Quantum Mechanics

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2025 年 1 月 5 日

目录

1 波函数和 Schrodinger 方程

1.1 波函数

1. 波函数:

$$\psi(\boldsymbol{r},t)=\psi_0\mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)} \tag{1.1}$$

2. 统计诠释:

$$P(\boldsymbol{r},t)=|\psi(\boldsymbol{r},t)|^2\mathrm{d}\tau \tag{1.2}$$

3. 归一化条件:

$$\int_{-\infty}^{+\infty}|\psi(\boldsymbol{r},t)|^2\mathrm{d}\tau=1 \tag{1.3}$$

1.2 Schrodinger 方程

1. 一维 Schrodinger 方程:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right]\psi(x,t)=\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(x,t) \tag{1.4}$$

2. 三维 Schrodinger 方程:

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{r},t)\right]\psi(\boldsymbol{r},t)=\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) \tag{1.5}$$

3. 概率密度:

$$\rho(\boldsymbol{r},t)=\psi^*(\boldsymbol{r},t)\psi(\boldsymbol{r},t) \tag{1.6}$$

4. 概率流密度:

$$\boldsymbol{j}(\boldsymbol{r},t)=\frac{\mathrm{i}\hbar}{2m}\left(\psi(\boldsymbol{r},t)\nabla\psi^*(\boldsymbol{r},t)-\psi^*(\boldsymbol{r},t)\nabla\psi(\boldsymbol{r},t)\right) \tag{1.7}$$

5. 概率连续性方程:

$$\frac{\partial\rho(\boldsymbol{r},t)}{\partial t}+\nabla\cdot\boldsymbol{j}(\boldsymbol{r},t)=0 \tag{1.8}$$

1.3 定态 Schrodinger 方程

1. 势场 $V(\boldsymbol{r})$ 不显含时间，Schrodinger 方程变为:

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{r})\right]\psi(\boldsymbol{r},t)=\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) \tag{1.9}$$

2. 分离变量:

$$\psi(\boldsymbol{r},t)=\psi(\boldsymbol{r})T(t) \tag{1.10}$$

$$\frac{\mathrm{i}\hbar}{T}\frac{\mathrm{d}T}{\mathrm{d}t}=\frac{1}{\psi}\left[-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{r})\right]\psi=E \tag{1.11}$$

3. 时间部分:

$$T(t)=T_0\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et} \tag{1.12}$$

4. 定态波函数:

$$\psi(\boldsymbol{r},t)=\psi(\boldsymbol{r})\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et} \tag{1.13}$$

5. 定态 Schrodinger 方程:

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{r})\right]\psi(\boldsymbol{r})=E\psi(\boldsymbol{r}) \tag{1.14}$$

2　一维势场中的粒子运动

2.1　一维无限深方势阱

1. 一维无限深方势阱：

$$V(x)=\begin{cases}0 & 0\leqslant x\leqslant a\\ +\infty & others.\end{cases} \tag{2.1}$$

2. Schrodinger 方程：

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+k^2\psi=0,\quad k^2=\frac{2mE}{\hbar^2} \tag{2.2}$$

$$\psi(x)=A\sin kx+B\cos kx \tag{2.3}$$

3. 边界条件：

$$\psi(0)=\psi(a)=0 \tag{2.4}$$

$$B=0,\quad ka=n\pi,\quad n=1,2,\dots \tag{2.5}$$

4. 本征函数：

$$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} \tag{2.6}$$

5. 能量：

$$E_n=\frac{k_n^2\hbar^2}{2m}=\frac{n^2\pi^2\hbar^2}{2ma^2} \tag{2.7}$$

2.2　一维有限深方势阱

1. 一维有限深方势阱：$E<V_0$

$$V(x)=\begin{cases}0 & -a\leqslant x\leqslant a\\ V_0 & others.\end{cases} \tag{2.8}$$

2. 当 $|x|\leqslant a$ 时：

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+k^2\psi=0,\quad k^2=\frac{2mE}{\hbar^2} \tag{2.9}$$

$$\psi(x)=A\sin kx+B\cos kx \tag{2.10}$$

3. 当 $|x|\geqslant a$ 时：

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}-\beta^2\psi=0,\quad \beta^2=\frac{2m(V_0-E)}{\hbar^2} \tag{2.11}$$

$$\psi(x)=\begin{cases}C\mathrm{e}^{\beta x} & x<-a\\ D\mathrm{e}^{-\beta x} & x>a\end{cases} \tag{2.12}$$

4. 偶宇称态：

$$\psi(x)=\begin{cases}D\mathrm{e}^{-\beta x} & x>a\\ B\cos kx & 0<x\leqslant a\\ \psi(-x) & x<0\end{cases} \tag{2.13}$$

边界条件：

$$D\mathrm{e}^{-\beta a}=B\cos ka,\quad -\beta D\mathrm{e}^{-\beta a}=-kB\sin ka \tag{2.14}$$

$$\beta=k\tan ka \tag{2.15}$$

$$k^2+\beta^2=\frac{2mV_0}{\hbar^2} \tag{2.16}$$

5. 奇宇称态：

$$\psi(x)=\begin{cases}De^{-\beta x} & x>a\\ A\sin kx & 0<x\leqslant a\\ -\psi(-x) & x<0\end{cases} \tag{2.17}$$

边界条件：

$$De^{-\beta a}=A\sin ka,\quad -\beta De^{-\beta a}=kA\cos ka \tag{2.18}$$

$$\beta=-k\cot ka \tag{2.19}$$

$$k^2+\beta^2=\frac{2mV_0}{\hbar^2} \tag{2.20}$$

2.3　方势垒的反射与穿透

1. 方势垒：$E<V_0$

$$V(x)=\begin{cases}V_0 & 0\leqslant x\leqslant a\\ 0 & others.\end{cases} \tag{2.21}$$

2. 当 $x<0$ 时：有入射波和反射波

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+k^2\psi=0,\quad k^2=\frac{2mE}{\hbar^2} \tag{2.22}$$

$$\psi(x)=Ae^{\mathrm{i}kx}+Be^{-\mathrm{i}kx} \tag{2.23}$$

3. 当 $0<x<a$ 时：

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}-\beta^2\psi=0,\quad \beta^2=\frac{2m(V_0-E)}{\hbar^2} \tag{2.24}$$

$$\psi(x)=Ce^{\beta x}+De^{-\beta x} \tag{2.25}$$

4. 当 $x>a$ 时：没有入射波

$$\psi(x)=Fe^{\mathrm{i}kx} \tag{2.26}$$

5. 边界条件：

$$A+B=C+D,\quad \mathrm{i}k(A-B)=\beta(C-D) \tag{2.27}$$

$$Ce^{\beta a}+De^{-\beta a}=Fe^{\mathrm{i}ka},\quad \beta(Ce^{\beta a}-De^{-\beta a})=\mathrm{i}kFe^{\mathrm{i}ka} \tag{2.28}$$

6. 透射系数：

$$\mathcal{T}=\frac{|F|^2}{|A|^2}=\frac{4k^2\beta^2}{(k^2+\beta^2)^2\mathrm{sh}^2\beta a+4k^2\beta^2}=\left[1+\frac{\mathrm{sh}^2\beta a}{\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)}\right]^{-1} \tag{2.29}$$

7. 反射系数：

$$\mathcal{R}=\frac{|B|^2}{|A|^2}=\frac{(k^2+\beta^2)^2\mathrm{sh}^2\beta a}{(k^2+\beta^2)^2\mathrm{sh}^2\beta a+4k^2\beta^2} \tag{2.30}$$

2.4　一维 δ 势

1. 一维 δ 势：

$$V(x)=\gamma\delta(x) \tag{2.31}$$

2. 当 $x=0$ 时：

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi=(E-\gamma\delta(x))\psi \tag{2.32}$$

$$\psi'(0^+)-\psi'(0^-)=\frac{2m\gamma}{\hbar^2}\psi(0) \tag{2.33}$$

3. 当 $x \neq 0$ 时:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + k^2\psi = 0, \quad k^2 = \frac{2mE}{\hbar^2} \tag{2.34}$$

$$\psi(x) = \begin{cases} Ae^{\mathrm{i}kx} + Be^{-\mathrm{i}kx} & x < 0 \\ Ce^{\mathrm{i}kx} & x > 0 \end{cases} \tag{2.35}$$

4. 边界条件:

$$A + B = C, \quad A - B = C\left(1 - \frac{2m\gamma}{\hbar^2 \mathrm{i}k}\right) \tag{2.36}$$

5. 透射系数:

$$\mathcal{T} = \frac{|C|^2}{|A|^2} = \frac{1}{1 + \mu^2\gamma^2/\hbar^2 k^2} = \frac{1}{1 + \mu\gamma^2/2\hbar^2 E} \tag{2.37}$$

6. 反射系数:

$$\mathcal{R} = \frac{|B|^2}{|A|^2} = \frac{\mu\gamma^2/2\hbar^2 E}{1 + \mu\gamma^2/1\hbar^2 E} \tag{2.38}$$

2.5 一维谐振子势

1. 一维谐振子势:

$$V(x) = \frac{1}{2}m\omega^2 x^2 \tag{2.39}$$

2. Schrodinger 方程:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + \frac{1}{2}m\omega^2 x^2\psi = E\psi \tag{2.40}$$

3. 当 $|x| \to \infty$ 时：只存在束缚态

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + \frac{1}{2}m\omega^2 x^2\psi = 0 \tag{2.41}$$

$$\psi(x) = e^{-\frac{1}{2}\alpha^2 x^2}, \quad \alpha^2 = \frac{m\omega}{\hbar} \tag{2.42}$$

4. 一般解:

$$\psi(x) = e^{-\frac{1}{2}\alpha^2 x^2} u(x) \tag{2.43}$$

5. 变量代换:

$$\xi = \alpha x \tag{2.44}$$

$$\frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} - 2\xi\frac{\mathrm{d}u}{\mathrm{d}\xi} + \left(\frac{2E}{\hbar\omega} - 1\right)u = 0 \tag{2.45}$$

6. 要求截断:

$$\frac{2E}{\hbar\omega} - 1 = 2n, \quad n = 0, 1, 2, \ldots \tag{2.46}$$

7. 能量:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, \ldots \tag{2.47}$$

8. 本征函数:

$$\psi_n(x) = N_n e^{-\frac{1}{2}\alpha^2 x^2} H_n(\alpha x), \quad N_n = \left(\frac{\alpha}{\sqrt{\pi}2^n n!}\right)^{\frac{1}{2}} \tag{2.48}$$

$$\psi_0(x) = \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-\frac{1}{2}\alpha^2 x^2} \tag{2.49}$$

$$\psi_1(x) = \frac{\sqrt{2\alpha}}{\pi^{1/4}} \alpha x e^{-\frac{1}{2}\alpha^2 x^2} \tag{2.50}$$

$$\psi_2(x) = \frac{\sqrt{\alpha/2}}{\pi^{1/4}} (2\alpha^2 x^2 - 1) e^{-\frac{1}{2}\alpha^2 x^2} \tag{2.51}$$

3 力学量和表象变换

3.1 力学量的算符表示

1. Hamilton 算符:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V \tag{3.1}$$

2. 能量算符:

$$\hat{E} = \mathrm{i}\hbar\frac{\partial}{\partial t} \tag{3.2}$$

3. 动量算符:

$$\boldsymbol{p} = -\mathrm{i}\hbar\nabla \tag{3.3}$$

4. 轨道角动量算符:

$$\hat{L}_x = y\hat{p}_z - z\hat{p}_y, \quad \hat{L}_y = z\hat{p}_x - x\hat{p}_z, \quad \hat{L}_z = x\hat{p}_y - y\hat{p}_x \tag{3.4}$$

$$\hat{L}_x = -\mathrm{i}\hbar\left(-\sin\varphi\frac{\partial}{\partial\theta} - \cos\varphi\cot\theta\frac{\partial}{\partial\varphi}\right) \tag{3.5}$$

$$\hat{L}_y = -\mathrm{i}\hbar\left(+\cos\varphi\frac{\partial}{\partial\theta} - \sin\varphi\cot\theta\frac{\partial}{\partial\varphi}\right) \tag{3.6}$$

$$\hat{L}_z = -\mathrm{i}\hbar\frac{\partial}{\partial\varphi} \tag{3.7}$$

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] \tag{3.8}$$

5. 对易关系:

$$[\hat{x}_\alpha, \hat{p}_\beta] = \mathrm{i}\hbar\delta_{\alpha\beta}, \quad [\hat{x}_\alpha, \hat{L}_\beta] = \varepsilon_{\alpha\beta\gamma}\mathrm{i}\hbar\hat{x}_\gamma, \quad [\hat{p}_\alpha, \hat{L}_\beta] = \varepsilon_{\alpha\beta\gamma}\mathrm{i}\hbar\hat{p}_\gamma \tag{3.9}$$

$$[\hat{L}_\alpha, \hat{L}_\beta] = \varepsilon_{\alpha\beta\gamma}\mathrm{i}\hbar\hat{L}_\gamma, \quad [\hat{L}^2, \hat{L}_\alpha] = 0 \tag{3.10}$$

6. 轨道角动量升降算符:

$$\hat{L}_+ = \hat{L}_x + \mathrm{i}\hat{L}_y, \quad \hat{L}_- = \hat{L}_x - \mathrm{i}\hat{L}_y \tag{3.11}$$

$$[\hat{L}_+, \hat{L}_-] = 2\hbar\hat{L}_z, \quad [\hat{L}_z, \hat{L}_\pm] = \pm\hbar\hat{L}_\pm \tag{3.12}$$

7. Heisenberg 不确定关系:

$$\Delta A\Delta B \geqslant \frac{1}{2}|\langle C\rangle|, \quad [\hat{A}, \hat{B}] = \mathrm{i}\hat{C} \tag{3.13}$$

8. 能量-时间不确定关系:

$$\Delta H\Delta O \geqslant \frac{1}{2}\left|\langle[\hat{H}, \hat{O}]\rangle\right| = \frac{\hbar}{2}\left|\frac{\mathrm{d}\langle O\rangle}{\mathrm{d}t}\right| \tag{3.14}$$

$$\Delta E\Delta t \geqslant \frac{\hbar}{2}, \quad \Delta t = \frac{\Delta O}{|\mathrm{d}\langle O\rangle/\mathrm{d}t|} \tag{3.15}$$

9. Baker-Campbell-Hausdorff 公式:

$$\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \cdots \tag{3.16}$$

$$\mathrm{e}^{\hat{A}+\hat{B}} = \mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}}\mathrm{e}^{-\frac{1}{2}[\hat{A},\hat{B}]} = \mathrm{e}^{\hat{B}}\mathrm{e}^{\hat{A}}\mathrm{e}^{\frac{1}{2}[\hat{A},\hat{B}]}, \quad [[\hat{A}, \hat{B}], \hat{A}] = [[\hat{A}, \hat{B}], \hat{B}] = 0 \tag{3.17}$$

10. Schneden 公式:

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{\hat{A}(x)} = \int_0^1 \mathrm{d}y\mathrm{e}^{(1-y)\hat{A}}\hat{A}'\mathrm{e}^{y\hat{A}} \tag{3.18}$$

$$\mathrm{e}^{-\hat{A}(x)}\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{\hat{A}(x)} = \hat{A}' + \frac{1}{2!}[\hat{A}', \hat{A}] + \frac{1}{3!}[[\hat{A}', \hat{A}], \hat{A}] + \cdots \tag{3.19}$$

3.2 力学量与测量

1. Hermite 算符：

$$\hat{O}^{\dagger}=\hat{O} \Rightarrow \langle\psi|\hat{O}\phi\rangle=\langle\hat{O}\psi|\phi\rangle \tag{3.20}$$

(1) 本征值为实数：

$$\lambda_n^*=\lambda_n \tag{3.21}$$

(2) 本征态正交归一：

$$\langle\psi_n|\psi_m\rangle=\delta_{nm} \tag{3.22}$$

2. 广义统计诠释：

(1) 量子态展开为力学量本征态的线性组合：

$$|\psi\rangle=\sum_n c_n\,|\phi_n\rangle\,,\quad c_n=\langle\phi_n|\psi\rangle \tag{3.23}$$

(2) 观测到 λ_n 的概率为 $|c_n|^2$：

$$\langle O\rangle=\sum_{nm}c_m^*c_n\,\langle\phi_m|\hat{O}|\phi_n\rangle=\sum_{nm}c_m^*c_n\lambda_n\delta_{nm}=\sum_n|c_n|^2\lambda_n \tag{3.24}$$

3. 守恒量：

(1) 平均值不随时间改变：

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\langle O\rangle=\frac{1}{\mathrm{i}\hbar}\left\langle\left[\hat{O},\hat{H}\right]\right\rangle+\left\langle\frac{\partial\hat{O}}{\partial t}\right\rangle=0 \tag{3.25}$$

(2) 测值概率分布不随时间改变：

$$\frac{\mathrm{d}}{\mathrm{d}t}|a_n(t)|^2=\langle\frac{1}{\mathrm{i}\hbar}\hat{H}\psi(t)|n\rangle\,\langle n|\psi(t)\rangle+h.c.=0 \tag{3.26}$$

4. Feynman-Hellmann 定理：

$$\frac{\partial E_n}{\partial\lambda}=\left\langle n\left|\frac{\partial\hat{H}}{\partial\lambda}\right|n\right\rangle \tag{3.27}$$

3.3 力学量的矩阵表示

1. 力学量的矩阵表示：

$$\boldsymbol{O}=\begin{pmatrix}O_{11}&O_{12}&\cdots\\O_{21}&O_{22}&\cdots\\\vdots&\vdots&\ddots\end{pmatrix},\quad O_{ij}=\langle\psi_i|\hat{O}|\psi_j\rangle \tag{3.28}$$

2. Schrodinger 方程的矩阵形式：

(1) 量子态在本征态展开：

$$|\psi\rangle=\sum_n a_n\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\,|n\rangle \tag{3.29}$$

(2) 代入 Schrodinger 方程：

$$E\sum_n a_n\,|n\rangle=\sum_n a_n\hat{H}\,|n\rangle \tag{3.30}$$

(3) 左乘本征函数 $\langle\psi_m|$：

$$Ea_m=\sum_n a_n\,\langle m|\hat{H}|n\rangle=\sum_n H_{mn}a_n \tag{3.31}$$

(4) 久期方程组：

$$\begin{pmatrix}H_{11}-E&H_{12}&\cdots\\H_{21}&H_{22}-E&\cdots\\\vdots&\vdots&\ddots\end{pmatrix}\begin{pmatrix}a_1\\a_2\\\vdots\end{pmatrix}=0 \tag{3.32}$$

3. 基底变换的矩阵表示：

$$\begin{pmatrix}\psi_1'\\ \psi_2'\\ \vdots\end{pmatrix}=\begin{pmatrix}U_{11} & U_{12} & \cdots\\ U_{21} & U_{22} & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\end{pmatrix},\quad U_{ij}=\langle\psi_j|\psi_i'\rangle \tag{3.33}$$

4. 不同基底下力学量矩阵相似：

$$\boldsymbol{O}'=\widetilde{\boldsymbol{U}}^{\dagger}\boldsymbol{O}\widetilde{\boldsymbol{U}},\quad \widetilde{\boldsymbol{U}}=\boldsymbol{U}^{T} \tag{3.34}$$

3.4　表象变换

1. 坐标表象：

(1) 坐标的本征方程：

$$\hat{x}\,|x'\rangle=x'\,|x'\rangle \tag{3.35}$$

(2) 坐标表象中坐标的本征函数：

$$\langle x|x'\rangle=\delta(x-x') \tag{3.36}$$

(3) 坐标表象中动量的本征函数：

$$\langle x|p'\rangle=\frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p'x} \tag{3.37}$$

2. 动量表象：

(1) 动量的本征方程：

$$\hat{p}\,|p'\rangle=p'\,|p'\rangle \tag{3.38}$$

(2) 动量表象中动量的本征函数：

$$\langle p|p'\rangle=\delta(p-p') \tag{3.39}$$

(3) 动量表象中坐标的本征函数：

$$\langle p|x'\rangle=\frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px'} \tag{3.40}$$

3. 波函数的表象变换：

$$\psi(x)=\langle x|\psi\rangle=\int\mathrm{d}p\,\langle x|p\rangle\,\langle p|\psi\rangle=\frac{1}{\sqrt{2\pi\hbar}}\int\mathrm{d}p\;\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}\,\langle p|\psi\rangle \tag{3.41}$$

$$\phi(p)=\langle p|\psi\rangle=\int\mathrm{d}x\,\langle p|x\rangle\,\langle x|\psi\rangle=\frac{1}{\sqrt{2\pi\hbar}}\int\mathrm{d}x\;\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px}\,\langle x|\psi\rangle \tag{3.42}$$

4. 坐标表象下力学量的矩阵元：

$$O_{x'x}=\langle x'|\hat{O}(x)|x\rangle=O(x)\delta(x'-x) \tag{3.43}$$

$$p_{x'x}=\langle x'|\hat{p}|x\rangle=-\mathrm{i}\hbar\frac{\partial}{\partial x}\delta(x-x') \tag{3.44}$$

