第6章：中心力场

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中心力场问题的一般表述

中心力场：力作用线过某点，场（势能）关于某一点对称

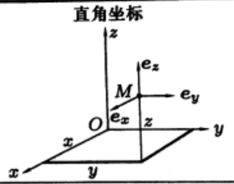
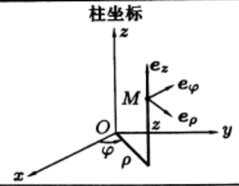
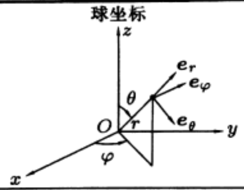
$$\hat{H}=\frac{\hat{p}}{2m}+V(r)$$

关于原点对称：

球坐标系 (r,θ,φ)

$$\begin{cases} x=r\sin\theta\cos\varphi \\ y=r\sin\theta\sin\varphi \\ z=r\cos\theta \end{cases} \qquad \begin{cases} r=\sqrt{x^2+y^2+z^2} \\ \theta=\arctan\left(\dfrac{\sqrt{x^2+y^2}}{z}\right) \\ \varphi=\arctan\left(\dfrac{y}{x}\right) \end{cases}$$

坐标系

	直角坐标	柱坐标	球坐标
			
定义	$U=U(x,y,z)$ $\boldsymbol{A}=A_x\boldsymbol{e}_x+A_y\boldsymbol{e}_y+A_z\boldsymbol{e}_z$ $A_x=A_x(x,y,z)$ $A_y=A_y(x,y,z)$ $A_z=A_z(x,y,z)$	$U=U(\rho,\varphi,z)$ $\boldsymbol{A}=A_\rho\boldsymbol{e}_\rho+A_\varphi\boldsymbol{e}_\varphi+A_z\boldsymbol{e}_z$ $A_\rho=A_x\cos\varphi+A_y\sin\varphi$ $A_\varphi=-A_x\sin\varphi+A_y\cos\varphi$	$U=U(r,\theta,\varphi)$ $\boldsymbol{A}=A_r\boldsymbol{e}_r+A_\theta\boldsymbol{e}_\theta+A_\varphi\boldsymbol{e}_\varphi$ $A_r=A_\rho\sin\theta+A_z\cos\theta$ $A_\theta=A_\rho\cos\theta-A_z\sin\theta$ $A_\varphi=-A_x\sin\varphi+A_y\cos\varphi$
梯度	$\nabla U=(\partial U/\partial x)\boldsymbol{e}_x$ $+(\partial U/\partial y)\boldsymbol{e}_y$ $+(\partial U/\partial z)\boldsymbol{e}_z$	$(\nabla U)_\rho=\partial U/\partial\rho$ $(\nabla U)_\varphi=[\partial U/\partial\varphi]/\rho$ $(\nabla U)_z=\partial U/\partial z$	$(\nabla U)_r=\partial U/\partial r$ $(\nabla U)_\theta=[\partial U/\partial\theta]/r$ $(\nabla U)_\varphi=[\partial U/\partial\varphi]/(r\sin\theta)$
拉普拉斯算符	$\Delta U=\frac{\partial^2U}{\partial x^2}+\frac{\partial^2U}{\partial y^2}+\frac{\partial^2U}{\partial z^2}$	$\Delta U=\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial U}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2U}{\partial\varphi^2}+\frac{\partial^2U}{\partial z^2}$	$\Delta U=\frac{1}{r}\frac{\partial^2}{\partial r^2}(rU)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial U}{\partial\theta}\right)$ $+\frac{1}{r^2\sin^2\theta}\frac{\partial^2U}{\partial\varphi^2}$
散度	$\nabla\cdot\boldsymbol{A}=\frac{\partial A_x}{\partial x}+\frac{\partial A_y}{\partial y}+\frac{\partial A_z}{\partial z}$	$\nabla\cdot\boldsymbol{A}=\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho A_\rho)+\frac{1}{\rho}\frac{\partial A_\varphi}{\partial\varphi}+\frac{\partial A_z}{\partial z}$	$\nabla\cdot\boldsymbol{A}=\frac{1}{r^2}\frac{\partial}{\partial r}(r^2A_r)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta A_\theta)$ $+\frac{1}{r\sin\theta}\frac{\partial A_\varphi}{\partial\varphi}$
旋度	$\nabla\times\boldsymbol{A}=(\partial A_z/\partial y-\partial A_y/\partial z)\boldsymbol{e}_x$ $+(\partial A_x/\partial z-\partial A_z/\partial x)\boldsymbol{e}_y$ $+(\partial A_y/\partial x-\partial A_x/\partial y)\boldsymbol{e}_z$	$(\nabla\times\boldsymbol{A})_\rho=(\partial A_z/\partial\varphi)/\rho-\partial A_\varphi/\partial z$ $(\nabla\times\boldsymbol{A})_\varphi=\partial A_\rho/\partial z-\partial A_z/\partial\rho$ $(\nabla\times\boldsymbol{A})_z=[\partial(\rho A_\varphi)/\partial\rho-\partial A_\rho/\partial\varphi]/\rho$	$(\nabla\times\boldsymbol{A})_r=[\partial(\sin\theta A_\varphi)/\partial\theta-\partial A_\theta/\partial\varphi]/(r\sin\theta)$ $(\nabla\times\boldsymbol{A})_\theta=[\partial A_r/\partial\varphi-\sin\theta\partial(rA_\varphi)/\partial r]/(r\sin\theta)$ $(\nabla\times\boldsymbol{A})_\varphi=[\partial(rA_\theta)/\partial r-\partial A_r/\partial\theta]/r$

