\boldsymbol{j}(\boldsymbol{r})=\frac{\hbar}{m}\rho(\boldsymbol{r})\nabla\xi(\boldsymbol{r})$.

(3) 如果两个波函数给出同一个概率密度为 $\rho(\boldsymbol{r})$ 和同一个概率流密度为 $\boldsymbol{j}(\boldsymbol{r})$, 则这两个波函数只相差一个总的相位因子.

解:

(1) 由于 $\xi(\boldsymbol{r})$ 为 $\psi(\boldsymbol{r})$ 的辐角, 则 $\psi(\boldsymbol{r})=|\psi(\boldsymbol{r})|e^{i\xi(\boldsymbol{r})}$, 而 $|\psi(\boldsymbol{r})|=\sqrt{\rho(\boldsymbol{r})}$, 所以 $\psi(\boldsymbol{r})=\sqrt{\rho(\boldsymbol{r})}e^{i\xi(\boldsymbol{r})}$.

(2) 证：已知概率流密度为

$$\boldsymbol{J}=\frac{1}{2m}\left(\psi^*(\boldsymbol{r},t)\hat{\boldsymbol{p}}\psi(\boldsymbol{r},t)-\psi(\boldsymbol{r},t)\hat{\boldsymbol{p}}\psi^*(\boldsymbol{r},t)\right) \tag{191}$$

$$=\frac{1}{m}\text{Re}\left(\psi^*(\boldsymbol{r},t)\hat{\boldsymbol{p}}\psi(\boldsymbol{r},t)\right) \tag{192}$$

$$=\frac{1}{m}\text{Re}\left(\psi^*(\boldsymbol{r},t)\hat{\boldsymbol{p}}\left(\sqrt{\rho(\boldsymbol{r})}e^{i\xi(\boldsymbol{r})}\right)\right) \tag{193}$$

这里

$$\hat{\boldsymbol{p}}\left(\sqrt{\rho(\boldsymbol{r})}e^{i\xi(\boldsymbol{r})}\right)=\frac{\hbar}{i}\nabla\left(\sqrt{\rho(\boldsymbol{r})}e^{i\xi(\boldsymbol{r})}\right) \tag{194}$$

$$=\frac{\hbar}{i}\left(\frac{1}{2}\frac{\nabla\rho}{\sqrt{\rho}}+i\sqrt{\rho}\nabla\xi\right)e^{i\xi} \tag{195}$$

所以

$$\boldsymbol{J}=\frac{1}{m}\text{Re}\left(\sqrt{\rho}e^{-i\xi}\frac{\hbar}{i}\left(\frac{1}{2}\frac{\nabla\rho}{\sqrt{\rho}}+i\sqrt{\rho}\nabla\xi\right)e^{i\xi}\right) \tag{196}$$

$$=\frac{1}{m}\text{Re}\left(\frac{\hbar}{i}\frac{1}{2}\nabla\rho+\hbar\rho\nabla\xi\right) \tag{197}$$

$$=\frac{\hbar}{m}\rho\nabla\xi \tag{198}$$

(3) 两个波函数的概率密度相同, 则可令 $\psi_1(\boldsymbol{r})=\sqrt{\rho}e^{i\xi_1}$, $\psi_2(\boldsymbol{r})=\sqrt{\rho}e^{i\xi_2}$. 如果两者的概率密度相同, 则

$$\frac{\hbar}{m}\rho\nabla\xi_1=\frac{\hbar}{m}\rho\nabla\xi_2 \tag{199}$$

即

$$\nabla(\xi_1-\xi_2)=0 \tag{200}$$

所以 $\xi_1-\xi_2=C$. C 为常数, 即 $\psi_1(\boldsymbol{r})$ 和 $\psi_1(\boldsymbol{r})$ 只差一个相位因子.

讨论: 本题进一步揭示了概率流密度和概率密度的联系. 波函数是复的, 这一点也有清晰的体现.

2. 假设 $t=0$ 时刻, 一个粒子的初始状态是能量本征态 $\psi_1(x)$, $\psi_2(x)$, $\psi_3(x)$ 的线性叠加: $\psi(x,0)=A\left(\psi_1(x)+\sqrt{2}i\psi_2(x)+\psi_3(x)\right)$ A 为归一化常数. $\psi_n(x)$ 对应的本征能量为 E_n, 满足 $n\neq m$ 时, $E_n\neq E_m$, 且 $(\psi_n,\psi_m)=\delta_{nm}$, 即正交归一, $m,n=1,2,3$.

(1) 已知粒子 Hamiltonian 算符为 $\hat{H}$, 计算它在 $\psi(x,0)$ 上的能量平均值;

(2) 求 $t>0$ 时刻粒子的波函数 $\psi(x,t)$, 验证它满足 Schrödinger 方程, 并计算能量的平均值;

(3) 若在 $t=0$ 时刻测量粒子的能量, 求测量值为 E_2 的概率. 求粒子在 $t>0$ 时刻的波函数, 并解释原因.