5. 动量表象下力学量的矩阵元：

$$O_{p'p}=\langle p'|\hat{O}(p)|p\rangle=O(p)\delta(p'-p) \tag{3.45}$$

$$x_{p'p}=\langle p'|\hat{x}|p\rangle=\mathrm{i}\hbar\frac{\partial}{\partial p}\delta(p-p') \tag{3.46}$$

6. 表象变换的矩阵表示：

$$\begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\end{pmatrix}=\begin{pmatrix}S_{11} & S_{12} & \cdots\\ S_{21} & S_{22} & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\\ \vdots\end{pmatrix},\quad S_{ij}=\langle\phi_j|\psi_i\rangle \tag{3.47}$$

7. 不同表象下力学量矩阵相似：

$$\boldsymbol{O}_{\Omega'}=\boldsymbol{S}\boldsymbol{O}_{\Omega}\boldsymbol{S}^{\dagger} \tag{3.48}$$

4 中心力场中的粒子运动

4.1 中心力场中粒子运动的一般性质

1. 定态 Schrodinger 方程：

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(r)\right]\psi(r,\theta,\varphi)=E\psi(r,\theta,\varphi) \tag{4.1}$$

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{\hat{L}^2}{2mr^2}+V(r)\right]\psi(r,\theta,\varphi)=E\psi(r,\theta,\varphi) \tag{4.2}$$

2. 分离变量：

$$\psi(r,\theta,\varphi)=R_l(r)Y_{lm}(\theta,\varphi) \tag{4.3}$$

3. 径向方程：

$$R_l''+\frac{2}{r}R_l'+\left[\frac{2m}{\hbar^2}\left(E-V(r)\right)-\frac{l(l+1)}{r^2}\right]R_l=0 \tag{4.4}$$

4. 变量代换：

$$R_l(r)=\frac{\chi_l(r)}{r} \tag{4.5}$$

$$\chi_l''+\left[\frac{2m}{\hbar^2}\left(E-V(r)\right)-\frac{l(l+1)}{r^2}\right]\chi_l=0 \tag{4.6}$$

5. 当 $r\to 0$ 时：

$$r^2V(r)\xrightarrow{r\to 0}0 \tag{4.7}$$

$$\chi_l''-\frac{l(l+1)}{r^2}\chi_l=0 \tag{4.8}$$

6. 试解指标方程：

$$\chi_l(r)=r^s\Rightarrow s(s-1)-l(l+1)=0\Rightarrow s_1=l+1,\ s_2=-l \tag{4.9}$$

7. 根据概率诠释，s 只能取 $l+1$：

$$\chi_l(r)=r^{l+1},\quad R_l(r)=r^l \tag{4.10}$$

4.2 无限深球方势阱

1. 无限深球方势阱：

$$V(r)=\begin{cases}0 & r<a\\ \infty & r>a\end{cases} \tag{4.11}$$

2. $l=0$ 的径向方程：

$$\chi_0''+k^2\chi_0=0,\quad k^2=\frac{2mE}{\hbar^2} \tag{4.12}$$

$$\chi_0(r)=A\sin kr+B\cos kr \tag{4.13}$$

3. 边界条件：

$$\chi_0(0)=\chi_0(a)=0 \tag{4.14}$$

$$B=0,\quad ka=n_r\pi,\quad n_r=1,2,\ldots \tag{4.15}$$

4. 径向波函数：

$$\chi_{n_r0}(r)=\sqrt{\frac{2}{a}}\sin\frac{n_r\pi r}{a} \tag{4.16}$$

5. 能量：

$$E_{n_r0}=\frac{n_r^2\pi^2\hbar^2}{2ma^2} \tag{4.17}$$

6. $l \neq 0$ 的径向方程:

$$R_l'' + \frac{2}{r}R_l' + \left(k^2 - \frac{l(l+1)}{r^2}\right)R_l = 0 \tag{4.18}$$

$$R_l = Cj_l(kr) \tag{4.19}$$

7. 边界条件:

$$R_l(a) = 0 \Rightarrow j_l(ka) = 0 \Rightarrow k_{n_rl}a = x_{n_rl} \tag{4.20}$$

8. 径向波函数:

$$R_{kl}(r) = \left(-\frac{2}{a}\Big/ j_{l-1}(ka)j(l+1)(ka)\right)^{\frac{1}{2}} j_l(kr) \tag{4.21}$$

9. 能量:

$$E_{n_rl} = \frac{\hbar^2}{2ma^2}x_{n_rl}^2 \tag{4.22}$$

4.3 三维各向同性谐振子

1. 三维各向同性谐振子势:

$$V(r) = \frac{1}{2}m\omega^2r^2 \tag{4.23}$$

2. 径向方程:

$$R_l'' + \frac{2}{r}R_l' + \left[\frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2r^2\right) - \frac{l(l+1)}{r^2}\right]R_l = 0 \tag{4.24}$$

3. 当 $r \to 0$ 时:

$$R_l(r) = r^l \tag{4.25}$$

4. 当 $r \to +\infty$ 时:

$$R_l''(r) - \frac{m^2\omega^2}{\hbar^2}r^2R_l(r) = 0 \tag{4.26}$$

$$R_l(r) = \exp\left(-\frac{m\omega}{2\hbar}r^2\right) \tag{4.27}$$

5. 假设试解:

$$R_l(r) = r^l\exp\left(-\frac{m\omega}{2\hbar}r^2\right)u_l(r) \tag{4.28}$$

$$u_l'' + \frac{2}{r}\left(l + 1 - \frac{m\omega}{\hbar}r^2\right)u_l' + \left(\frac{2mE}{\hbar^2} - \frac{3m\omega}{\hbar} - \frac{2lm\omega}{\hbar}\right)u_l = 0 \tag{4.29}$$

6. 变量代换:

$$\xi = \frac{m\omega}{\hbar}r^2 \tag{4.30}$$

$$\xi\frac{\mathrm{d}^2u_l}{\mathrm{d}\xi^2} + \left(l + \frac{3}{2} - \xi\right)\frac{\mathrm{d}u_l}{\mathrm{d}\xi} - \frac{1}{2}\left(l + \frac{3}{2} - \frac{E}{\hbar\omega}\right)u_l = 0 \tag{4.31}$$

$$u_l(r) = F(\alpha,\gamma,\xi), \quad \alpha = \frac{1}{2}\left(l + \frac{3}{2} - \frac{E}{\hbar\omega}\right), \quad \gamma = l + \frac{3}{2} \tag{4.32}$$

7. 要求截断:

$$\alpha + n_r = \frac{1}{2}\left(l + \frac{3}{2} - \frac{E}{\hbar\omega}\right) + n_r = 0, \quad n_r = 0,1,2,\ldots \tag{4.33}$$

8. 径向波函数:

$$R_{n_rl}(r) = \alpha^{\frac{3}{2}}\left(\frac{2^{l+2-n_r}(2l+2n_r+1)!!}{\sqrt{\pi}n_r!((2l+1)!!)^2}\right)^{\frac{1}{2}}(\alpha r)^l\mathrm{e}^{-\frac{1}{2}\alpha^2r^2}F\left(-n_r, l+\frac{3}{2}, \alpha^2r^2\right), \quad \alpha^2 = \frac{m\omega}{\hbar} \tag{4.34}$$

9. 能量:

$$E_N = \left(l + 2n_r + \frac{3}{2}\right)\hbar\omega = \left(N + \frac{3}{2}\right)\hbar\omega, \quad N = 0,1,2,\ldots \tag{4.35}$$

10. 能级简并度:

$$f_N = \frac{1}{2}(N+1)(N+2) \tag{4.36}$$

4.4 氢原子

1. Coulomb 作用势:

$$V(r) = -\frac{e^2}{r} \tag{4.37}$$

2. 径向方程:

$$\chi_l'' + \left[\frac{2m}{\hbar^2}\left(E + \frac{e}{r^2}\right) - \frac{l(l+1)}{r^2}\right]\chi_l = 0 \tag{4.38}$$

3. 当 $r \to 0$ 时:

$$\chi_l(r) = r^{l+1} \tag{4.39}$$

4. 当 $r \to +\infty$ 时:

$$\chi_l'' + \frac{2m}{\hbar^2}E\chi_l = 0, \quad E < 0 \tag{4.40}$$

$$\chi_l(r) = \mathrm{e}^{-\beta r}, \quad \beta = \sqrt{-\frac{2m}{\hbar^2}E} \tag{4.41}$$

5. 假设试解:

$$\chi_l(r) = r^{l+1}\mathrm{e}^{-\beta r}u_l(r) \tag{4.42}$$

$$ru_l'' + (2(l+1) - 2\beta r)\,u_l' - \left(2(l+1)\beta - \frac{2m}{\hbar^2}e^2\right)u_l = 0 \tag{4.43}$$

6. 变量代换:

$$\xi = 2\beta r \tag{4.44}$$

$$\xi\frac{\mathrm{d}^2u_l}{\mathrm{d}\xi^2} + (2(l+1) - \xi)\frac{\mathrm{d}u_l}{\mathrm{d}\xi} - \left((l+1) - \frac{me^2}{\hbar^2\beta}\right)u_l = 0 \tag{4.45}$$

$$u_l(r) = F(\alpha, \gamma, \xi), \quad \alpha = (l+1) - \frac{me^2}{\hbar^2\beta}, \quad \gamma = 2(l+1) \tag{4.46}$$

7. 要求截断:

$$\alpha + n_r = (l+1) - \frac{me^2}{\hbar^2\beta} + n_r = 0, \quad n_r = 0, 1, 2, \ldots \tag{4.47}$$

$$\frac{me^2}{\hbar^2\beta} = l + 1 + n_r = n, \quad n = 1, 2, \ldots \tag{4.48}$$

8. 径向波函数:

$$R_{nl}(r) = \frac{2}{a^{\frac{3}{2}}n^2(2l+1)!}\sqrt{\frac{(n+l)!}{(n-l-1)!}}\xi^l\mathrm{e}^{-\frac{1}{2}\xi}F(-n+l+1, 2l+2, \xi), \quad a = \frac{\hbar^2}{me^2} \tag{4.49}$$

9. 能量:

$$E_n = -\frac{me^4}{2\hbar^2}\frac{1}{n^2} = -\frac{e^2}{2a}\frac{1}{n^2}, \quad n = 1, 2, \ldots \tag{4.50}$$

10. 能级简并度:

$$f_n = \sum_{l=0}^{n-1}(2l+1) = n^2 \tag{4.51}$$

11. 径向概率分布:

$$P_{nl}(r)\mathrm{d}r = R_{nl}^2(r)r^2\mathrm{d}r = \chi_{nl}^2(r)\mathrm{d}r \tag{4.52}$$

12. 角向概率分布:

$$P_{lm}(\theta, \varphi)\mathrm{d}\Omega = |Y_l^m(\theta, \varphi)|^2\mathrm{d}\Omega = |P_l^m(\cos\theta)|^2\mathrm{d}\Omega \tag{4.53}$$

5 电磁场中的粒子运动

5.1 电磁场中粒子的 Schrodinger 方程

1. Hamilton 量:

$$\hat{H}=\frac{1}{2m}\left(\boldsymbol{P}-\frac{q}{c}\boldsymbol{A}\right)^2+q\varphi \tag{5.1}$$

2. Schrodinger 方程:

$$\left(-\frac{1}{2m}\boldsymbol{P}^2-\frac{q}{mc}\boldsymbol{A}\cdot\boldsymbol{P}+\frac{q^2}{2mc}\boldsymbol{A}^2+q\varphi\right)\psi=\mathrm{i}\hbar\frac{\partial}{\partial t}\psi \tag{5.2}$$

5.2 正常 Zeeman 效应

1. 均匀磁场:

$$\boldsymbol{A}=\frac{1}{2}\boldsymbol{B}\times\boldsymbol{r},\quad \boldsymbol{B}=B\boldsymbol{e}_z,\quad e\varphi(r)=V(r) \tag{5.3}$$

$$A_x=-\frac{1}{2}By,\quad A_y=\frac{1}{2}Bx,\quad A_z=0 \tag{5.4}$$

2. Hamilton 量:

$$\begin{aligned}\hat{H}&=\frac{1}{2m}\left[\left(\hat{P}_x-\frac{eB}{2c}y\right)^2+\left(\hat{P}_y+\frac{eB}{2c}x\right)^2+\hat{P}_z^2\right]+V(r)\\&=\frac{1}{2m}\left[\hat{P}^2+\frac{eB}{c}\hat{L}_z+\frac{e^2B^2}{4c^2}(x^2+y^2)\right]+V(r)\\&\approx\frac{1}{2m}\hat{P}^2+V(r)+\frac{eB}{2mc}\hat{L}_z\end{aligned} \tag{5.5}$$

3. 波函数:

$$\psi_{n_rlm}(r,\theta,\varphi)=R_{n_rl}(r)Y_{lm}(\theta,\varphi) \tag{5.6}$$

4. 能量:

$$E_{n_rlm}=E_{n_rl}+\frac{eB}{2mc}m\hbar=E_{n_rl}+m\hbar\omega_L \tag{5.7}$$

5.3 Landau 能级

1. 均匀磁场:

$$\boldsymbol{A}=\frac{1}{2}\boldsymbol{B}\times\boldsymbol{r},\quad \boldsymbol{B}=B\boldsymbol{e}_z,\quad \varphi(r)=0 \tag{5.8}$$

$$A_x=-\frac{1}{2}By,\quad A_y=\frac{1}{2}Bx,\quad A_z=0 \tag{5.9}$$

2. Hamilton 量:

$$\hat{H}=\frac{1}{2m}\left[\left(\hat{P}_x-\frac{eB}{2c}y\right)^2+\left(\hat{P}_y+\frac{eB}{2c}x\right)^2+\hat{P}_z^2\right]=\frac{1}{2m}\left[\hat{P}^2+\frac{eB}{c}\hat{L}_z+\frac{e^2B^2}{4c^2}(x^2+y^2)\right] \tag{5.10}$$

3. Schrodinger 方程:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right)\psi-\mathrm{i}\hbar\omega_L\frac{\partial}{\partial\varphi}\psi+\frac{1}{2}m\omega_L^2\rho^2\psi=E\psi \tag{5.11}$$

4. 分离变量:

$$\psi(\rho,\varphi,z)=R(\rho)\mathrm{e}^{\mathrm{i}m\varphi}\mathrm{e}^{\mathrm{i}kz},\quad m=0,\pm1,\pm2,\dots \tag{5.12}$$

5. 径向方程:

$$-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}+\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)R(\rho)+\frac{\hbar^2}{2m}\frac{m^2}{\rho^2}R(\rho)+\frac{1}{2}m\omega_L^2\rho^2R(\rho)=\left(E-\frac{\hbar^2k^2}{2m}-m\hbar\omega_L\right)R(\rho) \tag{5.13}$$

6. 当 $\rho \to +\infty$ 时:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}R(\rho)+\frac{1}{2}m\omega_L^2\rho^2R(\rho)=0 \tag{5.14}$$

$$R(\rho)=\exp\left(-\frac{m\omega_L}{2\hbar}\rho^2\right) \tag{5.15}$$

7. 当 $\rho \to 0$ 时:

$$-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}+\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)R(\rho)+\frac{\hbar^2}{2m}\frac{m^2}{\rho^2}R(\rho)=0 \tag{5.16}$$

$$R(\rho)=\rho^s\Rightarrow -s(s-1)+s+m^2=0\Rightarrow s=\pm m\Rightarrow R_m(\rho)=\rho^{|m|} \tag{5.17}$$

8. 假设试解:

$$R_m(\rho)=\rho^{|m|}\exp\left(-\frac{m\omega_L}{2\hbar}\rho^2\right)u_m(\rho) \tag{5.18}$$

$$u_m''+\frac{1}{\rho}\left((2|m|+1)-\frac{2m\omega_L}{\hbar}\rho^2\right)u_m'-\left((2|m|+2)\frac{m\omega_L}{\hbar}-\frac{2m}{\hbar}\widetilde{E}\right)u_m=0 \tag{5.19}$$

9. 变量代换:

$$\xi=\frac{m\omega_L}{\hbar}\rho^2 \tag{5.20}$$

$$\xi\frac{\mathrm{d}^2u_m}{\mathrm{d}\xi^2}+(|m|+1-\xi)\frac{\mathrm{d}u_m}{\mathrm{d}\xi}-\frac{1}{2}\left(|m|+1-\frac{\widetilde{E}}{\hbar\omega_L}\right)u_m=0 \tag{5.21}$$

$$u_m(\rho)=F(\alpha,\gamma,\xi),\quad \alpha=\frac{1}{2}\left(|m|+1-\frac{\widetilde{E}}{\hbar\omega_L}\right),\quad \gamma=|m|+1 \tag{5.22}$$

10. 要求截断:

$$\alpha+n_\rho=\frac{1}{2}\left(|m|+1-\frac{\widetilde{E}}{\hbar\omega_L}\right)+n_\rho=0,\quad n_\rho=0,1,2,\ldots \tag{5.23}$$

11. 波函数:

$$\psi_{n_\rho m}(\rho,\varphi,z)\sim\rho^{|m|}\exp\left(-\frac{m\omega_L}{2\hbar}\rho^2\right)F\left(-n_\rho,|m|+1,\frac{m\omega_L}{\hbar}\rho^2\right)\mathrm{e}^{\mathrm{i}m\rho}\mathrm{e}^{\mathrm{i}kz} \tag{5.24}$$

12. Landau 能级:

$$E_N=(2n_\rho+|m|+m+1)\hbar\omega_L+\frac{\hbar^2k^2}{2m}=(N+1)\hbar\omega_L+\frac{\hbar^2k^2}{2m},\quad N=0,2,4,\ldots \tag{5.25}$$

Remark. 上述结果不因规范选择而异。如选取 Landau 规范:

1. 均匀磁场:

$$A_x=-By,\quad A_y=A_z=0 \tag{5.26}$$

2. Schrodinger 方程:

$$\frac{1}{2m}\left[\left(\hat{P}_x-\frac{eB}{c}y\right)^2+\hat{P}_y^2+\hat{P}_z^2\right]\psi=E\psi \tag{5.27}$$

3. 分离变量:

$$\psi(\rho,\varphi,z)=\mathrm{e}^{\mathrm{i}k_xx}\phi(y)\mathrm{e}^{\mathrm{i}k_zz} \tag{5.28}$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\phi(y)}{\mathrm{d}y^2}+\frac{1}{2}m\omega_c^2(y-y_0)^2\phi(y)=\left(E-\frac{\hbar^2k_z^2}{2m}\right)\phi(y),\quad \omega_c=2\omega_L,\quad y_0=\frac{\hbar k_xc}{eB} \tag{5.29}$$

4. 波函数:

$$\phi_{y_0n}(y)\sim\mathrm{e}^{-\frac{1}{2}\alpha^2\hbar(y-y_0)^2}H_n(\alpha(y-y_0)),\quad \alpha^2=\frac{m\omega_c}{\hbar} \tag{5.30}$$

5. Landau 能级:

$$E_N=\left(n+\frac{1}{2}\right)\hbar\omega_c+\frac{\hbar^2k_z^2}{2m}=(N+1)\hbar\omega_L+\frac{\hbar^2k_z^2}{2m},\quad N=0,2,4,\ldots \tag{5.31}$$

6 自旋

6.1 电子自旋

1. 旋量波函数:

$$\psi(\boldsymbol{r},s_z)=\begin{pmatrix}\psi(\boldsymbol{r},\frac{\hbar}{2})\\ \psi(\boldsymbol{r},-\frac{\hbar}{2})\end{pmatrix} \tag{6.1}$$

2. Hamilton 量不显含自旋变量，可以分离变量:

$$\psi(\boldsymbol{r},s_z)=\varphi(\boldsymbol{r})\chi(s_z) \tag{6.2}$$

3. 自旋波函数:

$$\chi(s_z)=\begin{pmatrix}a\\ b\end{pmatrix}=a\begin{pmatrix}1\\ 0\end{pmatrix}+b\begin{pmatrix}0\\ 1\end{pmatrix}=a\alpha+b\beta \tag{6.3}$$

4. 自旋角动量算符:

$$\hat{S}_x=\frac{\hbar}{2}\begin{pmatrix}0&1\\ 1&0\end{pmatrix},\quad s_x=\pm\frac{\hbar}{2},\quad \chi_\uparrow(s_x)=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix},\quad \chi_\downarrow(s_x)=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix} \tag{6.4}$$

$$\hat{S}_y=\frac{\hbar}{2}\begin{pmatrix}0&-\mathrm{i}\\ \mathrm{i}&0\end{pmatrix},\quad s_y=\pm\frac{\hbar}{2},\quad \chi_\uparrow(s_y)=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \mathrm{i}\end{pmatrix},\quad \chi_\downarrow(s_y)=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -\mathrm{i}\end{pmatrix} \tag{6.5}$$

$$\hat{S}_z=\frac{\hbar}{2}\begin{pmatrix}1&0\\ 0&-1\end{pmatrix},\quad s_z=\pm\frac{\hbar}{2},\quad \chi_\uparrow(s_z)=\begin{pmatrix}1\\ 0\end{pmatrix}=\alpha,\quad \chi_\downarrow(s_z)=\begin{pmatrix}0\\ 1\end{pmatrix}=\beta \tag{6.6}$$

$$\left[\hat{S}_\alpha,\hat{S}_\beta\right]=\varepsilon_{\alpha\beta\gamma}\mathrm{i}\hbar\hat{S}_\gamma \tag{6.7}$$