$$\frac{\hat{p}^2}{2m}=-\frac{\hbar^2}{2m}\Delta=-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}r+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

角度部分（角动量）：

$$\begin{cases}\hat{l}_x=y\hat{p}_z-z\hat{p}_y=-i\hbar\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)\\ \hat{l}_y=z\hat{p}_x-x\hat{p}_z=-i\hbar\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right)\\ \hat{l}_z=x\hat{p}_y-y\hat{p}_x=-i\hbar\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)\end{cases}\qquad \begin{cases}\hat{l}_x=i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta}+\cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)\\ \hat{l}_y=i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta}+\cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)\\ \hat{l}_z=-i\hbar\frac{\partial}{\partial\varphi}\end{cases}$$

$$\hat{\boldsymbol{l}}^2=-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

径向部分（径向动量）：

$$\hat{p}_r=-i\hbar\left(\frac{1}{r}+\frac{\partial}{\partial r}\right)$$

$$\hat{H}=-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r+\frac{\hat{\boldsymbol{L}}^2}{2mr^2}+V(r)$$

$$=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+\frac{\hat{\boldsymbol{L}}^2}{2mr^2}+V(r)$$

$$=\frac{\hat{p}_r^2}{2m}+\frac{\hat{\boldsymbol{L}}^2}{2mr^2}+V(r)$$

空间旋转不变 → 角动量守恒 $[\hat{\boldsymbol{l}},\hat{H}]=0$

守恒量完全集 $\{\hat{H},\hat{l}^2,\hat{l}_z\}$. 所以 $\hat{l}^2$和$\hat{l}_z$的共同本征态$Y_l^m(\theta,\varphi)$

$$\hat{\boldsymbol{l}}^2 Y_l^m=l(l+1)\hbar^2 Y_l^m$$

$$\hat{l}_z Y_l^m=m\hbar Y_l^m$$

$$l=0,1,2,\cdots$$

$$|m|\leqslant l,\text{即 } m=-l,-l+1,\cdots,l-1,l$$

也是$\hat{H}$的本征态，但缺少径向自由度。于是三维问题的本征问题，可以通过分离变量求解：将本征函数分解为径向部分和角度部分

$$\hat{H}\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

$$\psi(r,\theta,\phi)=R(r)Y_l^m(\theta,\phi)$$

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r+\frac{\hat{L}^2}{2mr^2}+V(r)\right]R(r)Y_l^m(\theta,\phi)=ER(r)Y_l^m(\theta,\phi)$$

$$\Rightarrow\left[-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r+\frac{l(l+1)}{2mr^2}+V(r)\right]R(r)Y_l^m(\theta,\phi)=ER(r)Y_l^m(\theta,\phi)$$