解: (1) 首先确定归一化常数, 令

$$\begin{aligned}1 &= \left(\psi\left(x,0\right), \psi\left(x,0\right)\right) && (201)\\ &= \left(A\left(\psi_1(x)+\sqrt{2}i\psi_2(x)+\psi_3(x)\right), A\left(\psi_1(x)+\sqrt{2}i\psi_2(x)+\psi_3(x)\right)\right) && (202)\\ &= |A|^2\left(\psi_1(x)+\sqrt{2}i\psi_2(x)+\psi_3(x), \psi_1(x)+\sqrt{2}i\psi_2(x)+\psi_3(x)\right) && (203)\end{aligned}$$

由于 $(\psi_n,\psi_m)=\delta_{nm}$, 所以

$$\begin{aligned}1 &= |A|^2\left((\psi_1(x),\psi_1(x))+\left(\sqrt{2}i\psi_2(x),\sqrt{2}i\psi_2(x)\right)+(\psi_3(x),\psi_3(x))\right) && (204)\\ &= |A|^2\left(1+2+1\right) && (205)\end{aligned}$$

所以可取 $A=\frac{1}{2}$.

计算能量平均值: 为书写方便, 设 $\psi(x,0)=c_1\left(0\right)\psi_1(x)+c_2\left(0\right)\psi_2(x)+c_3\left(0\right)\psi_3(x)$,

$$\begin{aligned}\left\langle\hat{H}\right\rangle &= \left(\psi(x,0),\hat{H}\psi(x,0)\right) && (206)\\ &= \left(c_1\left(0\right)\psi_1(x)+c_2\left(0\right)\psi_2(x)+c_3\left(0\right)\psi_3(x), c_1\left(0\right)E_1\psi_1(x)+c_2\left(0\right)E_2\psi_2(x)+c_3\left(0\right)E_3\psi_3(x)\right) && (207)\end{aligned}$$

由于 $(\psi_n,\psi_m)=\delta_{nm}$,

$$\begin{aligned}\left\langle\hat{H}\right\rangle &= \left(c_1\left(0\right)\psi_1(x), c_1\left(0\right)E_1\psi_1(x)\right)+\left(c_2\left(0\right)\psi_2(x), c_2\left(0\right)E_2\psi_2(x)\right)+\left(c_3\left(0\right)\psi_3(x), c_3\left(0\right)E_3\psi_3(x)\right) && (208)\\ &= |c_1\left(0\right)|^2E_1+|c_2\left(0\right)|^2E_2+|c_3\left(0\right)|^2E_3 && (209)\end{aligned}$$

由于 $|c_1\left(0\right)|^2=\frac{1}{4}$, $|c_2\left(0\right)|^2=\frac{1}{2}$, $|c_3\left(0\right)|^2=\frac{1}{4}$, 所以

$$\left\langle\hat{H}\right\rangle=\frac{E_1+2E_2+E_3}{4} \qquad (210)$$

(2) 由非定态的公式可知:

$$\psi(x,t)=\frac{1}{2}\left(\psi_1(x)e^{-iE_1t/\hbar}+\sqrt{2}i\psi_2(x)e^{-iE_2t/\hbar}+\psi_3(x)e^{-iE_3t/\hbar}\right) \qquad (211)$$

验证满足 Schrödinger 方程

$$\begin{aligned}i\hbar\frac{\partial\psi(x,t)}{\partial t} &= \frac{1}{2}i\hbar\frac{\partial}{\partial t}\left(\psi_1(x)e^{-iE_1t/\hbar}+\sqrt{2}i\psi_2(x)e^{-iE_2t/\hbar}+\psi_3(x)e^{-iE_3t/\hbar}\right) && (212)\\ &= \frac{1}{2}i\hbar\left(\psi_1(x)\frac{\partial}{\partial t}e^{-iE_1t/\hbar}+\sqrt{2}i\psi_2(x)\frac{\partial}{\partial t}e^{-iE_2t/\hbar}+\psi_3(x)\frac{\partial}{\partial t}e^{-iE_3t/\hbar}\right) && (213)\\ &= \frac{1}{2}\left(\psi_1(x)E_1e^{-iE_1t/\hbar}+\sqrt{2}i\psi_2(x)E_2e^{-iE_2t/\hbar}+\psi_3(x)E_3e^{-iE_3t/\hbar}\right) && (214)\end{aligned}$$

由于 $\hat{H}\psi_i = E_i\psi_i$ $(i = 1, 2, 3)$, 则

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \frac{1}{2}\left(\hat{H}\psi_1(x)e^{-iE_1t/\hbar} + \sqrt{2}i\hat{H}\psi_2(x)e^{-iE_2t/\hbar} + \hat{H}\psi_3(x)e^{-iE_3t/\hbar}\right) \tag{215}$$

$$= \hat{H}\frac{1}{2}\left(\psi_1(x)e^{-iE_1t/\hbar} + \sqrt{2}i\psi_2(x)e^{-iE_2t/\hbar} + \psi_3(x)e^{-iE_3t/\hbar}\right) \tag{216}$$

$$= \hat{H}\psi(x,t) \tag{217}$$

即满足 Schrödinger 方程.