5. Pauli 矩阵:

$$\hat{\sigma}_x=\begin{pmatrix}0&1\\ 1&0\end{pmatrix},\quad \hat{\sigma}_y=\begin{pmatrix}0&-\mathrm{i}\\ \mathrm{i}&0\end{pmatrix},\quad \hat{\sigma}_z=\begin{pmatrix}1&0\\ 0&-1\end{pmatrix} \tag{6.8}$$

$$[\hat{\sigma}_\alpha,\hat{\sigma}_\beta]=\varepsilon_{\alpha\beta\gamma}2\mathrm{i}\hat{\sigma}_\gamma \tag{6.9}$$

$$\hat{\sigma}_x^2=\hat{\sigma}_y^2=\hat{\sigma}_z^2=\hat{I},\quad \hat{\sigma}_x^\dagger=\hat{\sigma}_x,\quad \hat{\sigma}_y^\dagger=\hat{\sigma}_y,\quad \hat{\sigma}_z^\dagger=\hat{\sigma}_z \tag{6.10}$$

$$\hat{\sigma}_x\hat{\sigma}_y=-\hat{\sigma}_y\hat{\sigma}_x=\mathrm{i}\hat{\sigma}_z,\quad \hat{\sigma}_y\hat{\sigma}_z=-\hat{\sigma}_z\hat{\sigma}_y=\mathrm{i}\hat{\sigma}_x,\quad \hat{\sigma}_z\hat{\sigma}_x=-\hat{\sigma}_x\hat{\sigma}_z=\mathrm{i}\hat{\sigma}y, \tag{6.11}$$

6. Pauli 升降算符:

$$\hat{\sigma}_+=\frac{1}{2}(\hat{\sigma}_x+\mathrm{i}\hat{\sigma}_y),\quad \hat{\sigma}_-=\frac{1}{2}(\hat{\sigma}_x-\mathrm{i}\hat{\sigma}_y) \tag{6.12}$$

$$[\hat{\sigma}_+,\hat{\sigma}_-]=\hat{\sigma}_z,\quad [\hat{\sigma}_z,\hat{\sigma}_\pm]=\pm2\hat{\sigma}_\pm \tag{6.13}$$

6.2 总角动量

1. 总角动量算符:

$$\hat{J}=\hat{L}+\hat{S} \tag{6.14}$$

2. 对易关系:

$$\left[\hat{J}_\alpha,\hat{J}_\beta\right]=\varepsilon_{\alpha\beta\gamma}\mathrm{i}\hbar\hat{J}_\gamma,\quad \left[\hat{J}^2,\hat{J}_\alpha\right]=0,\quad \left[\hat{J}^2,\hat{L}^2\right]=0 \tag{6.15}$$

3. 总角动量平方:

$$\begin{aligned}\hat{J}^2&=(\hat{L}+\hat{S})^2=\hat{L}^2+\hat{S}^2+2\hat{S}\cdot\hat{L}=\hat{L}^2+\frac{3}{4}\hbar^2+\hbar(\hat{\sigma}_x\hat{L}_x+\hat{\sigma}_y\hat{L}_y+\hat{\sigma}_z\hat{L}_z)\\ &=\begin{pmatrix}\hat{L}^2+\frac{3}{4}\hbar^2+\hbar\hat{L}_z & \hbar\hat{L}_-\\ \hbar\hat{L}_+ & \hat{L}^2+\frac{3}{4}\hbar^2-\hbar\hat{L}_z\end{pmatrix}\end{aligned} \tag{6.16}$$

4. 总角动量平方的本征方程:

$$\hat{J}^2\begin{pmatrix}aY_{lm}\\ bY_{l(m+1)}\end{pmatrix}=\lambda\hbar^2\begin{pmatrix}aY_{lm}\\ bY_{l(m+1)}\end{pmatrix} \tag{6.17}$$

5. 比较系数:

$$\left(l(l+1)+\frac{3}{4}+m-\lambda\right)a+\sqrt{l(l+1)-m(m+1)}b=0 \tag{6.18}$$

$$\sqrt{l(l+1)-m(m+1)}a+\left(l(l+1)+\frac{3}{4}-(m+1)-\lambda\right)b=0 \tag{6.19}$$

6. 总角动量的本征值:

$$\lambda_1=\left(l+\frac{1}{2}\right)\left(l+\frac{3}{2}\right),\quad \lambda_2=\left(l-\frac{1}{2}\right)\left(l+\frac{1}{2}\right) \tag{6.20}$$

$$\lambda\hbar^2=j(j+1)\hbar^2,\quad j=l\pm\frac{1}{2} \tag{6.21}$$

7. 总角动量的本征函数:

$$\phi_{ljm_j}(\theta,\varphi,s_z)=\frac{1}{\sqrt{2l+1}}\begin{pmatrix}\sqrt{l+m+1}Y_{lm}\\ \sqrt{l-m}Y_{l(m+1)}\end{pmatrix}=\sqrt{\frac{l+m+1}{2l+1}}Y_{lm}\chi_{\uparrow}+\sqrt{\frac{l-m}{2l+1}}Y_{l(m+1)}\chi_{\downarrow} \tag{6.22}$$

$$\phi_{ljm_j}(\theta,\varphi,s_z)=\frac{1}{\sqrt{2l+1}}\begin{pmatrix}-\sqrt{l-m}Y_{lm}\\ \sqrt{l+m+1}Y_{l(m+1)}\end{pmatrix}=-\sqrt{\frac{l-m}{2l+1}}Y_{lm}\chi_{\uparrow}+\sqrt{\frac{l+m+1}{2l+1}}Y_{l(m+1)}\chi_{\downarrow} \tag{6.23}$$

6.3 自旋单态和三重态

1. 非耦合表象自旋本征态:

$$|\uparrow\uparrow\rangle_{12},\quad |\uparrow\downarrow\rangle_{12},\quad |\downarrow\uparrow\rangle_{12},\quad |\downarrow\downarrow\rangle_{12} \tag{6.24}$$

2. 两个电子自旋角动量耦合:

$$\hat{S}^2=(\hat{S}_1+\hat{S}_2)^2=\hat{S}_1^1+\hat{S}_2^2+2\hat{S}_1\cdot\hat{S}_2=\frac{3}{2}\hbar^2+\frac{1}{2}\hbar^2\left(\hat{\sigma}_{1x}\hat{\sigma}_{2x}+\hat{\sigma}_{1y}\hat{\sigma}_{2y}+\hat{\sigma}_{1z}\hat{\sigma}_{2z}\right) \tag{6.25}$$

3. 自旋角动量平方作用于本征态:

$$\hat{S}^2|\uparrow\uparrow\rangle_{12}=2\hbar^2|\uparrow\uparrow\rangle_{12} \tag{6.26}$$

$$\hat{S}^2|\uparrow\downarrow\rangle_{12}=\hbar^2|\uparrow\downarrow\rangle_{12}+\hbar^2|\downarrow\uparrow\rangle_{12} \tag{6.27}$$

$$\hat{S}^2|\downarrow\uparrow\rangle_{12}=\hbar^2|\uparrow\downarrow\rangle_{12}+\hbar^2|\downarrow\uparrow\rangle_{12} \tag{6.28}$$

$$\hat{S}^2|\downarrow\downarrow\rangle_{12}=2\hbar^2|\downarrow\downarrow\rangle_{12} \tag{6.29}$$

4. 耦合表象自旋本征态:

$$\chi_{11}=|11\rangle=|\uparrow\uparrow\rangle_{12} \tag{6.30}$$

$$\chi_{1,-1}=|1-1\rangle=|\downarrow\downarrow\rangle_{12} \tag{6.31}$$

$$\chi_{10}=|10\rangle=\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle_{12}+|\downarrow\uparrow\rangle_{12}\right) \tag{6.32}$$

$$\chi_{00}=|00\rangle=\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle_{12}-|\downarrow\uparrow\rangle_{12}\right) \tag{6.33}$$

7 定态微扰论

7.1 非简并微扰论

1. 能量本征值和本征态逐级展开:

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}' \tag{7.1}$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \tag{7.2}$$

$$|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots \tag{7.3}$$

2. 代入 Schrodinger 方程比较同级系数:

$$\left(\hat{H}_0 - E_n^{(0)}\right) |n^{(1)}\rangle = \left(E_n^{(1)} - \hat{H}'\right) |n^{(0)}\rangle \tag{7.4}$$

$$\left(\hat{H}_0 - E_n^{(0)}\right) |n^{(2)}\rangle = \left(E_n^{(1)} - \hat{H}'\right) |n^{(1)}\rangle + E_n^{(2)} |n^{(0)}\rangle \tag{7.5}$$

3. 能量本征态在零级本征态展开:

$$|n^{(1)}\rangle = \sum_k a_k^{(1)} |k^{(0)}\rangle, \quad |n^{(2)}\rangle = \sum_k a_k^{(2)} |k^{(0)}\rangle \tag{7.6}$$

4. 左乘零级本征态 $\langle m^{(0)}|$:

$$a_m^{(1)} \left(E_m^{(0)} - E_n^{(0)}\right) = E_n^{(1)} \delta_{mn} - \langle m^{(0)}|\hat{H}'|n^{(0)}\rangle \tag{7.7}$$

$$a_m^{(2)} \left(E_m^{(0)} - E_n^{(0)}\right) = \sum_{k\neq n} a_k^{(1)} E_n^{(1)} \delta_{km} - \sum_{k\neq n} a_k^{(1)} \langle m^{(0)}|\hat{H}'|k^{(0)}\rangle + E_n^{(2)} \delta_{mn} \tag{7.8}$$

5. 能量本征值的一级修正:

$$E_n^{(1)} = \langle n^{(0)}|\hat{H}'|n^{(0)}\rangle \tag{7.9}$$

6. 能量本征态的一级修正:

$$|n^{(1)}\rangle = \sum_{m\neq n} \frac{\langle m^{(0)}|\hat{H}'|n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} |m^{(0)}\rangle \tag{7.10}$$

7. 能量本征值的二级修正:

$$E_n^{(2)} = \sum_{m\neq n} \frac{\left|\langle m^{(0)}|\hat{H}'|n^{(0)}\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}} \tag{7.11}$$

7.2 简并微扰论

1. 新零级本征态在原来零级本征态展开:

$$|n\widetilde{\nu}^{(0)}\rangle = \sum_{\nu=1}^{f_n} a_\nu(\widetilde{\nu}) |n\nu^{(0)}\rangle \tag{7.12}$$

2. 代入式(7.4):

$$\left(\hat{H}_0 - E_n^{(0)}\right) |n^{(1)}\rangle = \left(E_n^{(1)} - \hat{H}'\right) \sum_{\nu=1}^{f_n} a_\nu(\widetilde{\nu}) |n\nu^{(0)}\rangle \tag{7.13}$$

3. 左乘零级本征函数 $\langle n\mu^{(0)}|$:

$$\sum_{\nu=1}^{f_n} \left(H'_{\mu\nu} - E_n^{(1)} \delta_{\mu\nu}\right) a_\nu(\widetilde{\nu}) = 0 \tag{7.14}$$

4. 能量本征值的一级修正:

$$E_{n\widetilde{\nu}}^{(1)}, \quad \widetilde{\nu} = 1, \ldots, f_n \tag{7.15}$$

5. 能量零级本征态:

$$|n\widetilde{\nu}^{(0)}\rangle = \sum_{\nu=1}^{f_n} a_\nu(\widetilde{\nu}) |n\nu^{(0)}\rangle \tag{7.16}$$

7.3 氢原子精细结构

1. Hamilton 量的相对论修正：

$$\hat{H}_r' = \sqrt{\hat{p}^2c^2 + m^2c^4} - mc^2 - \frac{\hat{p}^2}{2m} \approx -\frac{\hat{p}^4}{8m^3c^2} \tag{7.17}$$

$$[\hat{H}_r', \hat{L}^2] = 0, \quad [\hat{H}_r', \hat{L}_z] = 0, \quad [\hat{H}_r', \hat{S}_z] = 0 \tag{7.18}$$

2. 能量本征值的相对论修正：

$$\begin{aligned} E_r^{(1)} &= -\frac{1}{8m^3c^2}\langle nlm|\hat{p}^4|nlm\rangle = -\frac{1}{2mc^2}\langle nlm|(E-V(r))^2|nlm\rangle \\ &= -\frac{1}{2mc^2}\left[E_n^2 - 2E_n\frac{e^2}{4\pi\varepsilon_0}\left\langle\frac{1}{r}\right\rangle + \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\left\langle\frac{1}{r^2}\right\rangle\right] \\ &= -\frac{E_n^2}{2mc^2}\left(\frac{4n}{1+1/2} - 3\right) \sim \alpha^4 mc^2 \end{aligned} \tag{7.19}$$

3. Hamilton 量的自旋轨道耦合修正：

$$\hat{H}_{so}' = -\frac{1}{2}\hat{\mu}\cdot\hat{B} = \frac{1}{2}\frac{e^2}{4\pi\varepsilon_0}\frac{1}{m^2c^2r^3}\hat{S}\cdot\hat{L} \tag{7.20}$$

$$[\hat{H}_{so}', \hat{L}^2] = 0, \quad [\hat{H}_{so}', \hat{J}^2] = 0 \tag{7.21}$$

4. 能量本征值的自旋轨道耦合修正：

$$\begin{aligned} E_{so}^{(1)} &= \frac{1}{2}\frac{e^2}{4\pi\varepsilon_0}\frac{1}{m^2c^2}\left\langle nlmm_s\left|\frac{1}{r^3}\frac{1}{2}(\hat{J}^2 - \hat{L}^2 - \hat{S}^2)\right|nlmm_s\right\rangle \\ &= \frac{e^2\hbar^2}{16\pi\varepsilon_0 m^2c^2}[j(j+1) - l(l+1) - s(s+1)]\left\langle\frac{1}{r^3}\right\rangle \\ &= \frac{E_n^2}{mc^2}\frac{n[j(j+1) - l(l+1) - 3/4]}{l(l+1/2)(l+1)} \sim \alpha^4 mc^2 \end{aligned} \tag{7.22}$$

5. 能量本征值的精细结构修正：

$$E_{fs}^{(1)} = E_r^{(1)} + E_{so}^{(1)} = \frac{E_n^2}{2mc^2}\left(3 - \frac{4n}{j+1/2}\right) \tag{7.23}$$

7.4 Zeeman 效应

1. Hamilton 量的 Zeeman 效应修正：

$$\hat{H}_z' = -(\hat{\mu}_l + \hat{\mu}_s)\cdot B_{ext} = \frac{e}{2m}(\hat{L} + 2\hat{S})\cdot B_{ext} \tag{7.24}$$

2. 弱场 Zeeman 效应：$B_{ext} \ll B_{int} \sim 10\mathrm{T}$

$$\widetilde{H}_0 = \hat{H}_0 + \hat{H}_{fs}', \quad \widetilde{H}' = \hat{H}_z' \tag{7.25}$$

$$\begin{aligned} E_z^{(1)} &= \frac{e}{2m}\hat{B}_{ext}\cdot\langle mljm_j|(\hat{L} + 2\hat{S})|nljm_j\rangle \\ &= \frac{e}{2m}\hat{B}_{ext}\cdot\left\langle mljm_j\left|\left(1 + \frac{\hat{S}\cdot\hat{J}}{\hat{J}^2}\right)\hat{J}\right|nljm_j\right\rangle \\ &= \mu_B B_{ext}\left(1 + \frac{j(j+1) - l(l+1) + 3/4}{j(j+1)}\right)m_j = \mu_B g_J m_j B_{ext} \end{aligned} \tag{7.26}$$

3. 强场 Zeeman 效应：$B_{ext} \gg B_{int} \sim 10\mathrm{T}$

$$\widetilde{H}_0 = \hat{H}_0 + \hat{H}_z', \quad \widetilde{H}' = \hat{H}_{fs}' \tag{7.27}$$

$$E_{nm_lm_s}^{(0)} = E_n + \mu_B B_{ext}(m_l + 2m_s) \tag{7.28}$$

4. 中间场 Zeeman 效应：

$$\widetilde{H}_0 = \hat{H}_0, \quad \widetilde{H}' = \hat{H}_{fs}' + \hat{H}_z' \tag{7.29}$$

8 量子跃迁

8.1 含时微扰论

1. 系统 Hamilton 量：

$$\hat{H}=\hat{H}_0+\lambda\hat{H}'(t) \tag{8.1}$$

2. 含时量子态在本征态展开：

$$|\psi(t)\rangle=\sum_n C_{nk}(t)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n t}|n\rangle\,,\quad |\psi(0)\rangle=|k\rangle \tag{8.2}$$

3. 代入 Schodinger 方程：

$$\mathrm{i}\hbar\sum_n \dot{C}_{nk}(t)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n t}|n\rangle=\lambda\sum_n C_{nk}(t)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n t}\hat{H}'(t)|n\rangle \tag{8.3}$$

4. 左乘本征态 $\langle k'|$：

$$\mathrm{i}\hbar\dot{C}_{k'k}(t)=\lambda\sum_n C_{nk}(t)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_{k'}-E_n)t}\langle k'|\hat{H}'(t)|n\rangle \tag{8.4}$$

5. 跃迁概率很小：

$$C_{nk}(t)=\delta_{nk}+\lambda C_{nk}^{(1)}(t) \tag{8.5}$$

6. 代入上式并比较一级系数：

$$\mathrm{i}\hbar\dot{C}_{k'k}^{(1)}(t)=\sum_n \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_{k'}-E_n)t}\delta_{nk}\langle k'|\hat{H}'(t)|n\rangle=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_{k'}-E_k)t}\langle k'|\hat{H}'(t)|k\rangle \tag{8.6}$$

7. 跃迁振幅：

$$C_{k'k}^{(1)}(t)=\frac{1}{\mathrm{i}\hbar}\int_0^t \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega_{k'k}t}H'_{k'k}(t) \tag{8.7}$$

8. 跃迁概率：

$$W_{k'k}(t)=\left|C_{k'k}^{(1)}(t)\right|^2=\frac{1}{\hbar^2}\left|\int_0^t \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega_{k'k}t}H'_{k'k}(t)\right|^2 \tag{8.8}$$

9. 跃迁速率：

$$w_{k'k}=\frac{\mathrm{d}}{\mathrm{d}t}W_{k'k}(t) \tag{8.9}$$

简并能级：初态求平均，末态求和

$$w_{k'k}=\frac{1}{f_k}\sum_{j=1}^{f_{k'}}\sum_{i=1}^{f_k}w_{k'_jk_i}=\frac{f_{k'}}{f_k}\sum_{i=1}^{f_k}w_{k'_jk_i} \tag{8.10}$$

8.2 周期微扰

1. 周期微扰：

$$\hat{H}'(t)=\hat{H}'\mathrm{e}^{-\mathrm{i}\omega t} \tag{8.11}$$

2. 跃迁振幅：

$$C_{k'k}^{(1)}(t)=\frac{1}{\mathrm{i}\hbar}\int_0^t \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega_{k'k}t}H_{k'k}(t)=-\frac{H'_{k'k}}{\hbar}\frac{\mathrm{e}^{\mathrm{i}(\omega_{k'k}-\omega)t}-1}{\omega_{k'k}-\omega} \tag{8.12}$$

3. 跃迁概率：

$$W_{k'k}(t)=\frac{|H'_{k'k}|^2}{\hbar^2}\left(\frac{\sin[(\omega_{k'k}-\omega)t/2]}{(\omega_{k'k}-\omega)/2}\right)^2\xrightarrow{t\to+\infty}\frac{2\pi t}{\hbar^2}|H'_{k'k}|^2\delta(\omega_{k'k}-\omega) \tag{8.13}$$

4. 跃迁速率：

$$w_{k'k}=\frac{2\pi}{\hbar^2}|H'_{k'k}|^2\delta(\omega_{k'k}-\omega)=\frac{2\pi}{\hbar}|H'_{k'k}|^2\delta(E_{k'}-E_k-\hbar\omega) \tag{8.14}$$

8.3 常微扰

1. 常微扰:

$$\hat{H}'(t) = \hat{H}'[\Theta(t) - \Theta(t-T)] \tag{8.15}$$

2. 跃迁振幅:

$$C_{k'k}^{(1)}(t) = \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t} \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega_{k'k}t} H_{k'k}(t) = -\frac{H'_{k'k}}{\hbar}\frac{\mathrm{e}^{\mathrm{i}\omega_{k'k}T}-1}{\omega_{k'k}} \tag{8.16}$$

3. 跃迁概率:

$$W_{k'k}(t) = \frac{|H'_{k'k}|^2}{\hbar^2}\left(\frac{\sin(\omega_{k'k}T/2)}{\omega_{k'k}/2}\right)^2 \xrightarrow{T\to+\infty} \frac{2\pi}{\hbar}|H'_{k'k}|^2\,\delta(E_{k'}-E_k)T \tag{8.17}$$