同除以$Y_l^m(\theta,\phi)$，可得径向方程

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r+\frac{l(l+1)}{2mr^2}+V(r)\right]R_l(r)=ER_l(r)$$

所以对于给定l，只需要求解径向方程就能确定能量E。即

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}[rR_l(r)]+\left[\frac{2m}{\hbar^2}(E-V)-\frac{l(l+1)}{r^2}\right]R_l(r)=0$$

或

$$R_l''(r)+\frac{2}{r}R_l'(r)+\left[\frac{2m}{\hbar^2}(E-V)-\frac{l(l+1)}{r^2}\right]R_l(r)=0$$

做变量代换 $R_l(r)=\chi(r)/r$，则径向方程变为

$$\chi_l''+\left[\frac{2m}{\hbar^2}(E-V)-\frac{l(l+1)}{r^2}\right]\chi_l=0$$

- ☐ 对于束缚态能量量子化，将出现径向量子数n_r, $n_r=0,1,2,\dots$,
- ☐ 轨道角动量量子数 $l=0,1,2,\dots$ s, p, d, f, ...
- ☐ E只依赖n_r和l，不依赖磁量子数m, 所以中心力场能级一般是$2l+1$重简并的

★三维中心力场问题求解小结

守恒量完全集 $\{\hat{H},\hat{l}^2,\hat{l}_z\}$

将本征函数分解为径向部分和角度部分

$$\psi(r,\theta,\phi)=R(r)Y_l^m(\theta,\phi)$$

角度方程

$$\hat{l}^2Y_l^m=l(l+1)\hbar^2Y_l^m$$

$$\hat{l}_zY_l^m=m\hbar Y_l^m$$

$$l=0,1,2,\cdots$$

$$|m|\leqslant l,\text{即 } m=-l,-l+1,\cdots,l-1,l$$

径向方程

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r+\frac{l(l+1)}{2mr^2}+V(r)\right]R_l(r)=ER_l(r)$$

变量代换 $R_l(r)=\chi(r)/r$

$$\chi_l''+\left[\frac{2m}{\hbar^2}(E-V)-\frac{l(l+1)}{r^2}\right]\chi_l=0$$

边界条件：$\chi_l(r)\xrightarrow{r\to\infty}0$, $\chi_l(0)=0$ (因为$R_l(r)$在0点有限)

本征态 $R_{n_rl}(r), n_r=0,1,2,\dots,$

☐ s态（s波）情况

$$\chi_l''+\left[\frac{2m}{\hbar^2}(E-V)\right]\chi_l=0$$

与一维定态问题类似，但注意边界条件不同。

☐ 中心力场在$r\to 0$ 邻域内的行为

假设 $\chi_l\xrightarrow{r\to 0}r^s$, 则有

$$s(s-1)r^{s-2}+\left[\frac{2m}{\hbar^2}(E-V)-\frac{l(l+1)}{r^2}\right]r^s=0$$

即

$$[s(s-1)-l(l+1)]+\frac{2m}{\hbar^2}(E-V)r^2=0$$

若 $r^2V\xrightarrow{r\to 0}0$, 则要求

$$s(s-1)-l(l+1)=0$$

即 $s=-l \; or \; l+1$

又，$\chi_l(0)=0$

所以 $s=l+1$, 即

$$\lim_{r\to 0} R_l(r)\approx r^l$$

满足 $r^2V\xrightarrow{r\to 0}0$的势

- 库仑势 $V\propto r^{-1}$
- 线性中心势 $V\propto r$
- 对数中心势 $V\propto \ln r$
- 谐振子势 $V\propto r^2$
- 汤川势 $V\propto r^{-1}r^{-\alpha r}$

