第6章：中心力场

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- [ ] 角动量守恒 → 径向方程
- [ ] 两体问题 → 单体问题
- [ ] 球方势阱
- [ ] 三维谐振子
- [ ] 氢原子

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

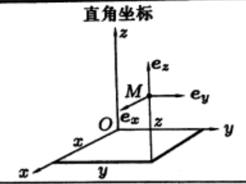
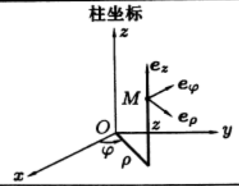
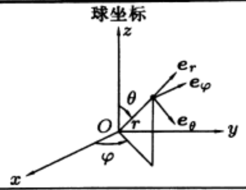
$$\widehat{H}=\frac{\hat{p}}{2m}+V(r)$$

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	$\Delta U=\dfrac{\partial^2U}{\partial x^2}+\dfrac{\partial^2U}{\partial y^2}+\dfrac{\partial^2U}{\partial z^2}$	$\Delta U=\dfrac{1}{\rho}\dfrac{\partial}{\partial\rho}\left(\rho\dfrac{\partial U}{\partial\rho}\right)+\dfrac{1}{\rho^2}\dfrac{\partial^2U}{\partial\varphi^2}+\dfrac{\partial^2U}{\partial z^2}$	$\Delta U=\dfrac{1}{r}\dfrac{\partial^2}{\partial r^2}(rU)+\dfrac{1}{r^2\sin\theta}\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial U}{\partial\theta}\right)$ $+\dfrac{1}{r^2\sin^2\theta}\dfrac{\partial^2U}{\partial\varphi^2}$
散度	$\nabla\cdot\boldsymbol{A}=\dfrac{\partial A_x}{\partial x}+\dfrac{\partial A_y}{\partial y}+\dfrac{\partial A_z}{\partial z}$	$\nabla\cdot\boldsymbol{A}=\dfrac{1}{\rho}\dfrac{\partial}{\partial\rho}(\rho A_\rho)+\dfrac{1}{\rho}\dfrac{\partial A_\varphi}{\partial\varphi}+\dfrac{\partial A_z}{\partial z}$	$\nabla\cdot\boldsymbol{A}=\dfrac{1}{r^2}\dfrac{\partial}{\partial r}(r^2A_r)+\dfrac{1}{r\sin\theta}\dfrac{\partial}{\partial\theta}(\sin\theta A_\theta)$ $+\dfrac{1}{r\sin\theta}\dfrac{\partial A_\varphi}{\partial\varphi}$
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$Y_l^m(\theta,\varphi)$

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

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

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

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

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

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

做变量代换 $R_l(r) \to \chi(r)/r$，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, $n_r = 0,1,2,\ldots$,
- 轨道角动量量子数 $l = 0,1,2,\ldots$ s, p, d, f, ...
- E只依赖n_r和l，不依赖磁量子数m

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

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

$$M = m_1 + m_2 \qquad \text{（总质量）}$$

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

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

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

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$\mu = Mm/(m+M)$