4. 跃迁速率:

$$w_{k'k} = \frac{W_{k'k}(t)}{T} = \frac{2\pi}{\hbar}|H'_{k'k}|^2\,\delta(E_{k'}-E_k) \tag{8.18}$$

5. Fermi 黄金规则:

$$w_{fi} = \int \mathrm{d}E_{k'} w_{k'k}\rho(E_{k'}) = \frac{2\pi}{\hbar}|H'_{k'k}|^2\,\rho(E_k) \tag{8.19}$$

8.4 光的吸收与辐射

8.4.1 受激吸收和受激辐射

1. 入射光:

$$\begin{cases} \boldsymbol{E}(\boldsymbol{r},t) = \boldsymbol{E}_0\cos(\omega t - \boldsymbol{k}\cdot\boldsymbol{r}) \\ \boldsymbol{B}(\boldsymbol{r},t) = \frac{1}{|\boldsymbol{k}|}\boldsymbol{k}\times\boldsymbol{E}(\boldsymbol{r},t) \end{cases} \tag{8.20}$$

Lorentz 力远小于电场力:

$$\frac{|\frac{e}{c}\boldsymbol{v}\times\boldsymbol{B}|}{|e\boldsymbol{E}|} \sim \frac{|\boldsymbol{v}|}{c} \ll 1 \tag{8.21}$$

电偶极近似:

$$\boldsymbol{E} = \boldsymbol{E}_0\cos\omega t \tag{8.22}$$

2. 入射光对电子的相互作用:

$$\hat{H}'(t) = -e\varphi = -\boldsymbol{d}\cdot\boldsymbol{E}_0\cos\omega t = \hat{H}'\cos\omega t, \quad \boldsymbol{d} = e\boldsymbol{r} \tag{8.23}$$

3. 跃迁振幅:

$$C_{k'k}^{(1)}(t) = \frac{1}{\mathrm{i}\hbar}\int_0^t \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega_{k'k}t}H_{k'k}(t) = -\frac{H_{k'k}}{2\hbar}\left(\frac{\mathrm{e}^{\mathrm{i}(\omega_{k'k}+\omega)t}-1}{\omega_{k'k}+\omega} + \frac{\mathrm{e}^{\mathrm{i}(\omega_{k'k}-\omega)t}-1}{\omega_{k'k}-\omega}\right) \tag{8.24}$$

4. 受激吸收的跃迁振幅:

$$C_{k'k}^{(1)}(t) = -\frac{H_{k'k}}{2\hbar}\frac{\mathrm{e}^{\mathrm{i}(\omega_{k'k}-\omega)t}-1}{\omega_{k'k}-\omega} \tag{8.25}$$

5. 受激吸收的跃迁概率:

$$W_{k'k}(t) = \frac{|H_{k'k}|^2}{4\hbar^2}\left(\frac{\sin[(\omega_{k'k}-\omega)t/2]}{(\omega_{k'k}-\omega)/2}\right)^2 \xrightarrow{t\to+\infty} \frac{\pi t}{2\hbar^2}|H'_{k'k}|^2\,\delta(\omega_{k'k}-\omega) \tag{8.26}$$

6. 受激吸收的跃迁速率:

$$\langle\cos^2\theta\rangle = \frac{1}{4\pi}\int_0^{2\pi}\mathrm{d}\varphi\int_0^{\pi}\cos^2\theta\sin\theta\mathrm{d}\theta = \frac{1}{3} \tag{8.27}$$

$$\rho(\omega) = \frac{1}{8\pi}\langle E^2+B^2\rangle = \frac{1}{4\pi}\langle E^2\rangle = \frac{E_0^2(\omega)}{4\pi}\frac{1}{T}\int_0^T\cos^2\omega t\mathrm{d}t = \frac{E_0^2(\omega)}{8\pi} \tag{8.28}$$

$$w_{k'k} = \frac{\pi}{2\hbar^2}|H'_{k'k}|^2\,\delta(\omega_{k'k}-\omega) = \frac{4\pi^2e^2}{3\hbar^2}|\boldsymbol{r}_{k'k}|^2\rho(\omega_{k'k}) \tag{8.29}$$

7. 电偶极辐射的选择定则：

$$\begin{cases} x = r\sin\theta\cos\varphi = \frac{r}{2}\sin\theta(\mathrm{e}^{\mathrm{i}\varphi} + \mathrm{e}^{-\mathrm{i}\varphi}) \\ y = r\sin\theta\sin\varphi = \frac{r}{2\mathrm{i}}\sin\theta(\mathrm{e}^{\mathrm{i}\varphi} - \mathrm{e}^{-\mathrm{i}\varphi}) \\ z = r\cos\theta \end{cases} \tag{8.30}$$

$$\cos\theta Y_{lm} = \sqrt{\frac{(l+1)^2 - m^2}{(2l+1)(2l+3)}} Y_{l+1,m} + \sqrt{\frac{l^2 - m^2}{(2l+1)(2l-1)}} Y_{l-1,m} \tag{8.31}$$

$$\sin\theta \mathrm{e}^{\pi\mathrm{i}\varphi} Y_{lm} = \pm\sqrt{\frac{(l\pm m+1)(l\pm m+2)}{(2l+1)(2l+3)}} Y_{l+1,m+1} + \sqrt{\frac{(l\mp m)(l\mp m+1)}{(2l-1)(2l+1)}} Y_{l-1,m\pm1} \tag{8.32}$$

$$\Delta l = l' - l = \pm1, \quad \Delta m = m' - m = 0,\ \pm1 \tag{8.33}$$

8.4.2 自发辐射

1. 受激吸收和受激辐射：

$$w_{k'k} = B_{k'k}\rho(\omega_{k'k}), \quad w_{kk'} = B_{kk'}\rho(\omega_{k'k}) \tag{8.34}$$

2. 自发辐射：

$$w_{kk'} = A_{kk'} \tag{8.35}$$

3. 粒子数 Boltzmann 分布：

$$\frac{n_k}{n'_k} = \mathrm{e}^{(E_{k'} - E_k)/kT} = \mathrm{e}^{\hbar\omega_{k'k}/kT} \tag{8.36}$$

4. 平衡的跃迁速率：

$$n_k B_{k'k}\rho(\omega_{k'k}) = n_{k'}(B_{kk'}\rho(\omega_{k'k}) + A_{kk'}) \tag{8.37}$$

5. 能量密度：

$$\rho(\omega_{k'k}) = \frac{A_{kk'}}{B_{kk'}} \frac{1}{\mathrm{e}^{\hbar\omega_{k'k}/kT} - 1} \xrightarrow{kT \gg \hbar\omega_{k'k}} \frac{A_{kk'}}{B_{kk'}} \frac{kT}{\hbar\omega_{k'k}} = \frac{\omega_{k'k}^2}{\pi^2 c^3} kT \tag{8.38}$$

6. 自发辐射系数：

$$A_{kk'} = \frac{\hbar\omega_{k'k}^2}{\pi^2 c^3} B_{kk'} = \frac{4e^2\omega_{k'k}^3}{3\hbar c^3} |\boldsymbol{r}_{kk'}|^2 \tag{8.39}$$

9 散射理论

9.1 Lippmann-Schwinger 方程

1. 传播子：

$$(\nabla^2 + \boldsymbol{k}^2)G(\boldsymbol{r}, \boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{9.1}$$

$$G(\boldsymbol{r}, \boldsymbol{r}') = \frac{\hbar^2}{2m}\left\langle \boldsymbol{r} \left| \frac{1}{E - \hat{H}_0 + \mathrm{i}\epsilon} \right| \boldsymbol{r}' \right\rangle = -\frac{1}{4\pi}\frac{\mathrm{e}^{\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|} \tag{9.2}$$

2. Lippmann-Schwinger 方程：

$$|\psi_{out}\rangle = |\psi_{in}\rangle + |\psi_{sc}\rangle = |\psi_{in}\rangle + \frac{1}{E - \hat{H}_0 + \mathrm{i}\epsilon}\hat{V}\,|\psi_{out}\rangle \tag{9.3}$$

$$\psi_{out}(\boldsymbol{r}) = \psi_{in}(\boldsymbol{r}) + \psi_{sc}(\boldsymbol{r}) = \psi_{in}(\boldsymbol{r}) + \frac{2m}{\hbar^2}\int \mathrm{d}\boldsymbol{r}' G(\boldsymbol{r}, \boldsymbol{r}')V(\boldsymbol{r}')\psi_{out}(\boldsymbol{r}') \tag{9.4}$$

3. 势场力程有限时：

$$|\boldsymbol{r} - \boldsymbol{r}'| \approx r\left(1 - \frac{\boldsymbol{r}\cdot\boldsymbol{r}'}{r^2}\right), \quad \mathrm{e}^{\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|} \approx \mathrm{e}^{\mathrm{i}(kr - \boldsymbol{k}'\cdot\boldsymbol{r}')}, \quad \boldsymbol{k}' = k\frac{\boldsymbol{r}}{r} \tag{9.5}$$

$$\psi_{out}(\boldsymbol{r}) \approx \psi_{in}(\boldsymbol{r}) - \frac{1}{4\pi}\frac{2m}{\hbar^2}\frac{\mathrm{e}^{\mathrm{i}kr}}{r}\int \mathrm{d}\boldsymbol{r}'\mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\psi_{out}(\boldsymbol{r}') = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{\mathrm{e}^{\mathrm{i}kr}}{r}f(\theta) \tag{9.6}$$

4. 散射振幅：

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}\boldsymbol{r}'\mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\psi_{out}(\boldsymbol{r}') \tag{9.7}$$

5. 入射波概率流密度：

$$j_{in} = \left|\frac{\mathrm{i}\hbar}{2m}\left(\psi_{in}\nabla\psi_{in}^* - \psi_{in}^*\nabla\psi_{in}\right)\right| = \left|\frac{\mathrm{i}\hbar}{2m}(-2\mathrm{i}\boldsymbol{k})\right| = \frac{\hbar k}{m} \tag{9.8}$$

6. 出射波概率流密度：

$$j_{sc}^r(\theta) = \left|\frac{\mathrm{i}\hbar}{2m}\left(\psi_{sc}\frac{\partial}{\partial r}\psi_{sc}^* - \psi_{sc}^*\frac{\partial}{\partial r}\psi_{sc}\right)\right| = \left|\frac{\mathrm{i}\hbar}{2m}(-2\mathrm{i}\boldsymbol{k})\frac{|f(\theta)|^2}{r^2}\right| = \frac{\hbar k}{m}\frac{|f(\theta)|^2}{r^2} \tag{9.9}$$

7. 微分散射截面：

$$\sigma_c(\theta) = \frac{w_{k'k}}{j_{in}\mathrm{d}\Omega} = \frac{j_{sc}r^2}{j_{in}} = |f(\theta)|^2 \tag{9.10}$$

9.2 高能散射：Born 近似

1. 转移动量：

$$\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}, \quad q = 2k\sin\frac{\theta}{2} \tag{9.11}$$

2. Born 近似：

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}\boldsymbol{r}'\mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\psi_{in}(\boldsymbol{r}') = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}\boldsymbol{r}'\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}'}V(\boldsymbol{r}') = \frac{m}{2\pi\hbar^2}\widetilde{V}(\boldsymbol{q}) \tag{9.12}$$

3. 微分散射截面：

$$\sigma_c(\theta) = |f(\theta)|^2 = \frac{m^2}{4\pi^2\hbar^2}\left|\int \mathrm{d}\boldsymbol{r}'\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\right|^2 = \frac{4m^2}{\hbar^4 q^2}\left|\int_0^{+\infty} r'V(r')\sin qr'\mathrm{d}r'\right|^2 \tag{9.13}$$

4. Yukawa 势的微分散射截面：

$$V(r) = \frac{Ze^2}{r}\mathrm{e}^{-\alpha r} \Rightarrow \sigma_c(\theta) = \frac{4m^2Z^2e^2}{\hbar^4}\frac{1}{(\alpha^2 + q^2)^2} \tag{9.14}$$

5. Rutherford 散射公式：

$$\sigma_c(\theta) = \frac{4m^2Z^2e^2}{\hbar^4}\frac{1}{q^4} = \frac{Z^2e^2}{16E^2}\frac{1}{\sin^4\frac{\theta}{2}} \tag{9.15}$$

9.3 低能散射：分波法

1. 入射波函数：

$$\psi_{in}(\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}kz} = \mathrm{e}^{kr\cos\theta} = \sum_{l=0}^{+\infty}(2l+1)\mathrm{i}^l \cdot j_l(kr)P_l(\cos\theta) = \sum_{l=0}^{+\infty}\sqrt{4\pi(2l+1)}\mathrm{i}^l \cdot j_l(kr)Y_{l0}(\theta)$$

$$\xrightarrow{r\to\infty} \sum_{l=0}^{+\infty}\sqrt{4\pi(2l+1)}\mathrm{i}^l\frac{1}{2\mathrm{i}kr}\left[\mathrm{e}^{\mathrm{i}(kr-l\pi/2)} - \mathrm{e}^{-\mathrm{i}(kr-l\pi/2)}\right]Y_{l0}(\theta) \tag{9.16}$$

2. 出射波函数：

$$\psi_{out}(\boldsymbol{r}) = \psi_{in}(\boldsymbol{r}) + \psi_{sc}(\boldsymbol{r}) \xrightarrow{r\to+\infty} \sum_{l=0}^{+\infty}\sqrt{4\pi(2l+1)}\mathrm{i}^l\frac{1}{2\mathrm{i}kr}\left[(1+a_l)\mathrm{e}^{\mathrm{i}(kr-l\pi/2)} - \mathrm{e}^{-\mathrm{i}(kr-l\pi/2)}\right]Y_{l0}(\theta) \tag{9.17}$$

3. 各分波的振幅不变：

$$|1+a_l| = 1 \Rightarrow a_l = \mathrm{e}^{2\mathrm{i}\delta_l} - 1 = 2\mathrm{i}\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l \tag{9.18}$$

4. 散射波函数：

$$\psi_{sc}(\boldsymbol{r}) = \sum_{l=0}^{+\infty}\sqrt{4\pi(2l+1)}\mathrm{i}^l\frac{1}{kr}\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l\mathrm{e}^{\mathrm{i}(kr-l\pi/2)}Y_{l0}(\theta) = \sum_{l=0}^{+\infty}\frac{\sqrt{4\pi(2l+1)}}{k}\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l Y_{l0}(\theta)\frac{\mathrm{e}^{\mathrm{i}kr}}{r} \tag{9.19}$$

5. 散射振幅：

$$f(\theta) = \sum_{l=0}^{+\infty}f_l(\theta) = \sum_{l=0}^{+\infty}\frac{\sqrt{4\pi(2l+1)}}{k}\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l Y_{l0}(\theta) = \sum_{l=0}^{+\infty}\frac{2l+1}{k}\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l P_l(\cos\theta) \tag{9.20}$$

6. 微分散射截面：

$$\sigma_c(\theta) = |f(\theta)|^2 = \frac{4\pi}{k^2}\left|\sum_{l=0}^{+\infty}\sqrt{2l+1}\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l Y_{l0}(\theta)\right|^2 \tag{9.21}$$

7. 总散射截面：

$$\sigma_{tot} = \int\sigma_c(\theta)\mathrm{d}\Omega = \frac{4\pi}{k^2}\sum_{l=0}^{+\infty}(2l+1)\sin^2\delta_l \tag{9.22}$$

8. 光学定理：

$$\mathrm{Im}f(0) = \sum_{l=0}^{+\infty}\frac{2l+1}{k}\sin^2\delta_l = \frac{k}{4\pi}\sigma_{tot} \tag{9.23}$$

9. 求解相移 δ_l：

(1) 求解散射区域径向方程：

$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R_l}{\mathrm{d}r}\right) + \left(k^2 - \frac{l(l+1)}{r^2} - \frac{2mV(r)}{\hbar^2}\right)R_l = 0 \tag{9.24}$$

(2) 与边界条件比较：

$$R_l(kr) \xrightarrow{r\to\infty} \sqrt{4\pi(2l+1)}\mathrm{i}^l\frac{1}{2\mathrm{i}kr}\left[\mathrm{e}^{2\mathrm{i}\delta_l}\mathrm{e}^{\mathrm{i}(kr-l\pi/2)} - \mathrm{e}^{-\mathrm{i}(kr-l\pi/2)}\right] = D_l\frac{1}{kr}\sin\left(kr - \frac{l\pi}{2} + \delta_l\right) \tag{9.25}$$

10　力学量本征值的代数解法

10.1　一维谐振子能量的本征谱

1. 谐振子升降算符:

$$\hat{a}^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} - \mathrm{i}\hat{p}), \quad \hat{a} = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} + \mathrm{i}\hat{p}) \tag{10.1}$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a}), \quad \hat{p} = \mathrm{i}\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}^\dagger - \hat{a}) \tag{10.2}$$

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \tag{10.3}$$

2. 对易关系:

$$[\hat{a}, \hat{a}^\dagger] = 1, \quad [\hat{n}, \hat{a}] = -\hat{a}, \quad [\hat{n}, \hat{a}^\dagger] = \hat{a}^\dagger \tag{10.4}$$

3. 能量本征态:

$$\hat{n}\left|n\right\rangle = n\left|n\right\rangle, \quad \left|n\right\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n\left|0\right\rangle, \quad \left\langle n|n'\right\rangle = \delta_{nn'} \tag{10.5}$$

$$\hat{a}^\dagger\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle, \quad \hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle \tag{10.6}$$

4. 本征函数:

$$\hat{a}\left|0\right\rangle = 0 \Rightarrow \left\langle x|\hat{a}|0\right\rangle = 0 \Rightarrow \int \mathrm{d}x' \left\langle x|\hat{a}|x'\right\rangle \left\langle x'|0\right\rangle = 0 \tag{10.7}$$

$$\Rightarrow \frac{1}{\sqrt{2\hbar m\omega}}\left(m\omega x + \hbar\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_0(x) = 0 \Rightarrow \psi_0(x) = \frac{\sqrt{\alpha}}{\pi^{1/4}}\mathrm{e}^{-\frac{1}{2}\alpha^2x^2} \tag{10.8}$$

$$\psi_n(x) = \left\langle x|n\right\rangle = \frac{1}{\sqrt{n!}}\left\langle x\right|\left(\hat{a}^\dagger\right)^n\left|0\right\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n\psi_0(x) = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n\frac{\sqrt{\alpha}}{\pi^{1/4}}\mathrm{e}^{-\frac{1}{2}\alpha^2x^2} \tag{10.9}$$

5. 能量:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, \ldots \tag{10.10}$$

10.2　角动量算符的本征谱

1. 角动量升降算符:

$$\hat{J}_+ = \hat{J}_x + \hat{J}_y, \quad \hat{J}_- = \hat{J}_x - \mathrm{i}\hat{J}_y \tag{10.11}$$

$$\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-), \quad \hat{J}_y = \frac{1}{2\mathrm{i}}(\hat{J}_+ - \hat{J}_-) \tag{10.12}$$

2. 对易关系:

$$\left[\hat{J}_+, \hat{J}_-\right] = 2\hbar\hat{J}_z, \quad \left[\hat{J}_z, \hat{J}_\pm\right] = \pm\hbar\hat{J}_\pm \tag{10.13}$$

3. 角动量本征态:

$$\hat{J}^2\left|jm\right\rangle = j(j+1)\hbar^2\left|jm\right\rangle, \quad j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots \tag{10.14}$$

$$\hat{J}_z\left|jm\right\rangle = m\hbar\left|jm\right\rangle, \quad m = 0, \pm1, \ldots, \pm j \tag{10.15}$$

4. 矩阵元公式:

$$\left\langle j(m+1)|\hat{J}_+|jm\right\rangle = \hbar\sqrt{j(j+1) - m(m+1)} \tag{10.16}$$

$$\left\langle j(m-1)|\hat{J}_-|jm\right\rangle = \hbar\sqrt{j(j+1) - m(m-1)} \tag{10.17}$$

$$\left\langle j(m+1)|\hat{J}_x|jm\right\rangle = \frac{\hbar}{2}\sqrt{j(j+1) - m(m+1)} \tag{10.18}$$

$$\left\langle j(m-1)|\hat{J}_x|jm\right\rangle = \frac{\hbar}{2}\sqrt{j(j+1) - m(m-1)} \tag{10.19}$$

$$\left\langle j(m+1)|\hat{J}_y|jm\right\rangle = -\frac{\mathrm{i}\hbar}{2}\sqrt{j(j+1) - m(m+1)} \tag{10.20}$$

$$\left\langle j(m-1)|\hat{J}_y|jm\right\rangle = \frac{\mathrm{i}\hbar}{2}\sqrt{j(j+1) - m(m-1)} \tag{10.21}$$