两体问题化为单体问题

中心力场往往是两体问题。比如两个质量分别为m_1和m_2的粒子，坐标为$\boldsymbol{r}_1$和$\boldsymbol{r}_2$。

如果相互作用$V(|\boldsymbol{r}_1-\boldsymbol{r}_2|)$只依赖二者之间的距离，是否可以化成中心力场问题

这个二粒子的能量本征方程为

$$\left[-\frac{\hbar^2}{2m_1}\nabla_1^2-\frac{\hbar^2}{2m_2}\nabla_2^2+V(|\boldsymbol{r}_1-\boldsymbol{r}_2|)\right]\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)=E_T\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)$$

引进质心坐标$\boldsymbol{R}$及相对坐标$\boldsymbol{r}$为

$$\boldsymbol{r}=\boldsymbol{r}_1-\boldsymbol{r}_2 \qquad \boldsymbol{R}=\frac{m_1\boldsymbol{r}_1+m_2\boldsymbol{r}_2}{m_1+m_2}$$

由此可得

$$\frac{1}{m_1}\nabla_1^2+\frac{1}{m_2}\nabla_2^2=\frac{1}{M}\nabla_R^2+\frac{1}{\mu}\nabla^2$$

$$M=m_1+m_2 \qquad \text{(总质量)}$$

$$\mu=m_1m_2/(m_1+m_2) \qquad \text{(约化质量)}$$

$$\nabla_R^2=\frac{\partial^2}{\partial X^2}+\frac{\partial^2}{\partial Y^2}+\frac{\partial^2}{\partial Z^2}$$

$$\nabla^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$$

于是有

$$\left[-\frac{\hbar^2}{2M}\nabla_R^2-\frac{\hbar^2}{2\mu}\nabla^2+V(r)\right]\Psi=E_T\Psi$$

于是可以把质心运动与相对运动分离变量

$$\Psi=\phi(\boldsymbol{R})\psi(\boldsymbol{r})$$

质心方程

$$-\frac{\hbar^2}{2M}\nabla_R^2\phi(\boldsymbol{R})=E_C\phi(\boldsymbol{R})$$

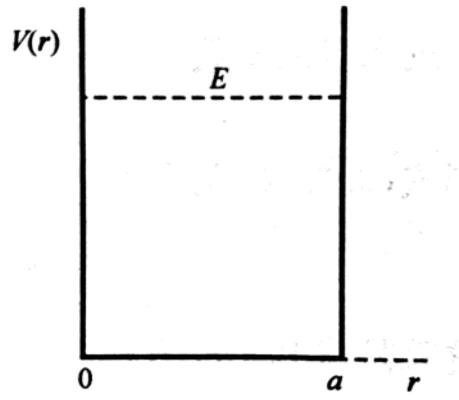
相对运动方程

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2+V(\boldsymbol{r})\right)\psi(\boldsymbol{r})=(E_T-E_C)\psi(\boldsymbol{r})=E\psi(\boldsymbol{r})$$

与前面的中心力场方程相一致。例如在原子物理中，我们研究氢原子中电子的运动，可以将原子核看作静止来研究电子的绕核运动。所需要做的改变就是将电子质量变为约化

质量$\mu = Mm/(m+M)$

例：无限深球方势阱



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

s态 ($l = 0$)

$$\chi_l'' + \left[\frac{2m}{\hbar^2}(E - V)\right]\chi_l = 0$$

$$\chi_l'' + k^2\chi_l = 0\ (r \le a)$$

$$k = \frac{\sqrt{2mE}}{\hbar}(E > 0)$$

边界条件+连续性条件：$\begin{cases} \chi(0) = 0 \\ \chi(a) = 0 \end{cases}$

于是有量子化条件

$ka = (n_r + 1)\pi, n_r = 0,1,2,3,\cdots$

能量本征值：$E_n = \frac{(n_r+1)^2\pi^2\hbar^2}{2\mu a^2}$

本征波函数：$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{(n_r+1)\pi x}{a}$

$l \neq 0$

$$R_l'' + \frac{2}{r}R_l' + \left[k^2 - \frac{l(l+1)}{r}\right]R_l = 0 \qquad (r < a) \qquad (6.2.10)$$

而在边界上要求

$$R_l(r)\big|_{r=a} = 0 \qquad (6.2.11)$$

引进无量纲变数

$$\rho = kr \qquad (6.2.12)$$

则式(6.2.10)化为

$$\frac{d^2R_l}{d\rho^2} + \frac{2}{\rho}\frac{dR_l}{d\rho} + \left[1 - \frac{l(l+1)}{\rho^2}\right]R_l = 0 \qquad (6.2.13)$$