计算能量平均值: 与 (1) 中类似, 设 $\psi(x,t) = c_1(t)\,\psi_1(x) + c_2(t)\,\psi_2(x) + c_3(t)\,\psi_3(x)$, 与 (1) 中推导类似,

$$\left\langle \hat{H} \right\rangle = \left(\psi(x,t), \hat{H}\psi(x,t)\right) \tag{218}$$

$$= |c_1(t)|^2 E_1 + |c_2(t)|^2 E_2 + |c_3(t)|^2 E_3 \tag{219}$$

由于 $|c_1(t)|^2 = \frac{1}{4}$, $|c_2(t)|^2 = \frac{1}{2}$, $|c_3(t)|^2 = \frac{1}{4}$, 所以

$$\left\langle \hat{H} \right\rangle = \frac{E_1 + 2E_2 + E_3}{4} \tag{220}$$

(3) $t = 0$ 时, 测得能量为 E_2 的概率为 $|(\psi_2, \psi(x,0))|^2 = \frac{1}{2}$. $t > 0$ 时刻, 粒子的波函数为 $\psi(x, t > 0) = \psi_2 e^{-iE_2t/\hbar}$. 测量后, 粒子坍缩到能量为 E_2 的本征态上, 此后的演化将以此为初态.

讨论:

(1) 由初态 $\psi(x,0)$ 得到 $\psi(x,t)$ 是量子力学上重要的问题.

(2) 能量的平均值不依赖时间是能量守恒的体现.

3. 算符 $\hat{A}$ 表示力学量 A, 它有两个正交归一的本征态 ψ_1 和 ψ_2, 本征值分别为 a_1 和 a_2. $a_1 \neq a_2$. 算符 $\hat{B}$ 表示力学量 B, 它有两个正交归一的本征态 ϕ_1 和 ϕ_2, 本征值分别为 b_1 和 b_2. $b_1 \neq b_2$. 它们的本征态由下式联系:

$$\psi_1 = c_1\left(\sqrt{2}\phi_1 + i\phi_2\right)$$
$$\psi_2 = c_2\left(\phi_1 - \sqrt{2}i\phi_2\right)$$

这里 c_1, c_2 为归一化常数.

(1) 开始时, 先对力学量 A 进行测量, 测量值为 a_2. 当测量刚刚完成时, 体系的状态如何表示? 简述原因.

(2) 接下来, 测量力学量 B, 可能的测量值是什么？它们出现的概率是多少?

(3) 最后, 再次测量力学量 A, 测量值为 a_2 的概率是多少?

解:

(1) 对力学量 A 进行测量, 测量值为 a_2, 体系将坍缩到 a_2 对应的本征态 ψ_2 上. 原因: 测量引起量子态的本征坍缩.

(2) $\psi_2 = c_2\left(\phi_1 - \sqrt{2}i\phi_2\right)$, 由归一化可得 $c_2 = \frac{1}{\sqrt{3}}$, 测量力学量 B, 可能的测量值为 b_1 和 b_2. 测量值为 b_1 的概率为 $|(\phi_1, \psi_2)|^2 = \frac{1}{3}$, 测量值为 b_2 的概率为 $|(\phi_2, \psi_2)|^2 = \frac{2}{3}$.

(3) 利用归一化, 可取 $c_1 = \frac{1}{\sqrt{3}}$, 于是

$$\phi_1 = \frac{\sqrt{6}\psi_1 + \sqrt{3}\psi_2}{3} \tag{221}$$

$$\phi_2 = \frac{-\sqrt{3}i\psi_1 + \sqrt{6}i\psi_2}{3} \tag{222}$$

若力学量 B 的测量值为 b_1, 进而测量力学量 A, 测量值为 a_2 的概率为 $\frac{1}{3}\frac{1}{3} = \frac{1}{9}$; 若力学量 B 的测量值为 b_2, 进而测量力学量 A, 测量值为 a_2 的概率为 $\frac{2}{3}\frac{2}{3} = \frac{4}{9}$; 测量值为 a_2 总概率为上述两种可能性之和, 即 $\frac{1}{9} + \frac{4}{9} = \frac{5}{9}$.

讨论: 本题为两个力学量的连续测量. 对于一个力学量, 单次测量结果具有随机性, 多次测量结果的平均值是可预测的.