10.3　角动量耦合和 CG 系数

1. 两个角动量耦合:

$$\hat{J} = \hat{J}_1 + \hat{J}_2 \tag{10.22}$$

2. 耦合表象角动量本征态:

$$\hat{J}_1^2 |j,m\rangle = j_1(j_1+1)\hbar^2 |j,m\rangle \tag{10.23}$$

$$\hat{J}_2 |j,m\rangle = j_2(j_2+1)\hbar^2 |j,m\rangle \tag{10.24}$$

$$\hat{J}^2 |j,m\rangle = j(j+1)\hbar^2 |j,m\rangle \tag{10.25}$$

$$\hat{J}_z |j,m\rangle = m\hbar |j,m\rangle \tag{10.26}$$

3. CG 系数:

$$|jm\rangle = \sum_{m_1 m_2} \langle j_1 m_1, j_2 m_2 | jm\rangle |j_1 m_1\rangle \otimes |j_2 m_2\rangle \tag{10.27}$$

4. CG 系数的性质:

(1) 非零性:

$$\langle j_1 m_1, j_2 m_2 | jm\rangle = \delta_{m(m_1+m_2)} \langle j_1 m_1, j_2(m-m_1) | jm\rangle \tag{10.28}$$

(2) 幺正性:

$$\sum_{m_1 m_2} \langle j_1 m_1, j_2 m_2 | j' m\rangle \langle j_1 m_1, j_2 m_2 | jm\rangle = \delta_{j'j} \tag{10.29}$$

(3) 实数性:

$$\sum_{jm} \langle j_1 m_1, j_2 m_2 | jm\rangle \langle j_1 m_1', j_2 m_2' | jm\rangle = \delta_{m_1 m_1'} \delta_{m_2 m_2'} \tag{10.30}$$

(4) 对称性:

$$\langle j_1 m_1, j_2 m_2 | j_3 m_3\rangle = (-1)^{j_1+j_2-j_3} \langle j_1 m_1, j_2 - m_2 | j_3 - m_3\rangle \tag{10.31}$$

$$= (-1)^{j_1+j_2-j_3} \langle j_2 m_2, j_1 m_1 | j_3 m_3\rangle \tag{10.32}$$

$$= (-1)^{j_1-m_1} \sqrt{\frac{2j_3+1}{2j_2+1}} \langle j_1 m_1, j_3 - m_3 | j_2 - m_2\rangle \tag{10.33}$$

$$= (-1)^{j_2+m_2} \sqrt{\frac{2j_3+1}{2j_2+1}} \langle j_3 - m_3, j_2 m_2 | j_1 - m_1\rangle \tag{10.34}$$

$$= (-1)^{j_1-m_1} \sqrt{\frac{2j_3+1}{2j_2+1}} \langle j_3 m_3, j_1 - m_1 | j_2 m_2\rangle \tag{10.35}$$

$$= (-1)^{j_2+m_2} \sqrt{\frac{2j_3+1}{2j_1+1}} \langle j_2 - m_2, j_3 m_3 | j_1 m_1\rangle \tag{10.36}$$

11 二次量子化

11.1 粒子数表象

11.1.1 多体波函数

1. 单粒子波函数：箱归一化

$$\widetilde{\varphi}_{n_1,n_2,n_3,\uparrow}(x,y,z,\uparrow)=\frac{1}{\sqrt{V}}\exp\left(\mathrm{i}\frac{2\pi}{L}(n_1x+n_2y+n_3z)\right)\begin{pmatrix}1\\0\end{pmatrix} \tag{11.1}$$

$$\widetilde{\varphi}_{n_1,n_2,n_3,\downarrow}(x,y,z,\downarrow)=\frac{1}{\sqrt{V}}\exp\left(\mathrm{i}\frac{2\pi}{L}(n_1x+n_2y+n_3z)\right)\begin{pmatrix}0\\1\end{pmatrix} \tag{11.2}$$

2. Bose 子多体波函数表象：

$$\psi_{k_1,\ldots,k_N}(q_1,\ldots,q_N)=\sqrt{\frac{n_1!n_2!\cdots n_N!}{N!}}\sum_{\{\hat{P}\}}\varphi_{k_1}\left(q_{P(1)}\right)\cdots\varphi_{k_N}\left(q_{P(N)}\right) \tag{11.3}$$

3. Fermi 子多体波函数表象：

$$\psi_{k_1,\ldots,k_N}(q_1,\ldots,q_N)=\frac{1}{\sqrt{N!}}\sum_{\hat{P}}(-1)^{\hat{P}}\varphi_{k_1}\left(q_{P(1)}\right)\cdots\varphi_{k_N}\left(q_{P(N)}\right) \tag{11.4}$$

$$=\frac{1}{\sqrt{N!}}\begin{vmatrix}\varphi_{k_1}(q_1) & \varphi_{k_1}(q_1) & \cdots & \varphi_{k_N}(q_1)\\ \varphi_{k_2}(q_2) & \varphi_{k_1}(q_2) & \cdots & \varphi_{k_N}(q_2)\\ \vdots & \vdots & \ddots & \vdots\\ \varphi_{k_1}(q_N) & \varphi_{k_1}(q_N) & \cdots & \varphi_{k_N}(q_N)\end{vmatrix} \tag{11.5}$$

11.1.2 产生和湮灭算符

1. 产生和湮灭算符：

$$\hat{a}_\alpha^\dagger\left|0\right\rangle=\left|n_\alpha=1\right\rangle,\quad \hat{a}_\alpha\left|n_\alpha=1\right\rangle=\left|0\right\rangle,\quad \hat{a}_\alpha\left|0\right\rangle=0 \tag{11.6}$$

2. 粒子数算符：

$$\hat{n}_\alpha=\hat{a}_\alpha^\dagger\hat{a}_\alpha \tag{11.7}$$

3. 对易关系：

$$[\hat{a}_\alpha,\hat{a}_\beta^\dagger]=\delta_{\alpha\beta},\quad [\hat{a}_\alpha,\hat{a}_\beta]=[\hat{a}_\alpha^\dagger,\hat{a}_\beta^\dagger]=0 \tag{11.8}$$

$$\{\hat{c}_\alpha,\hat{c}_\beta^\dagger\}=\delta_{\alpha\beta},\quad \{\hat{c}_\alpha,\hat{c}_\beta\}=\{\hat{c}_\alpha^\dagger,\hat{c}_\beta^\dagger\}=0 \tag{11.9}$$

4. Bose 子多体粒子数表象：

$$\left|n_1\cdots n_N\right\rangle=\frac{1}{\sqrt{n_1!\cdots n_N!}}(\hat{a}_1^\dagger)^{n_1}\cdots(\hat{a}_N^\dagger)^{n_N}\left|0\right\rangle \tag{11.10}$$

$$\hat{a}_\alpha^\dagger\left|n_1\cdots n_\alpha\cdots n_N\right\rangle=\sqrt{n_\alpha+1}\left|n_1\cdots(n_\alpha+1)\cdots n_N\right\rangle \tag{11.11}$$

$$\hat{a}_\alpha\left|n_1\cdots n_\alpha\cdots n_N\right\rangle=\sqrt{n_\alpha}\left|n_1\cdots(n_\alpha-1)\cdots n_N\right\rangle \tag{11.12}$$

5. Fermi 子多体粒子数表象：

$$\left|n_1\cdots n_N\right\rangle,\quad n_k=1\text{ or }0 \tag{11.13}$$

$$\hat{a}_\alpha^\dagger\left|n_1\cdots n_\alpha\cdots n_N\right\rangle=(-1)^{\sum\limits_{i=1}^{\alpha-1}n_i}\left|n_1\cdots 1_\alpha\cdots n_N\right\rangle\delta_{n_\alpha 0} \tag{11.14}$$

$$\hat{a}_\alpha\left|n_1\cdots n_\alpha\cdots n_N\right\rangle=(-1)^{\sum\limits_{i=1}^{\alpha-1}n_i}\left|n_1\cdots 0_\alpha\cdots n_N\right\rangle\delta_{n_\alpha 1} \tag{11.15}$$

11.2 Bose 子单体和二体算符的表达式

11.2.1 单体算符

1. 单体算符：

$$\hat{F}=\sum_{\alpha\beta}f_{\alpha\beta}\hat{a}_{\alpha}^{\dagger}\hat{a}_{\beta} \tag{11.16}$$

$$f_{\alpha\beta}=\langle\varphi_{k_\alpha}(q_1)|\hat{f}(q_1)|\varphi_{k_\beta}(q_1)\rangle \tag{11.17}$$

2. 单体算符的矩阵元：

$$\langle\psi_{n_1'\cdots n_N'},\hat{F}\psi_{n_1\cdots n_N}\rangle=N\langle\psi_{n_1'\cdots n_N'},\hat{f}(q_1)\psi_{n_1\cdots n_N}\rangle \tag{11.18}$$

(1) F 的对角矩阵元：

$$\langle F\rangle=\langle\cdots n_j\cdots n_i\cdots|\hat{F}|\cdots n_i\cdots n_j\cdots\rangle=\sum_i n_i f_{ii} \tag{11.19}$$

(2) F 的非对角矩阵元：

$$\langle\cdots(n_j-1)\cdots(n_i+1)\cdots|\hat{F}|\cdots n_i\cdots n_j\cdots\rangle=\sqrt{(n_i+1)n_j}f_{ij} \tag{11.20}$$

11.2.2 二体算符

1. 二体算符：

$$\hat{G}=\frac{1}{2}\sum_{\alpha'\beta'}\sum_{\alpha\beta}g_{\alpha'\beta',\alpha\beta}\hat{a}_{\alpha'}^{\dagger}\hat{a}_{\beta'}^{\dagger}\hat{a}_{\beta}\hat{a}_{\alpha} \tag{11.21}$$

$$g_{\alpha'\beta',\alpha\beta}=\langle\varphi_{k_{\alpha'}}(q_1)\varphi_{k_{\beta'}}(q_2)\left|\hat{g}(q_1,q_2)\right|\varphi_{k_\alpha}(q_1)\varphi_{k_\beta}(q_2)\rangle \tag{11.22}$$

2. 二体算符的矩阵元：

$$\langle\psi_{n_1'\cdots n_N'},\hat{G}\psi_{n_1\cdots n_N}\rangle=\frac{N(N-1)}{2}\left\langle\psi_{n_1'\cdots n_N'},\hat{g}(q_1,q_2)\psi_{n_1\cdots n_N}\right\rangle \tag{11.23}$$

(1) G 的对角矩阵元：

$$\langle G\rangle=\langle\cdots n_j\cdots n_i\cdots|\hat{G}|\cdots n_i\cdots n_j\cdots\rangle=\frac{1}{2}\sum_{i\neq j}n_in_j(g_{ij,ij}+g_{ij,ji})+\frac{1}{2}\sum_i n_i(n_i-1)g_{ii,ii} \tag{11.24}$$

(2) G 的非对角矩阵元：

a. $(i,j)\to(k,l)$：

$$\begin{aligned}&\langle\cdots(n_l+1)\cdots(n_k+1)\cdots(n_j-1)\cdots(n_i-1)\cdots|\hat{G}|\cdots n_i\cdots n_j\cdots n_k\cdots n_l\cdots\rangle\\&=\sqrt{n_in_j(n_k+1)(n_l+1)}(g_{kl,ij}+g_{kl,ji})\end{aligned} \tag{11.25}$$

b. $(i,j)\to(k,k)$：

$$\begin{aligned}&\langle\cdots(n_k+2)\cdots(n_j-1)\cdots(n_i-1)\cdots|\hat{G}|\cdots n_i\cdots n_j\cdots n_k\cdots\rangle\\&=\sqrt{n_in_j(n_k+1)(n_k+2)}g_{kk,ij}\end{aligned} \tag{11.26}$$

c. $(i,i)\to(k,k)$：

$$\begin{aligned}&\langle\cdots(n_k+2)\cdots(n_i-2)\cdots|\hat{G}|\cdots n_i\cdots n_k\cdots\rangle\\&=\frac{1}{2}\sqrt{n_i(n_i-1)(n_k+1)(n_k+2)}g_{kk,ii}\end{aligned} \tag{11.27}$$

d. $j\to k$：

$$\begin{aligned}&\langle\cdots(n_k+1)\cdots(n_j-1)\cdots|\hat{G}|\cdots n_j\cdots n_k\cdots\rangle\\&=\sum_{\alpha\neq j,k}\sqrt{n_j(n_k+1)n_\alpha(g_{k\alpha,j\alpha}+g_{\alpha k,j\alpha})}+\sqrt{n_k^2(n_k+1)}n_jg_{kk,kj}+\sqrt{(n_j-1)^2n_j(n_k+1)}g_{jk,jj}\end{aligned} \tag{11.28}$$

11.3 Fermi 子单体和二体算符的表达式

11.3.1 单体算符

1. 单体算符:

$$\hat{F} = \sum_{\alpha\beta} f_{\alpha\beta} \hat{c}_\alpha^\dagger \hat{c}_\beta \tag{11.29}$$

$$f_{\alpha\beta} = \langle \varphi_{k_\alpha}(q_1) | \hat{f}(q_1) | \varphi_{k_\beta}(q_1) \rangle \tag{11.30}$$

2. 单体算符的矩阵元:

$$\langle \psi_{n_1' \cdots n_N'}, \hat{F} \psi_{n_1 \cdots n_N} \rangle = N \langle \psi_{n_1' \cdots n_N'}, \hat{f}(q_1) \psi_{n_1 \cdots n_N} \rangle \tag{11.31}$$

(1) F 的对角矩阵元:

$$\langle F \rangle = \langle \cdots n_j \cdots n_i \cdots | \hat{F} | \cdots n_i \cdots n_j \cdots \rangle = \sum_i n_i f_{ii}, \quad n_i = 1 \text{ or } 0 \tag{11.32}$$

(2) F 的非对角矩阵元:

$$\langle \cdots 0_k \cdots 1_j \cdots | \hat{F} | \cdots 0_j \cdots 1_k \cdots \rangle = (-1)^{\sum\limits_{i=j+1}^{k-1} n_i} f_{jk} \tag{11.33}$$

11.3.2 二体算符

1. 二体算符:

$$\hat{G} = \frac{1}{2} \sum_{\alpha'\beta'} \sum_{\alpha\beta} g_{\alpha'\beta',\alpha\beta} \hat{c}_{\alpha'}^\dagger \hat{c}_{\beta'}^\dagger \hat{c}_\beta \hat{c}_\alpha \tag{11.34}$$

$$g_{\alpha'\beta',\alpha\beta} = \langle \varphi_{k_{\alpha'}}(q_1) \varphi_{k_{\beta'}}(q_2) | \hat{g}(q_1, q_2) | \varphi_{k_\alpha}(q_1) \varphi_{k_\beta}(q_2) \rangle \tag{11.35}$$

2. 二体算符的矩阵元:

$$\langle \psi_{n_1' \cdots n_N'}, \hat{G} \psi_{n_1 \cdots n_N} \rangle = \frac{N(N-1)}{2} \langle \psi_{n_1' \cdots n_N'}, \hat{g}(q_1, q_2) \psi_{n_1 \cdots n_N} \rangle \tag{11.36}$$

(1) G 的对角矩阵元:

$$\langle G \rangle = \langle \cdots n_2 n_1 | \hat{G} | n_1 n_2 \cdots \rangle = \frac{1}{2} \sum_{i \neq j} n_i n_j (g_{ij,ij} + g_{ij,ji}) \tag{11.37}$$

(2) G 的非对角矩阵元:$(i,j) \to (k,l)$

$$\begin{aligned} &\langle \cdots 1_l \cdots 1_k \cdots 0_j \cdots 0_i \cdots | \hat{G} | \cdots 1_i \cdots 1_j \cdots 0_k \cdots 0_l \cdots \rangle \\ &= (-1)^{\sum\limits_{\nu=i+1}^{j-1} n_\nu + \sum\limits_{\nu=k+1}^{l-1} n_\nu} (g_{kl,ij} - g_{kl,ji}) \end{aligned} \tag{11.38}$$

11.4 粒子数表象与二次量子化的关系

1. Bose 子的场算符:

$$\hat{\psi}(\boldsymbol{r}) = \sum_k \hat{a}_k \varphi_k(\boldsymbol{r}) \tag{11.39}$$

$$\left[\hat{\psi}(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r})\right] = \delta(\boldsymbol{r} - \boldsymbol{r}'), \quad \left[\hat{\psi}^\dagger(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r})\right] = \left[\hat{\psi}(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r})\right] = 0 \tag{11.40}$$

2. Fermi 子的场算符:

$$\hat{\psi}(\boldsymbol{r}) = \sum_k \hat{c}_k \varphi_k(\boldsymbol{r}) \tag{11.41}$$

$$\left\{\hat{\psi}(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r})\right\} = \delta(\boldsymbol{r} - \boldsymbol{r}'), \quad \left\{\hat{\psi}^\dagger(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r})\right\} = \left\{\hat{\psi}(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r})\right\} = 0 \tag{11.42}$$

3. 相关函数:

$$G(\boldsymbol{r}_1, \boldsymbol{r}_2; t_1, t_2) = -\mathrm{i}\Theta(t_1 - t_2) \langle i | \hat{\psi}(\boldsymbol{r}_1, t_1) \hat{\psi}^\dagger(\boldsymbol{r}_2, t_2) | i \rangle \tag{11.43}$$

12 形式微扰论

12.1 绘景理论

12.1.1 Schrodinger 绘景

1. 波函数:

$$|\psi_S(t)\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}|\psi_S(0)\rangle \tag{12.1}$$

2. 波函数随时间的演化:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi_S(t)\rangle = \hat{H}|\psi_S(t)\rangle \tag{12.2}$$

3. 力学量随时间的演化:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}_S = 0 \tag{12.3}$$

4. 力学量的平均值随时间的演化:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle O_S\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle\left[\hat{O}_S, \hat{H}\right]\right\rangle \tag{12.4}$$

12.1.2 Heisenberg 绘景

1. 波函数:

$$|\psi_H(t)\rangle = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}|\psi_S(t)\rangle \tag{12.5}$$

2. 波函数随时间的演化:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi_H(t)\rangle = 0 \tag{12.6}$$

3. 力学量:

$$\hat{O}_H(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{O}_S\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t} \tag{12.7}$$

4. 力学量随时间的演化:Heisenberg 运动方程

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}_H(t) = \frac{1}{\mathrm{i}\hbar}\left[\hat{O}_H(t), \hat{H}\right] \tag{12.8}$$

5. 对易关系:必须等时

$$\hat{a}_{\alpha H}(t)\hat{a}^\dagger_{\beta H}(t) - \hat{a}^\dagger_{\beta H}(t)\hat{a}_{\alpha H}(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\left(\hat{a}_{\alpha S}\hat{a}^\dagger_{\beta S} - \hat{a}^\dagger_{\beta S}\hat{a}_{\alpha S}\right)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t} = \delta_{\alpha\beta} \tag{12.9}$$

12.1.3 相互作用绘景

1. 波函数:

$$|\psi_I(t)\rangle = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0 t}|\psi_S(t)\rangle \tag{12.10}$$

2. 波函数随时间的演化:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = \hat{H}'_I(t)|\psi_I(t)\rangle \tag{12.11}$$

3. 力学量:

$$\hat{O}_I(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0 t}\hat{O}_S\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0 t} \tag{12.12}$$

4. 力学量随时间的演化:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}_I(t) = \frac{1}{\mathrm{i}\hbar}\left[\hat{O}_I(t), \hat{H}_0\right] \tag{12.13}$$

5. 对易关系:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{a}_{\alpha I}(t) = \frac{1}{\mathrm{i}\hbar}\left[\hat{a}_{\alpha I}(t), \sum_\beta \frac{\hbar^2 k_\beta^2}{2m}\hat{a}^\dagger_{\beta I}(t)\hat{a}_{\beta I}(t)\right] = \frac{1}{\mathrm{i}\hbar}\frac{\hbar^2 k_\alpha^2}{2m}\hat{a}_{\alpha I}(t) \tag{12.14}$$

$$\Rightarrow \hat{a}_{\alpha I}(t) = \hat{a}_{\alpha I}(0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon_\alpha t} = \hat{a}_{\alpha S}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\varepsilon_\alpha t}, \quad \varepsilon_\alpha = \frac{\hbar^2 k_\alpha^2}{2m} \tag{12.15}$$

$$\hat{a}_{\alpha I}(t)\hat{a}^\dagger_{\beta I}(t') - \hat{a}^\dagger_{\beta I}(t')\hat{a}_{\alpha I}(t) = \delta_{\alpha\beta}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\varepsilon_\alpha(t'-t)} \tag{12.16}$$

12.2 形式微扰论

1. 相互作用绘景下的时间演化算符:

$$|\psi_I(t)\rangle = \hat{U}(t,t_0)\,|\psi_I(t_0)\rangle \tag{12.17}$$

$$\hat{U}(t_0,t_0)=\hat{I},\quad \hat{U}(t,t_0)=\hat{U}(t,t_1)\hat{U}(t_1,t_0),\quad \hat{U}^\dagger(t,t_0)\hat{U}(t,t_0)=\hat{I} \tag{12.18}$$

2. 时间演化算符的方程:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0)=\hat{V}_I(t)\hat{U}(t,t_0) \tag{12.19}$$

$$\hat{U}(t,t_0)=\hat{I}+\frac{1}{\mathrm{i}\hbar}\int_{t_0}^{t}\mathrm{d}t'\hat{V}_I(t')\hat{U}(t',t_0) \tag{12.20}$$