这就是球 Bessel 方程. 令

$$R_l = u_l(\rho)/\sqrt{\rho} \qquad (6.2.14)$$

经过计算，可求出 u_l 满足下列方程：

$$u_l'' + \frac{1}{\rho}u_l' + \left[1 - \frac{(l+1/2)^2}{\rho^2}\right]u_l = 0 \qquad (6.2.15)$$

这正是半奇数$(l+1/2)$阶 Bessel 方程($l=0,1,2,\cdots$)，它的两个线性无关解可以表示为

$$J_{l+1/2}(\rho), \qquad J_{-l-1/2}(\rho)$$

所以径向波函数的两个解是

$$R_l \propto \frac{1}{\sqrt{\rho}}J_{l+1/2}(\rho), \quad \frac{1}{\sqrt{\rho}}J_{-l-1/2}(\rho)$$

例：三维各向同性谐振子

$$V(r) = \frac{1}{2}Kr^2 = \frac{1}{2}\mu\omega^2r^2, \qquad \omega = \sqrt{K/\mu}$$

$$R_l''(r) + \frac{2}{r}R_l'(r) + \left[\frac{2\mu}{\hbar^2}\left(E - \frac{1}{2}\mu\omega^2r^2\right) - \frac{l(l+1)}{r^2}\right]R_l(r) = 0$$

先分析渐近行为再求解

1. $r \to 0$

$$R_l''(r) + \frac{2}{r}R_l'(r) - \frac{l(l+1)}{r^2}R_l(r) = 0$$
$$R_l(r) \propto r^l$$

2. $r \to \infty$

$$R_l''(r) + \frac{\mu^2\omega^2 r^2}{\hbar^2}R_l(r) = 0$$
$$R_l(r) \propto e^{\pm\frac{\alpha^2 r^2}{2}} \quad \left(\alpha = \sqrt{\mu\omega/\hbar}\right)$$
$$R_l(r) \xrightarrow{r\to\infty} 0 \Rightarrow R_l(r) \propto e^{-\frac{\alpha^2 r^2}{2}}$$

再利用渐近解构造解为

$$R_l(r) \propto r^l e^{-\frac{\alpha^2 r^2}{2}} u_l(r)$$

则

$$u_l'' + \frac{2}{r}(l+1-r^2)u_l' + [2E-(2l+3)]u_l = 0$$

再令

$$\xi = r^2$$

方程(6.3.10)化为

$$\xi\frac{\mathrm{d}^2 u_l}{\mathrm{d}\xi^2} + \left[\left(l+\frac{3}{2}\right)-\xi\right]\frac{\mathrm{d}u_l}{\mathrm{d}\xi} + \left(\frac{E}{2} - \frac{l+3/2}{2}\right)u_l = 0$$

这正是合流超几何方程

$$u_l \propto F(\alpha,\gamma,\xi)$$

$$E = 2n_r + l + 3/2$$

$$E = (2n_r + l + 3/2)\hbar\omega$$

$$N = 2n_r + l$$

$$E = E_N = (N + 3/2)\hbar\omega$$
$$N = 0,1,2,\cdots$$

直角坐标系解法

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2}\mu^2\omega^2 r^2 = H_x + H_y + H_z$$

$$H_x = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\mu\omega^2 x^2$$

守恒量完全集 $(\hat{H}_x, \hat{H}_y, \hat{H}_z)$

$$\Phi_{n_x n_y n_z}(x,y,z) = \varphi_{n_x}(x)\varphi_{n_y}(y)\varphi_{n_z}(z)$$
$$n_x, n_y, n_z = 0,1,2,\cdots$$

$$E_{n_x n_y n_z} = \left(n_x + \frac{1}{2}\right)\hbar\omega + \left(n_y + \frac{1}{2}\right)\hbar\omega + \left(n_z + \frac{1}{2}\right)\hbar\omega = (N + 3/2)\hbar\omega$$