3. 迭代求解:

$$\hat{U}(t,t_0)=\hat{I}+\frac{1}{\mathrm{i}\hbar}\int_{t_0}^{t}\mathrm{d}t'\hat{V}_I(t')+\left(\frac{1}{\mathrm{i}\hbar}\right)^2\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t'}\mathrm{d}t''\hat{V}_I(t')\hat{V}_I(t'')+\cdots \tag{12.21}$$

4. 编时算符:

$$\hat{P}\,\hat{V}_I(t_1)\cdots\hat{V}(t_n)=\hat{V}_I(t_{\max})\cdots\hat{V}_I(t_{\min}) \tag{12.22}$$

$$\hat{P}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\cdots\int_{t_0}^{t}\mathrm{d}t_n\hat{V}_I(t_1)\cdots\hat{V}_I(t_n)=n!\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\cdots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n\hat{V}_I(t_1)\cdots\hat{V}_I(t_n) \tag{12.23}$$

5. 时间演化算符的形式解:

$$\hat{U}(t,t_0)=\hat{P}\exp\left(\frac{1}{\mathrm{i}\hbar}\int_{t_0}^{t}\mathrm{d}t'\hat{V}_I(t')\right) \tag{12.24}$$

6. 微扰的绝热近似:

$$\hat{V}_I(t)=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0 t}\hat{V}_S\mathrm{e}^{-s|t|}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0 t},\quad s\to 0^+ \tag{12.25}$$

7. 形式微扰论:

(1) 散射问题:

$$|\psi_I(+\infty)\rangle=\hat{U}(+\infty,-\infty)\,|\psi_I(-\infty)\rangle \tag{12.26}$$

(2) 一般微扰问题:

$$|\psi_I(0,s)\rangle=\hat{U}(0,-\infty)\,|\psi_I(-\infty)\rangle \tag{12.27}$$

12.3 散射矩阵

12.3.1 跃迁矩阵

1. 入射态和出射态:

$$|\psi_{in}\rangle=|\boldsymbol{k}\rangle\,,\quad |\psi_{out}\rangle=|\psi_{in}\rangle+\frac{1}{E_\alpha-\hat{H}_0+\mathrm{i}\epsilon}\hat{V}\,|\psi_{out}\rangle \tag{12.28}$$

2. 跃迁算符:

$$\hat{T}\,|\psi_{in}\rangle=\hat{V}\,|\psi_{out}\rangle \tag{12.29}$$

$$\hat{T}=\hat{V}+\hat{V}\frac{1}{E_\alpha-\hat{H}_0+\mathrm{i}\epsilon}\hat{T} \tag{12.30}$$

$$\hat{T}=\hat{V}+\hat{V}\frac{1}{E-\hat{H}_0+\mathrm{i}\epsilon}\hat{V}+\hat{V}\frac{1}{E-\hat{H}_0+\mathrm{i}\epsilon}\hat{V}\frac{1}{E-\hat{H}_0+\mathrm{i}\epsilon}\hat{V}+\cdots \tag{12.31}$$

3. 散射振幅:

$$f(\theta)=-\frac{m}{2\pi\hbar^2}\int\mathrm{d}\boldsymbol{r}'\mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\psi_{out}(\boldsymbol{r}')=-\frac{m}{2\pi\hbar^2}\langle\boldsymbol{k}'|\hat{V}|\psi_{out}\rangle=-\frac{m}{2\pi\hbar^2}\langle\boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle \tag{12.32}$$

4. 微分散射截面:

$$\sigma_c(\theta)=|f(\theta)|^2=\frac{m^2}{4\pi^2\hbar^4}\left|\langle\boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2 \tag{12.33}$$

12.3.2 散射矩阵

1. 入射态和出射态:

$$|\psi_I(-\infty)\rangle = |\boldsymbol{k}_\alpha\rangle\,, \quad |\psi_I(+\infty)\rangle = \sum_\beta b_\beta\,|\boldsymbol{k}_\beta\rangle \tag{12.34}$$

2. 散射算符:

$$\hat{S} = \hat{U}(+\infty, -\infty), \quad \hat{S}^\dagger\hat{S} = \hat{I} \tag{12.35}$$

3. 散射概率:

$$W_{\beta\alpha} = |b_\beta|^2 = |S_{\beta\alpha}|^2 \tag{12.36}$$

4. 散射算符的形式解:

$$\hat{S} = \hat{I} + \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{+\infty}\mathrm{d}t'\hat{V}_I(t') + \left(\frac{1}{\mathrm{i}\hbar}\right)^2\int_{-\infty}^{+\infty}\mathrm{d}t'\int_{-\infty}^{+\infty}\mathrm{d}t''\hat{V}_I(t')\hat{V}_I(t'') + \cdots \tag{12.37}$$

5. 散射矩阵元的各级近似: $\epsilon = \hbar s$

$$S_{\beta\alpha}^{(0)} = \delta_{\alpha\beta} \tag{12.38}$$

$$S_{\beta\alpha}^{(1)} = -2\pi\mathrm{i}\delta(E_\beta - E_\alpha)\langle\boldsymbol{k}_\beta|\hat{V}|\boldsymbol{k}_\alpha\rangle \tag{12.39}$$

$$S_{\beta\alpha}^{(2)} = -2\pi\mathrm{i}\delta(E_\beta - E_\alpha)\left\langle\boldsymbol{k}_\beta\left|\hat{V}\frac{1}{E_\alpha - \hat{H}_0 + \mathrm{i}\epsilon}\hat{V}\right|\boldsymbol{k}_\alpha\right\rangle \tag{12.40}$$

$$S_{\beta\alpha}^{(n)} = -2\pi\mathrm{i}\delta(E_\beta - E_\alpha)\left\langle\boldsymbol{k}_\beta\left|\hat{V}\frac{1}{E_\alpha - \hat{H}_0 + \mathrm{i}\epsilon}\hat{V}\frac{1}{E_\alpha - \hat{H}_0 + \mathrm{i}\epsilon}\hat{V}\cdots\hat{V}\right|\boldsymbol{k}_\alpha\right\rangle \tag{12.41}$$

6. 散射矩阵元:

$$S_{\beta\alpha} = \delta_{\beta\alpha} - 2\pi\mathrm{i}\delta(E_\beta - E_\alpha)\langle\boldsymbol{k}_\beta|\hat{T}|\boldsymbol{k}_\alpha\rangle \tag{12.42}$$

$$\hat{T} = \hat{V} + \hat{V}\frac{1}{E_\alpha - \hat{H}_0 + \mathrm{i}\epsilon}\hat{V} + \hat{V}\frac{1}{E_\alpha - \hat{H}_0 + \mathrm{i}\epsilon}\hat{V}\frac{1}{E_\alpha - \hat{H}_0 + \mathrm{i}\epsilon}\hat{V} + \cdots \tag{12.43}$$

7. 在壳条件:

$$E_\beta = E_\alpha \tag{12.44}$$

12.4 散射截面

12.4.1 箱归一化波函数的散射截面

1. 箱归一化波函数:

$$\langle\boldsymbol{r}|\boldsymbol{k}\rangle = \frac{1}{\sqrt{V}}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \tag{12.45}$$

2. 微分散射截面:

$$\sigma_c(\theta) = V^2|f(\theta)|^2 = \frac{m^2V^2}{4\pi^2\hbar^4}\left|\langle\boldsymbol{k}_\beta|\hat{T}|\boldsymbol{k}_\alpha\rangle\right|^2 \tag{12.46}$$

12.4.2 球对称波函数的散射截面

1. 球对称波函数:

$$\langle\boldsymbol{r}|E\boldsymbol{n}\rangle = C\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} = \sqrt{\frac{km}{(2\pi)^3\hbar^2}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \tag{12.47}$$

2. 微分散射截面:

$$\sigma_c(\theta) = \frac{1}{|C|^4}|f(\theta)|^2 = \frac{1}{|C|^4}\frac{m^2}{4\pi^2\hbar^4}\left|\langle E_\beta\boldsymbol{n}_\beta|\hat{T}|E_\alpha\boldsymbol{n}_\alpha\rangle\right|^2 = \frac{(2\pi)^4}{k^4}\left|\langle E_\beta\boldsymbol{n}_\beta|\hat{T}|E_\alpha\boldsymbol{n}_\alpha\rangle\right|^2 \tag{12.48}$$

12.5 分波法

1. 散射矩阵对于 $|lm\rangle$ 是对角化的:

$$\langle E_\beta l'm'|\hat{S}|E_\alpha lm\rangle = S_{\beta\alpha}^{(l)}\delta_{l'l}\delta_{m'm} \tag{12.49}$$

2. 弹性散射矩阵元:

$$\begin{aligned}\langle E_\alpha \boldsymbol{n}_\beta|\hat{S}|E_\alpha \boldsymbol{n}_\alpha\rangle &= \sum_{lm}\sum_{l'm'}\langle \boldsymbol{n}_\beta|l'm'\rangle\langle l'm'|\hat{S}_{\alpha\alpha}(E_\alpha)|lm\rangle\langle lm|\boldsymbol{n}_\alpha\rangle \\ &= \sum_{lm}\sum_{l'm'} Y_{l'm'}(\boldsymbol{n}_\beta)S_{\alpha\alpha}^{(l)}(E_\alpha)\delta_{l'l}\delta_{m'm}Y_{lm}^*(\boldsymbol{n}_\alpha) \\ &= \sum_{lm} Y_{lm}(\boldsymbol{n}')Y_{lm}^*(\boldsymbol{n})S_{\alpha\alpha}^{(l)}(E_\alpha) = \sum_l \frac{2l+1}{4\pi}S_{\alpha\alpha}^{(l)}(E_\alpha)P_l(\cos\theta)\end{aligned} \tag{12.50}$$

3. 弹性微分散射截面:

$$\begin{aligned}\sigma_c(\theta) &= \frac{(2\pi)^4}{k^4}\left|\langle E_\beta \boldsymbol{n}_\beta|\hat{T}|E_\alpha \boldsymbol{n}_\alpha\rangle\right|^2 = \frac{(2\pi)^4}{k^4}\left|\left\langle E_\beta \boldsymbol{n}_\beta\left|\frac{\hat{S}-\hat{I}}{2\pi\mathrm{i}}\right|E_\alpha \boldsymbol{n}_\alpha\right\rangle\right|^2 \\ &= \frac{4\pi^2}{k^4}\left|\sum_l \frac{2l+1}{4\pi}S_{\alpha\alpha}^{(l)}(E_\alpha)P_l(\cos\theta) - \sum_{lm}\langle \boldsymbol{n}_\beta|lm\rangle\langle lm|\boldsymbol{n}_\alpha\rangle\right|^2 \\ &= \frac{1}{4k^2}\left|\sum_l (2l+1)\left(1-S_{\alpha\alpha}^{(l)}(E_\alpha)\right)P_l(\cos\theta)\right|^2\end{aligned} \tag{12.51}$$

4. 弹性总散射截面:

$$\sigma_e = \int_0^{2\pi}\int_0^{\pi}\sigma_c(\theta)\sin\theta\mathrm{d}\theta\mathrm{d}\varphi = \frac{\pi}{k^2}\sum_l (2l+1)\left|1-S_{\alpha\alpha}^{(l)}(E_\alpha)\right|^2 = \sum_l \sigma_e^{(l)} \tag{12.52}$$

5. 非弹性总散射截面:

$$\sigma_r = \frac{\pi}{k^2}\sum_l (2l+1)\sum_{\beta\neq\alpha}\left|S_{\beta\alpha}^{(l)}\right|^2 = \frac{\pi}{k^2}\sum_l (2l+1)\left(1-\left|S_{\alpha\alpha}^{(l)}(E_\alpha)\right|^2\right) = \sum_l \sigma_r^{(l)} \tag{12.53}$$

6. 总散射截面:

$$\sigma_{tot} = \sigma_e + \sigma_r = \frac{2\pi}{k^2}\sum_l (2l+1)(1-\mathrm{Re}S_{\alpha\alpha}^{(l)}(E_\alpha)) \tag{12.54}$$

7. 光学定理:

$$\mathrm{Im}f(0) = \frac{1}{2k}\sum_l (2l+1)(1-\mathrm{Re}S_{\alpha\alpha}^{(l)}(E_\alpha)) = \frac{k}{4\pi}\sigma_{tot} \tag{12.55}$$

8. l 分波弹性散射总截面:

$$\sigma_r^{(l)} = 0 \Rightarrow \left|S_{\alpha\alpha}^{(l)}(E_\alpha)\right| = 1 \Rightarrow S_{\alpha\alpha}^{(l)}(E_\alpha) = \mathrm{e}^{\mathrm{i}2\delta_l(E_\alpha)} \tag{12.56}$$

$$\sigma_e^{(l)} = \frac{\pi}{k^2}(2l+1)\left|1-\mathrm{e}^{\mathrm{i}2\delta_l(E_\alpha)}\right|^2 = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l(E_\alpha) \tag{12.57}$$

13 角动量理论

13.1 三维空间转动群及其表示

13.1.1 转动算符

1. 轨道角动量转动算符：

$$\hat{R}(\boldsymbol{n},\theta)=\exp\left(-\mathrm{i}\theta\boldsymbol{n}\cdot\hat{\boldsymbol{L}}\right) \tag{13.1}$$

2. 总角动量转动算符：

$$\hat{R}(\boldsymbol{n},\theta)=\exp\left(-\mathrm{i}\theta\boldsymbol{n}\cdot\hat{\boldsymbol{J}}\right) \tag{13.2}$$

13.1.2 角动量本征态的转动和 D 函数

1. 角动量本征态的转动：

$$\begin{aligned}\hat{R}(\boldsymbol{n},\theta)\left|jm\right\rangle &= \mathrm{e}^{-\mathrm{i}\theta\boldsymbol{n}\cdot\hat{\boldsymbol{J}}}\left|jm\right\rangle=\sum_{j'm'}\left|j'm'\right\rangle\left\langle j'm'\right|\mathrm{e}^{-\mathrm{i}\theta\boldsymbol{n}\cdot\hat{\boldsymbol{J}}}\left|jm\right\rangle\delta_{jj'}\\ &=\sum_{m'}\left|jm'\right\rangle\left\langle jm'\right|\mathrm{e}^{-\mathrm{i}\theta\boldsymbol{n}\cdot\hat{\boldsymbol{J}}}\left|jm\right\rangle=\sum_{m'}D^{j}_{m'm}(\boldsymbol{n},\theta)\left|jm'\right\rangle\end{aligned} \tag{13.3}$$

2. 转动算符分解为三个 Euler 角转动的乘积：

$$\hat{R}(\boldsymbol{n},\theta)=\mathrm{e}^{-\mathrm{i}\gamma\hat{J}_{z''}}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\beta\hat{J}_{y'}}\mathrm{e}^{-\mathrm{i}\alpha\hat{J}_{z}}=\mathrm{e}^{-\mathrm{i}\alpha\hat{J}_{z}}\mathrm{e}^{-\mathrm{i}\beta\hat{J}_{y}}\mathrm{e}^{-\mathrm{i}\gamma\hat{J}_{z}} \tag{13.4}$$

3. D 函数：

$$\begin{aligned}D^{j}_{m'm}(\alpha,\beta,\gamma)&=\left\langle jm'\right|\mathrm{e}^{-\mathrm{i}\theta\boldsymbol{n}\cdot\hat{\boldsymbol{J}}}\left|jm\right\rangle=\left\langle jm'\right|\mathrm{e}^{-\mathrm{i}\alpha\hat{J}_{z}}\mathrm{e}^{-\mathrm{i}\beta\hat{J}_{y}}\mathrm{e}^{-\mathrm{i}\alpha\hat{J}_{z}}\left|jm\right\rangle\\ &=\mathrm{e}^{-\mathrm{i}(m'\alpha+m\gamma)}\left\langle jm'\right|\mathrm{e}^{-\mathrm{i}\beta\hat{J}_{y}}\left|jm\right\rangle=\mathrm{e}^{-\mathrm{i}(m'\alpha+m\gamma)}d^{j}_{m'm}(\beta)\end{aligned} \tag{13.5}$$

4. d 函数的一般表达式：ν 的取值应保证各因子为非负整数

$$\begin{aligned}d^{j}_{m'm}(\beta)&=[(j+m)!(j-m)!(j+m')!(j-m')!]^{1/2}\\ &\quad\times\sum_{\nu}[(-1)^{\nu}(j-m'-\nu)!(j+m-\nu)!(\nu+m'-m)!\nu!]^{-1}\\ &\quad\times\left(\cos\frac{\beta}{2}\right)^{2j+m-m'-2\nu}\left(-\sin\frac{\beta}{2}\right)^{m'-m+2\nu}\end{aligned} \tag{13.6}$$

5. d 函数的性质：

(1)
$$d^{j}_{m'm}(-\beta)=d^{j}_{mm'}(\beta) \tag{13.7}$$

(2)
$$d^{j}_{m'm}(-\beta)=(-1)^{m'-m}d^{j}_{m'm}(\beta) \tag{13.8}$$

(3)
$$d^{j}_{mm'}(\beta)=(-1)^{m'-m}d^{j}_{m'm}(\beta) \tag{13.9}$$

(4)
$$d^{j}_{-m,-m'}(\beta)=d^{j}_{m'm}(\beta) \tag{13.10}$$

(5)
$$d^{j}_{m'm}(\pi)=d^{j}_{m'm}(-\pi)=(-1)^{j-m}\delta_{m',-m} \tag{13.11}$$

(6)
$$d^{j}_{m'm}(\beta+\pi)=(-1)^{j+m'}d^{j}_{-m',m}(\beta) \tag{13.12}$$

6. D 函数的性质：

(1)
$$D^{j}_{m'm}(-\gamma,-\beta,-\alpha)=D^{j*}_{mm'}(\alpha,\beta,\gamma) \tag{13.13}$$

(2)
$$D^{j*}_{mm'}(\alpha,\beta,\gamma)=(-1)^{m-m'}D^{j}_{-m,-m'}(\alpha,\beta,\gamma) \tag{13.14}$$

(3)
$$D^{j}_{m'm}(-\gamma,-\beta,-\alpha)=(-1)^{m-m'}D^{j}_{-m,-m'}(\alpha,\beta,\gamma) \tag{13.15}$$

(4)
$$\sum_{m_1}D^{j*}_{m_1m'}(\alpha,\beta,\gamma)D^{j}_{m_1m}(\alpha,\beta,\gamma)=\delta_{m'm} \tag{13.16}$$

7. D 函数的耦合公式：

$$\langle j_1\mu_1, j_2(\mu-\mu_1)|j\mu\rangle D^j_{\mu m} = \sum_{m_1} \langle j_1 m_1, j_2(m-m_1)|jm\rangle D^{j_1}_{sm_1} D^{j_2}_{\mu-\mu_1,m-m_1} \tag{13.17}$$

8. D 函数的分解公式：

$$\sum_j \langle j_1\mu_1, j_2\mu_2|j(\mu_1+\mu_2)\rangle \langle j_1 m_1, j_2 m_2|j(m_1+m_2)\rangle D^j_{\mu_1+\mu_2,m_1+m_2} = D^{j_1}_{\mu_1 m_1} D^{j_2}_{\mu_2 m_2} \tag{13.18}$$

9. D 函数的积分公式：

$$K = \int_0^{2\pi} \mathrm{d}\alpha \int_0^{\pi} \sin\beta \mathrm{d}\beta \int_0^{2\pi} \mathrm{d}\gamma D^{j_1 *}_{m_1 k_1}(\alpha,\beta,\gamma) D^{j_2}_{m_2 k_2}(\alpha,\beta,\gamma) = \frac{8\pi^2}{2j_1+1}\delta_{j_1 j_2}\delta_{m_1 m_2}\delta_{k_1 k_2} \tag{13.19}$$

13.2 陀螺的转动谱

13.2.1 陀螺角动量的对易关系

1. 粒子固定于实验室系，主轴系从实验室系旋转到特定位置：粒子被动旋转

$$\langle \theta,\varphi|jm\rangle = \langle \theta',\varphi'|\psi'\rangle = \mathrm{e}^{\mathrm{i}\theta \boldsymbol{n}\cdot\hat{\boldsymbol{J}}} \langle \theta',\varphi'|jm\rangle = \sum_k D^{j*}_{mk}(\alpha,\beta,\gamma) \langle \theta',\varphi'|jk\rangle \tag{13.20}$$

2. 粒子固定于实验室系，主轴系绕 $\boldsymbol{n}_1$ 转动无穷小角度：刚体主动旋转，粒子被动旋转

$$\langle \theta,\varphi|jm\rangle = \sum_k \left(\mathrm{e}^{-\mathrm{i}\delta \boldsymbol{n}_1\cdot\hat{\boldsymbol{I}}} D^{j*}_{mk}(\alpha,\beta,\gamma)\right)\left(\mathrm{e}^{\mathrm{i}\delta \boldsymbol{n}_1\cdot\hat{\boldsymbol{J}}} \langle \theta',\varphi'|jk\rangle\right) \tag{13.21}$$

$$\Rightarrow \sum_k \left(\boldsymbol{n}_1\cdot\hat{\boldsymbol{I}}\right) D^{j*}_{mk}(\alpha,\beta,\gamma)\,|jk\rangle = \sum_k D^{j*}_{mk}(\alpha,\beta,\gamma)\left(\boldsymbol{n}_1\cdot\hat{\boldsymbol{J}}\right)|jk\rangle \tag{13.22}$$

3. $\boldsymbol{n}_1$ 向主轴投影：

$$\hat{I}_\zeta D^{j*}_{mk} = k D^{j*}_{mk} \tag{13.23}$$

$$\hat{I}_\xi D^{j*}_{mk} = \frac{1}{2}\left(\sqrt{j(j+1)-k(k-1)}D^{j*}_{m(k-1)} + \sqrt{j(j+1)-k(k+1)}D^{j*}_{m(k+1)}\right) \tag{13.24}$$

$$\hat{I}_\eta D^{j*}_{mk} = \frac{1}{2\mathrm{i}}\left(\sqrt{j(j+1)-k(k-1)}D^{j*}_{m(k-1)} - \sqrt{j(j+1)-k(k+1)}D^{j*}_{m(k+1)}\right) \tag{13.25}$$

4. 主轴系中刚体角动量的对易关系：

$$\left[\hat{I}_\xi, \hat{I}_\eta\right] = -\mathrm{i}\hbar\hat{I}_\zeta, \quad \left[\hat{I}_\eta, \hat{I}_\zeta\right] = -\mathrm{i}\hbar\hat{I}_\xi, \quad \left[\hat{I}_\zeta, \hat{I}_\xi\right] = -\mathrm{i}\hbar\hat{I}_\eta \tag{13.26}$$

5. 粒子固定于主轴系，实验室系绕 $\boldsymbol{n}_2$ 转动无穷小角度：刚体被动旋转，粒子被动旋转

$$\mathrm{e}^{\mathrm{i}\delta \boldsymbol{n}_2\cdot\hat{\boldsymbol{J}}} \langle \theta,\varphi|jm\rangle = \sum_k \mathrm{e}^{-\mathrm{i}\delta \boldsymbol{n}_1\cdot\hat{\boldsymbol{I}}} D^{j*}_{mk}(\alpha,\beta,\gamma) \langle \theta',\varphi'|jk\rangle \tag{13.27}$$

$$\Rightarrow \left(\boldsymbol{n}_2\cdot\hat{\boldsymbol{J}}\right)\langle \theta,\varphi|jm\rangle = \sum_k \left(\boldsymbol{n}_2\cdot\hat{\boldsymbol{I}}\right) D^{j*}_{mk}(\alpha,\beta,\gamma) \langle \theta'\varphi'|jk\rangle \tag{13.28}$$

6. $\boldsymbol{n}_2$ 向实验室系坐标轴投影：

$$\hat{I}_z D^{j*}_{mk} = m D^{l*}_{mk} \tag{13.29}$$

$$\hat{I}_x D^{j*}_{mk} = \frac{1}{2}\left(\sqrt{j(j+1)-m(m+1)}D^{j*}_{(m+1)k} + \sqrt{j(j+1)-m(m-1)}D^{j*}_{(m-1)k}\right) \tag{13.30}$$

$$\hat{I}_y D^{j*}_{mk} = \frac{1}{2\mathrm{i}}\left(\sqrt{j(j+1)-m(m+1)}D^{j*}_{(m+1)k} - \sqrt{j(j+1)-m(m-1)}D^{j*}_{(m-1)k}\right) \tag{13.31}$$

7. 实验室系中刚体角动量的对易关系：

$$\left[\hat{I}_x, \hat{I}_y\right] = \mathrm{i}\hbar\hat{I}_z, \quad \left[\hat{I}_y, \hat{I}_z\right] = \mathrm{i}\hbar\hat{I}_x, \quad \left[\hat{I}_z, \hat{I}_x\right] = \mathrm{i}\hbar\hat{I}_y \tag{13.32}$$

13.2.2 陀螺角动量的量子化

1. 陀螺的 Hamilton 量：

$$\hat{H}=\frac{\hat{I}_\xi^2}{2J_\xi}+\frac{\hat{I}_\eta^2}{2J_\eta}+\frac{\hat{I}_\zeta^2}{2J_\zeta} \tag{13.33}$$

2. 陀螺的角动量：

$$\hat{I}_x=-\mathrm{i}\hbar\left(\sin\alpha\frac{\partial}{\partial\beta}+\cot\beta\cos\alpha\frac{\partial}{\partial\alpha}+\frac{\cos\alpha}{\sin\beta}\frac{\partial}{\partial\gamma}\right) \tag{13.34}$$

$$\hat{I}_y=-\mathrm{i}\hbar\left(\cos\alpha\frac{\partial}{\partial\beta}-\cot\beta\sin\alpha\frac{\partial}{\partial\alpha}-\frac{\sin\alpha}{\sin\beta}\frac{\partial}{\partial\gamma}\right) \tag{13.35}$$

$$\hat{I}_z=-\mathrm{i}\hbar\frac{\partial}{\partial\alpha},\quad \hat{I}_\zeta=-\mathrm{i}\hbar\frac{\partial}{\partial\gamma} \tag{13.36}$$

$$\hat{I}^2=-\hbar^2\left(\frac{1}{\sin\beta}\frac{\partial}{\partial\beta}\left(\sin\beta\frac{\partial}{\partial\beta}\right)+\frac{1}{\sin^2\beta}\left(\frac{\partial^2}{\partial\alpha^2}+2\cos\beta\frac{\partial^2}{\partial\alpha\partial\gamma}+\frac{\partial^2}{\partial\gamma^2}\right)\right) \tag{13.37}$$

13.2.3 对称陀螺的转动谱

1. 对称陀螺的 Hamilton 量：

$$\hat{H}=\frac{1}{2J}\left(\hat{I}_\xi^2+\hat{I}_\eta^2\right)+\frac{1}{2J_\zeta}\hat{I}_\zeta^2=\frac{1}{2J}\hat{I}^2+\left(\frac{1}{2J_\zeta}-\frac{1}{2J}\right)\hat{I}_\zeta^2 \tag{13.38}$$

2. $\hat{I}^2$，$\hat{I}_z$，$\hat{I}_\zeta$ 的共同本征态：

$$|IKM\rangle=\sqrt{\frac{2I+1}{8\pi^2}}D^{I*}_{MK}(\alpha,\beta,\gamma) \tag{13.39}$$

3. 对称陀螺的转动动能：

$$E_{IK}=\frac{\hbar^2}{2J}I(I+1)+\frac{\hbar^2K^2}{2}\left(\frac{1}{J_\zeta}-\frac{1}{J}\right) \tag{13.40}$$

4. 在适当相位规定下：

$$\hat{R}_\xi(\pi)\left|IMK\right\rangle=(-1)^I\left|IM(-K)\right\rangle \tag{13.41}$$

5. $\hat{I}^2$，$\hat{I}_z$，$\hat{I}_\zeta^2$，$\hat{R}_\xi(\pi)$ 的共同本征态：$K>0$

$$|IMK,+1\rangle=\frac{1}{\sqrt{2}}\left(\left|IMK\right\rangle+(-1)^I\left|IM(-K)\right\rangle\right) \tag{13.42}$$

$$|IMK,-1\rangle=\frac{1}{\sqrt{2}}\left(\left|IMK\right\rangle-(-1)^I\left|IM(-K)\right\rangle\right) \tag{13.43}$$

6. 旋称：

$$\hat{R}_\xi(\pi)\left|IMKr\right\rangle=r\left|IMKr\right\rangle,\quad r=\pm1 \tag{13.44}$$

13.2.4 非对称陀螺的转动谱

1. 非对称陀螺的 Hamilton 量：

$$\hat{H}=\alpha_1\hat{I}_\xi^2+\alpha_2\hat{I}_\eta^2+\alpha_3\hat{I}_\zeta^2=\left[\frac{1}{2}(\alpha_1+\alpha_2)\left(\hat{I}^2-\hat{I}_\zeta^2\right)+\alpha_3\hat{I}_\zeta^2\right]+\frac{1}{4}(\alpha_1-\alpha_2)(\hat{I}_+^2+\hat{I}_-^2) \tag{13.45}$$

2. $\hat{H}$ 的对角元：

$$\langle IMK|\hat{H}|IMK\rangle=\frac{1}{2}(\alpha_1+\alpha_2)\left[I(I+1)-K^2\right]+\alpha_3K^2 \tag{13.46}$$

3. $\hat{H}$ 的非对角元：

$$\langle IM(K+2)|\hat{H}|IMK\rangle=\frac{1}{4}(\alpha_1-\alpha_2)\sqrt{I(I+1-K(K+1))}\sqrt{I(I+1)-(K+1)(K+2)} \tag{13.47}$$

$$\langle IM(K-2)|\hat{H}|IMK\rangle=\frac{1}{4}(\alpha_1-\alpha_2)\sqrt{I(I+1-K(K-1))}\sqrt{I(I+1)-(K-1)(K-2)} \tag{13.48}$$

13.3 不可约张量算符

1. 不可约张量算符族：

$$\hat{R}\hat{T}^j_m\hat{R}^{-1} = \sum_{m'=-j}^{j} D^j_{m'm}(\hat{R})\hat{T}^j_{m'} \tag{13.49}$$

2. 不可约张量算符族的等价定义：

$$\left[\hat{J}_z, \hat{T}^j_m\right] = \sum_{m'} \langle jm'|\hat{J}_z|jm\rangle \hat{T}^j_{m'} = m\hat{T}^j_m \tag{13.50}$$

$$\left[\hat{J}_+, \hat{T}^j_m\right] = \sum_{m'} \langle jm'|\hat{J}_+|jm\rangle \hat{T}^j_{m'} = \sqrt{j(j+1)-m(m+1)}\hat{T}^j_{m+1} \tag{13.51}$$

$$\left[\hat{J}_-, \hat{T}^j_m\right] = \sum_{m'} \langle jm'|\hat{J}_-|jm\rangle \hat{T}^j_{m'} = \sqrt{j(j+1)-m(m-1)}\hat{T}^j_{m-1} \tag{13.52}$$

3. 一阶不可约张量算符族：

$$\hat{T}^1_{-1} = \frac{1}{\sqrt{2}}\left(\hat{T}_x - \mathrm{i}\hat{T}_y\right) = \frac{1}{\sqrt{2}}\hat{T}_-, \quad \hat{T}^1_0 = \hat{T}_z, \quad \hat{T}^1_1 = -\frac{1}{\sqrt{2}}\left(\hat{T}_x + \mathrm{i}\hat{T}_y\right) = -\frac{1}{\sqrt{2}}\hat{T}_+ \tag{13.53}$$

4. 两个不可约张量算符族的张量积：

$$\hat{T}^j_m = \left[\hat{T}^{j_1} \times \hat{T}^{j_2}\right]^j_m = \sum_{m_1=-j_1}^{j_1} \langle j_1m_1, j_2(m-m_1)|jm\rangle \hat{T}^{j_1}_{m_1}\hat{T}^{j_2}_{m-m_1} \tag{13.54}$$

5. 同阶不可约张量算符族的内积：

$$\left\langle \hat{T}^j, \hat{S}^j \right\rangle = \sum_{m=-j}^{j} (-1)^{-m}\hat{T}^j_m\hat{T}^j_{-m} \tag{13.55}$$

$$\left[\hat{T}^j, \hat{S}^j\right]^0_0 = \sum_m \langle jm, j(-m)|00\rangle \hat{T}^j_m\hat{T}^j_{-m} = \sum_m \frac{(-1)^{j-m}}{\sqrt{2j+1}}\hat{T}^j_m\hat{T}^j_{-m} = \frac{(-1)^j}{\sqrt{2j+1}}\left\langle \hat{T}^j, \hat{S}^j \right\rangle \tag{13.56}$$

6. 不可约张量算符和角动量本征态的耦合：是 $(\hat{J}^2, \hat{J}_z)$ 的本征态

$$|\widetilde{\alpha}jm\rangle = \sum_q \langle j_1q, j_2(m-q)|jm\rangle \hat{T}^{j_1}_q |\alpha j_2(m-q)\rangle \tag{13.57}$$

13.4 Wigner-Eckart 定理

1. Wigner-Eckart 定理：

$$\langle \alpha'j'm'|\hat{T}^k_q|\widetilde{\alpha}jm\rangle = \frac{1}{\sqrt{2j'+1}} \langle kq, jm|j'm'\rangle \langle \alpha'j'\|\hat{T}^k\|\widetilde{\alpha}j\rangle \tag{13.58}$$

2. 约化矩阵元：与磁量子数无关

$$\langle \alpha'j'\|\hat{T}^k\|\widetilde{\alpha}j\rangle = \frac{1}{\sqrt{2j'+1}} \sum_\mu \langle \alpha'j'\mu|\widetilde{\alpha}j'\mu\rangle \tag{13.59}$$

3. 一阶不可约张量的投影定理：

$$\delta_{J'J}\delta_{M'(M+\mu)} \langle J'M'|\hat{T}_\mu|JM\rangle = \frac{\langle JM'|\hat{J}_\mu \langle \hat{J}, \hat{T}\rangle |JM\rangle}{J(J+1)} \tag{13.60}$$

4. 一阶不可约张量的因式分解定理：

$$\langle JM'|\hat{J}_\mu \langle \hat{J}, \hat{T}\rangle |JM\rangle = \frac{1}{\sqrt{2J+1}} \langle JM'|\hat{J}_\mu|JM\rangle \langle J\| \langle \hat{J}, \hat{T}\rangle \|J\rangle \tag{13.61}$$

5. 一阶不可约张量矩阵元的一般公式：

$$\delta_{J'J}\delta_{M'(M+\mu)} \langle J'M'|\hat{T}_\mu|JM\rangle = \frac{\langle J\| \langle \hat{J}, \hat{T}\rangle \|J\rangle}{J(J+1)\sqrt{2J+1}} \langle JM'|\hat{J}_\mu|JM\rangle \tag{13.62}$$

14 量子体系的对称性

14.1 对称性与守恒量

1. 对称变换：

$$\boldsymbol{r}' = \hat{\rho}(\boldsymbol{r}), \quad \psi' = \hat{Q}\psi \tag{14.1}$$

$$\psi'(\boldsymbol{r}') = \psi(\boldsymbol{r}), \quad \hat{H}(\boldsymbol{r}') = \hat{H}(\boldsymbol{r}) \tag{14.2}$$

$$[\hat{Q}, \hat{H}] = 0 \tag{14.3}$$

2. Wigner 定理：对称变换只能是幺正变换或反幺正变换

(1) 幺正变换：$\langle \hat{Q}\psi | \hat{Q}\phi \rangle = \langle \psi | \phi \rangle \Rightarrow \hat{Q}(a\,|\phi_1\rangle + b\,|\phi_2\rangle) = a\hat{Q}\,|\phi_1\rangle + b\hat{Q}\,|\phi_2\rangle$ (14.4)

(2) 反幺正变换：$\langle \hat{Q}\psi | \hat{Q}\phi \rangle = \langle \psi | \phi \rangle^* \Rightarrow \hat{Q}(a\,|\phi_1\rangle + b\,|\phi_2\rangle) = a^*\hat{Q}\,|\phi_1\rangle + b^*\hat{Q}\,|\phi_2\rangle$ (14.5)

3. 平移算符：

$$\hat{D}(\boldsymbol{r}) = \exp\left(-\frac{\mathrm{i}}{\hbar}\boldsymbol{r}\cdot\hat{\boldsymbol{p}}\right) \tag{14.6}$$

4. 空间平移对称性：

$$\boldsymbol{r}' = \boldsymbol{r} + \delta\boldsymbol{r}, \quad \psi' = \hat{D}\psi \tag{14.7}$$

$$\psi'(\boldsymbol{r}') = \psi(\boldsymbol{r}) \Rightarrow \hat{D}\psi(\boldsymbol{r}) = \psi(\boldsymbol{r} - \delta\boldsymbol{r}) = \left[\hat{I} - \delta\boldsymbol{r}\nabla + \mathcal{O}(\delta\boldsymbol{r}^2)\right]\psi(\boldsymbol{r}) \tag{14.8}$$

$$\left[\hat{D}, \hat{H}\right] = 0 \Rightarrow \left[-\delta\boldsymbol{r}\nabla + \mathcal{O}(\delta\boldsymbol{r}^2), \hat{H}\right] = 0 \Rightarrow \left[-\nabla, \hat{H}\right] = 0 \Rightarrow \left[\hat{\boldsymbol{p}}, \hat{H}\right] = 0 \tag{14.9}$$

5. 转动算符：

$$\hat{R}(\boldsymbol{n}, \theta) = \exp\left(-\frac{\mathrm{i}}{\hbar}\theta\boldsymbol{n}\cdot\hat{\boldsymbol{L}}\right) \tag{14.10}$$

6. 空间转动对称性：

$$\boldsymbol{r}' = \boldsymbol{r} + \delta\theta\boldsymbol{n}\times\boldsymbol{r}, \quad |\psi'\rangle = \hat{R}\,|\psi\rangle \tag{14.11}$$

$$\psi'(\boldsymbol{r}') = \psi(\boldsymbol{r}) \Rightarrow \hat{R}\psi(\boldsymbol{r}) = \psi(\boldsymbol{r} - \delta\theta\boldsymbol{n}\times\boldsymbol{r}) = \left[\hat{I} - (\delta\theta\boldsymbol{n}\times\boldsymbol{r})\cdot\nabla + \mathcal{O}(\delta\theta^2)\right]\psi(\boldsymbol{r}) \tag{14.12}$$

$$\left[\hat{R}, \hat{H}\right] = 0 \Rightarrow \left[-(\delta\theta\boldsymbol{n}\times\boldsymbol{r})\cdot\nabla + \mathcal{O}(\delta\theta^2)\right] = 0 \Rightarrow \left[-\boldsymbol{n}\cdot(\boldsymbol{r}\times\nabla), \hat{H}\right] = 0 \Rightarrow \left[\boldsymbol{n}\cdot\hat{\boldsymbol{L}}, \hat{H}\right] = 0 \tag{14.13}$$

14.2 对称性与量子态的分类

1. 对称变换后的本征态：

$$|\widetilde{\psi^i_\nu}\rangle = \hat{Q}\,|\psi^i_\nu\rangle = \sum_\mu D^i_{\mu\nu}(\hat{Q})\,|\psi^i_\mu\rangle \tag{14.14}$$

2. $D^i(\hat{Q})$ 构成对称群 G 的一个 f_i 维幺正线性表示：

(1) 群表示：

$$\hat{Q}_1\hat{Q}_2\,|\psi^i_\nu\rangle = \sum_\mu D_{\mu\nu}(\hat{Q}_1\hat{Q}_2)\,|\psi^i_\mu\rangle \tag{14.15}$$

$$\hat{Q}_1\hat{Q}_2\,|\psi^i_\nu\rangle = \sum_{\mu_1} D^i_{\mu_1\nu}(\hat{Q}_2)(\hat{Q}_1\,|\psi^i_{\mu_1}\rangle) = \sum_\mu\sum_{\mu_1} D^i_{\mu\mu_1}(\hat{Q})D^i_{\mu_1\nu}(\hat{Q}_2)\,|\psi^i_\mu\rangle \tag{14.16}$$

$$\Rightarrow D^i_{\mu\nu}(\hat{Q}_1\hat{Q}_2) = \sum_{\mu_1} D^i_{\mu\mu_1}(\hat{Q})D^i_{\mu_1\nu}(\hat{Q}_2) = \left[D^i(\hat{Q}_1)D^i(\hat{Q}_2)\right]_{\mu\nu} \tag{14.17}$$

(2) 幺正性：

$$\langle \psi^i_\nu | \psi^i_\mu \rangle = \langle \hat{Q}\psi^i_\nu | \hat{Q}\psi^i_\mu \rangle = \delta_{\nu\mu} \tag{14.18}$$

$$\langle \hat{Q}\psi^i_\nu | \hat{Q}\psi^i_\mu \rangle = \sum_\alpha\sum_\beta D^{i*}_{\beta\nu}(\hat{Q})D^i_{\alpha\mu}(\hat{Q})\,\langle \psi^i_\beta | \psi^i_\alpha \rangle = \sum_\alpha D^{i*}_{\alpha\nu}(\hat{Q})D^i_{\alpha\mu}(\hat{Q}) \tag{14.19}$$

$$\Rightarrow \sum_\alpha D^{i\dagger}_{\nu\alpha}(\hat{Q})D^i_{\alpha\mu} = \sum_\alpha D^{i*}_{\alpha\nu}(\hat{Q})D_{\alpha\mu}(\hat{Q}) = \delta_{\nu\mu} \tag{14.20}$$

14.3 对称性与选择定则

1. 不等价不可约对称群表示波函数的内积：

$$\langle\psi_\nu^i|\phi_\mu^i\rangle = \delta_{ij}\delta_{\nu\mu}C_i \tag{14.21}$$

2. 标量算符的矩阵元：

$$\langle\psi_\nu^i|\hat{F}\phi_\mu^i\rangle = \delta_{ij}\delta_{\mu\nu}F_i \tag{14.22}$$

3. 不可约张量算符的矩阵元：若 $D^k \otimes D_j$ 不含表示 D^i

$$\langle\psi_\nu^i|\hat{T}_q^k\psi_\mu^i\rangle = 0 \tag{14.23}$$

4. 实际问题中算符可以写成若干不可约张量算符之和：

$$\hat{O} = \sum_{kq} C_{kq}\hat{O}_q^k \tag{14.24}$$

14.4 对称性与简并微扰论

1. 微扰下体系的 Hamilton 量：

$$\hat{H} = \hat{H}_0 + \hat{H}' \tag{14.25}$$

2. 微扰下 $F|_G$ 按照 $G \subset G_0$ 的不可约表示 L 分解：

$$F|_G = \bigoplus_k a_k L_k \tag{14.26}$$

3. 能级劈裂条数：

$$N = \sum_k a_k \tag{14.27}$$

4. 能级的剩余简并度：

$$f_k = \dim(L_k) \tag{14.28}$$

15 时间反演对称性

15.1 时间反演态

1. 时间反演的经典力学对应：

$$\langle\psi|\hat{r}|\psi\rangle = \langle\psi'|\hat{r}|\psi'\rangle, \quad \langle\psi|\hat{p}|\psi\rangle = -\langle\psi'|\hat{p}|\psi'\rangle, \quad \langle\psi|\hat{L}|\psi\rangle = -\langle\psi'|\hat{L}|\psi'\rangle \tag{15.1}$$

2. 时间反演不变性：

$$\hat{H}^* = \hat{U}^\dagger \hat{H} \hat{U} \Rightarrow [\hat{T}, \hat{H}] = 0 \tag{15.2}$$

3. 复共轭算符：

$$\hat{K}\,|\psi\rangle = |\psi\rangle^* \tag{15.3}$$

4. 时间反演算符：

$$\hat{T} = \hat{U}\hat{K} \tag{15.4}$$

15.2 $\hat{T}^2$ 本征值与统计性

1. $\hat{T}^2$ 的本征值：

$$\hat{T}^2 = c\hat{I}, \quad c = \pm 1 \tag{15.5}$$

2. 无自旋粒子：

$$\hat{T} = \hat{K}, \quad \hat{T}^2 = \hat{I}, \quad c = 1 \tag{15.6}$$

3. 自旋 1/2 粒子：

$$\hat{T} = -\mathrm{i}\sigma_y\hat{K}, \quad \hat{T}^2 = -\hat{I}, \quad c = -1 \tag{15.7}$$

4. Bose 子组成的多体系 $c = 1$，N 个 Fermi 子组成的多体系 $c = (-1)^N$
5. 角动量为 J 的体系：

$$\hat{T}\,|JM\rangle = (-1)^{J-M}\,|J(-M)\rangle \tag{15.8}$$

$$\hat{T}^2\,|JM\rangle = (-1)^{2J}\,|JM\rangle \tag{15.9}$$

15.3 Kramers 简并

1. 奇数个 Fermi 子体系：$|\hat{T}\psi\rangle$ 和 $|\psi\rangle$ 正交

$$\langle\hat{T}\psi|\psi\rangle = -\langle\hat{T}\psi|\psi\rangle = 0 \tag{15.10}$$

2. 时间反演不变性：$|\hat{T}\psi\rangle$ 和 $|\psi\rangle$ 的能量本征值相同

$$[\hat{T}, \hat{H}] = 0 \tag{15.11}$$

3. Kramers 简并：这一能级至少是二重简并的

15.4 力学量的分类

1. 力学量的分类：

$$\hat{T}\hat{F}\hat{T}^{-1} = \eta\hat{F}, \quad \eta = \pm 1 \tag{15.12}$$

2. 涉及时间反演态的矩阵元：

$$\langle\widetilde{\mu}|\hat{F}|\widetilde{\nu}\rangle = \eta\,\langle\mu|\hat{F}|\nu\rangle^* \tag{15.13}$$

$$\langle\mu|\hat{F}|\widetilde{\nu}\rangle = c\eta\,\langle\widetilde{\mu}|\hat{F}|\nu\rangle^* \tag{15.14}$$

16 混合系综

16.1 量子态的描述

1. 投影算符：

$$\hat{P}_n = |n\rangle \langle n| \tag{16.1}$$

$$\hat{P}_n^\dagger = \hat{P}_n, \quad \hat{P}_n^2 = \hat{P}_n, \quad \hat{P}_n \hat{P}_{n'} = \hat{P}_n \delta_{nn'} \tag{16.2}$$

2. 算符的谱表示：

$$\hat{F} = \hat{F} \sum_n |n\rangle \langle n| = \sum_n F_n |n\rangle \langle n| = \sum_n F_n \hat{P}_n \tag{16.3}$$

3. 量子态在本征态展开：

$$|\psi\rangle = \sum_n |n\rangle \langle n|\psi\rangle = \sum_n \hat{P}_n |\psi\rangle = \sum_n C_n |n\rangle \tag{16.4}$$

4. 量子态随时间的演化：

$$|\psi(t)\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t} |\psi(0)\rangle = \sum_n C_n \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n t} |n\rangle \tag{16.5}$$

16.2 密度矩阵

16.2.1 纯态的密度矩阵

1. 纯态密度算符：

$$\hat{\rho}(t) = |\psi(t)\rangle \langle \psi(t)| \tag{16.6}$$

$$\hat{\rho}(t) = \sum_n \sum_{n'} |n\rangle \langle n|\psi(t)\rangle \langle \psi(t)|n'\rangle \langle n'| = \sum_n \sum_{n'} \rho_{nn'}(t) |n\rangle \langle n'| \tag{16.7}$$

$$\hat{\rho}^\dagger(t) = \hat{\rho}(t), \quad \hat{\rho}^2(t) = \hat{\rho}(t) \tag{16.8}$$

2. 纯态密度矩阵：

$$\rho_{nn'}(t) = \langle n|\psi(t)\rangle \langle \psi(t)|n'\rangle = C_n(t) C_{n'}^*(t) \tag{16.9}$$

$$\mathrm{tr}(\boldsymbol{\rho}) = \sum_n |C_n(t)|^2 = 1 \tag{16.10}$$

3. 力学量的平均值：

$$\langle O\rangle = \mathrm{tr}(\boldsymbol{\rho}\boldsymbol{O}) = \mathrm{tr}(\boldsymbol{O}\boldsymbol{\rho}) \tag{16.11}$$

4. 密度算符随时间的演化：

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}(t) = \frac{1}{\mathrm{i}\hbar}\left[\hat{H}, \hat{\rho}(t)\right] \tag{16.12}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{nn'}(t) = \frac{1}{\mathrm{i}\hbar}(E_n - E_{n'})\rho_{nn'}(t) \Rightarrow \rho_{nn'}(t) = \rho_{nn'}(0)\mathrm{e}^{-\mathrm{i}\omega_{nn'}t} \tag{16.13}$$

5. 坐标表象下的密度矩阵元：

$$\rho_{rr'} = \langle \boldsymbol{r}|\psi\rangle \langle \psi|\boldsymbol{r}'\rangle = \psi^*(\boldsymbol{r}')\psi(\boldsymbol{r}) \tag{16.14}$$

$$W(\boldsymbol{r}) = \rho_{rr} = \psi^*(\boldsymbol{r})\psi(\boldsymbol{r}) \tag{16.15}$$

6. 动量表象下的密度矩阵元：

$$\rho_{pp'} = \langle \boldsymbol{p}|\psi\rangle \langle \psi|\boldsymbol{p}'\rangle = \phi^*(\boldsymbol{p}')\phi(\boldsymbol{p}) \tag{16.16}$$

$$W(\boldsymbol{p}) = \rho_{pp} = \phi^*(\boldsymbol{p})\phi(\boldsymbol{p}) \tag{16.17}$$

16.2.2　混合态的密度矩阵

1. 混合态密度算符：

$$\hat{\rho}(t)=\sum_k p_k\,|\psi_k(t)\rangle\,\langle\psi_k(t)|=\sum_k p_k\hat{\rho}_k(t) \tag{16.18}$$

$$\hat{\rho}^\dagger(t)=\hat{\rho}(t),\quad \hat{\rho}^2(t)\leqslant\hat{\rho}(t) \tag{16.19}$$

2. 混合态密度矩阵：

$$\rho_{nn'}(t)=\sum_k p_k\,\langle n|\psi_k(t)\rangle\,\langle\psi_k(t)|n'\rangle=\sum_k p_k C_n^k(t)C_{n'}^{k*}(t) \tag{16.20}$$

$$\mathrm{tr}(\boldsymbol{\rho})=\sum_k p_k\mathrm{tr}(\boldsymbol{\rho}_k)=\sum p_k=1 \tag{16.21}$$

3. 纯度和混乱度：

$$P(\hat{\rho})=\mathrm{tr}(\hat{\rho}^2),\quad M(\hat{\rho})=1-P(\hat{\rho}) \tag{16.22}$$

4. 力学量的平均值：

$$\langle O\rangle=\mathrm{tr}(\boldsymbol{\rho}\boldsymbol{O})=\mathrm{tr}(\boldsymbol{O}\boldsymbol{\rho}) \tag{16.23}$$

5. 密度算符随时间的演化：

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}(t)=\frac{1}{\mathrm{i}\hbar}\left[\hat{H},\hat{\rho}(t)\right] \tag{16.24}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{nn'}(t)=\frac{1}{\mathrm{i}\hbar}(E_n-E_{n'})\rho_{nn'}(t)\Rightarrow\rho_{nn'}(t)=\rho_{nn'}(0)\mathrm{e}^{-\mathrm{i}\omega_{nn'}t} \tag{16.25}$$

16.3　复合体系

16.3.1　约化密度矩阵

1. 复合体系的线性展开：

$$|\psi\rangle_{AB}=\sum_{i\mu}a_{i\mu}\,|i\rangle_A\,|\mu\rangle_B \tag{16.26}$$

2. 复合体系的密度算符：

$$\hat{\rho}_{AB}=|\psi\rangle_{AB\,AB}\,\langle\psi|=\sum_{i\mu j\nu}a_{j\nu}^*a_{i\mu}\,|i\rangle_A\,|\mu\rangle_{B\,A}\,\langle j|_B\,\langle\nu| \tag{16.27}$$

3. A 的可观测量的平均值：

$$\langle O_A\rangle=\mathrm{tr}_{AB}(\boldsymbol{\rho}_{AB}\boldsymbol{O})=\mathrm{tr}_A(\boldsymbol{\rho}_A\boldsymbol{O}_A) \tag{16.28}$$

4. A 的约化密度算符：

$$\hat{\rho}_A=\sum_{ij\mu}a_{i\mu}a_{j\mu}^*\,|i\rangle_{A\,A}\,\langle j|=\mathrm{tr}_B(\hat{\rho}_{AB}) \tag{16.29}$$

$$\hat{\rho}_A^\dagger=\hat{\rho}_A,\quad \mathrm{tr}(\hat{\rho}_A)=1,\quad \rho_A\geqslant 0 \tag{16.30}$$

$$\mathrm{tr}_B(|a_1b_1\rangle\,\langle a_2b_2|)=\mathrm{tr}_B(|a_1\rangle\,\langle a_2|\otimes|b_1\rangle\,\langle b_2|)=|a_1\rangle\,\langle a_2|\cdot\langle b_2|b_1\rangle \tag{16.31}$$

16.3.2　Schmidt 分解和纯化

1. Schmidt 分解定理：纯态

$$|\psi\rangle_{AB}=\sum_i\lambda_i\,|i\rangle_A\,|i\rangle_B\,,\quad \sum_i\lambda_i^2=1 \tag{16.32}$$

2. 约化密度算符：

$$\hat{\rho}_A=\sum_i\lambda_i^2\,|i\rangle_{A\,A}\,\langle i|\,,\quad \hat{\rho}_B=\sum_i\lambda_i^2\,|i\rangle_{B\,B}\,\langle i| \tag{16.33}$$

3. 纯化：混合态 $\rho_A\to$ 纯态 $|AR\rangle$

$$|AR\rangle\equiv\sum_i\lambda_i\,|i\rangle_A\,|i\rangle_R\Rightarrow\hat{\rho}_A=\mathrm{tr}_R(|AR\rangle\,\langle AR|) \tag{16.34}$$

16.4 纠缠态

16.4.1 双电子纠缠态

1. 双电子非耦合表象本征态：$(\hat{S}_{1z}, \hat{S}_{2z})$

$$|\uparrow\uparrow\rangle_{12}\,,\quad |\uparrow\downarrow\rangle_{12}\,,\quad |\downarrow\uparrow\rangle_{12}\,,\quad |\downarrow\downarrow\rangle_{12} \tag{16.35}$$

2. 双电子耦合表象本征态：$(\hat{S}^2, \hat{S}_z)$

$$|11\rangle = |\uparrow\uparrow\rangle_{12}\,,\quad |1-1\rangle = |\downarrow\downarrow\rangle_{12}\,,\quad |10\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle_{12} + |\downarrow\uparrow\rangle_{12}\right),\quad |00\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle_{12} - |\downarrow\uparrow\rangle_{12}\right) \tag{16.36}$$

3. Bell 基：$(\hat{\sigma}_{1x}\hat{\sigma}_{2x})(\hat{\sigma}_{1y}\hat{\sigma}_{2y})(\hat{\sigma}_{1z}\hat{\sigma}_{2z}) = -1$

$$|\psi^{\pm}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle_{12} \pm |\downarrow\uparrow\rangle_{12}\right),\quad |\varphi^{\pm}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle_{12} \pm |\downarrow\downarrow\rangle_{12}\right) \tag{16.37}$$

$$\boldsymbol{\rho}_1 = \boldsymbol{\rho}_2 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\quad E = 1 \tag{16.38}$$

16.4.2 双光子纠缠态

1. 单光子偏振态分量：

$$\begin{pmatrix} |x(\theta)\rangle \\ |y(\theta)\rangle \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} |x\rangle \\ |y\rangle \end{pmatrix} = \hat{R}_z(\theta)\begin{pmatrix} |x\rangle \\ |y\rangle \end{pmatrix} \tag{16.39}$$

$$|R\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix},\quad |L\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathrm{i} \\ 1 \end{pmatrix} \tag{16.40}$$

$$\hat{S}_z\,|R\rangle = |R\rangle\,,\quad \hat{S}_z\,|L\rangle = -\,|L\rangle \tag{16.41}$$

2. 单光子偏振态：右旋和左旋光子态

$$|+\rangle = \frac{1}{\sqrt{2}}(|x\rangle + \mathrm{i}\,|y\rangle),\quad |-\rangle = \frac{1}{\sqrt{2}}(|x\rangle - \mathrm{i}\,|y\rangle) \tag{16.42}$$

$$\hat{S}_y\,|+\rangle = |+\rangle\,,\quad \hat{S}_y\,|-\rangle = -\,|-\rangle \tag{16.43}$$

3. 双光子非耦合表象本征态：

$$|+-\rangle_{12}\,,\quad |-+\rangle_{12} \tag{16.44}$$

4. 双光子耦合表象本征态：

$$|\psi^{\pm}\rangle_{12} = -\frac{1}{\sqrt{2}}(|+-\rangle_{12} \pm |-+\rangle_{12}) \tag{16.45}$$

$$\tau(\theta) = |x(\theta)\rangle\,\langle x(\theta)| - |y(\theta)\rangle\,\langle y(\theta)| \tag{16.46}$$

$$\tau(\theta)\,|x(\theta)\rangle = +\,|x(\theta)\rangle\,,\quad \tau(\theta)\,|y(\theta)\rangle = -\,|y(\theta)\rangle \tag{16.47}$$

16.4.3 GHZ 态

1. 3Q-bit 非耦合表象本征态：

$$|\uparrow\uparrow\uparrow\rangle,\quad |\uparrow\downarrow\uparrow\rangle,\quad |\uparrow\uparrow\downarrow\rangle,\quad |\uparrow\downarrow\downarrow\rangle,\quad |\downarrow\uparrow\downarrow\rangle,\quad |\downarrow\downarrow\uparrow\rangle,\quad |\downarrow\downarrow\downarrow\rangle \tag{16.48}$$

2. 3Q-bit GHZ 态：$(\hat{\sigma}_{1x}\hat{\sigma}_{2y}\hat{\sigma}_{3y})(\hat{\sigma}_{1y}\hat{\sigma}_{2x}\hat{\sigma}_{3y})(\hat{\sigma}_{1y}\hat{\sigma}_{2y}\hat{\sigma}_{3x})(\hat{\sigma}_{1x}\hat{\sigma}_{2x}\hat{\sigma}_{3x}) = -1$

$$\frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\rangle \pm |\downarrow\downarrow\downarrow\rangle),\quad \frac{1}{\sqrt{2}}(|\uparrow\downarrow\uparrow\rangle \pm |\downarrow\uparrow\downarrow\rangle),\quad \frac{1}{\sqrt{2}}(|\uparrow\uparrow\downarrow\rangle \pm |\downarrow\downarrow\uparrow\rangle),\quad \frac{1}{\sqrt{2}}(|\uparrow\downarrow\downarrow\rangle \pm |\downarrow\uparrow\uparrow\rangle) \tag{16.49}$$

16.5 纠缠度量

1. 两体纯态的纠缠度：

$$E(|\psi\rangle_{AB}) = S(\boldsymbol{\rho}_A) = S(\boldsymbol{\rho}_B) = -\sum_n \lambda_n \log_2 \lambda_n \tag{16.50}$$

2. 一般混合态的纠缠度：

$$E(\boldsymbol{\rho}) = \min \sum_k p_k E(|\psi_k\rangle) \tag{16.51}$$

3. 两体二维混合态的 Concurrence：

$$C(\boldsymbol{\rho}_{AB}) = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\} \tag{16.52}$$

4. 两体高维混合态的 Negativity：

$$N(\boldsymbol{\rho}_{AB}) = \sum_i |\mu_i| = \frac{|\boldsymbol{\rho}_{AB}^{T_A}| - 1}{2} \tag{16.53}$$

5. 两体高维混合态的 Logarithmic Negativity：

$$LN(\boldsymbol{\rho}_{AB}) = \log_2 |\boldsymbol{\rho}_{AB}^{T_A}| \tag{16.54}$$

6. 两体连续混合态的 Logarithmic Negativity：利用协方差矩阵

$$LN(\boldsymbol{\rho}_{AB}) = \max\{-\log_2 2\widetilde{\nu}_-, 0\} \tag{16.55}$$

$$\widetilde{\nu}_-^2 = \frac{1}{2}\left(\widetilde{A}(\boldsymbol{\sigma}) - \sqrt{\widetilde{A}^2(\boldsymbol{\sigma}) - 4|\boldsymbol{\sigma}|}\right), \quad \widetilde{A}(\boldsymbol{\sigma}) = |\boldsymbol{A}| + |\boldsymbol{B}| - 2|\boldsymbol{C}| \tag{16.56}$$

$$\boldsymbol{\sigma} = \begin{pmatrix} \boldsymbol{A} & \boldsymbol{C} \\ \boldsymbol{C}^T & \boldsymbol{B} \end{pmatrix}, \quad \sigma_{ij} = \langle\{\hat{R}_i, \hat{R}_j\}\rangle - 2\langle\hat{R}_i\rangle\langle\hat{R}_j\rangle, \quad \hat{R} = (\hat{x}_1, \hat{p}_1, \hat{x}_2, \hat{p}_2)^T \tag{16.57}$$

$$\hat{x}_1 = \frac{1}{\sqrt{2}}(\hat{a}_1 + \hat{a}_1^\dagger), \quad \hat{p}_1 = \frac{1}{\mathrm{i}\sqrt{2}}(\hat{a}_1 - \hat{a}_1^\dagger), \quad \hat{x}_2 = \frac{1}{\sqrt{2}}(\hat{a}_2 + \hat{a}_2^\dagger), \quad \hat{p}_2 = \frac{1}{\mathrm{i}\sqrt{2}}(\hat{a}_2 - \hat{a}_2^\dagger) \tag{16.58}$$

17 量子测量

17.1 量子测量基本概念

17.1.1 一般测量

1. 一般测量结果 m_i 的概率：

$$p_i = \langle\psi|\hat{M}_i^\dagger \hat{M}_i|\psi\rangle\,, \quad \sum_i \hat{M}_i^\dagger \hat{M}_i = \hat{I} \tag{17.1}$$

2. 一般测量后系统的量子态：

$$|\psi'\rangle = \frac{\hat{M}_i\,|\psi\rangle}{\sqrt{\langle\psi|\hat{M}_i^\dagger \hat{M}_i|\psi\rangle}} \tag{17.2}$$

3. 一般测量后的密度矩阵：非选择

$$\boldsymbol{\rho}' = \sum_i \hat{M}_i \boldsymbol{\rho} \hat{M}_i^\dagger \tag{17.3}$$

17.1.2 投影测量

1. 投影测量结果 m_i 的概率：

$$p_i = \langle\psi|\hat{P}_i|\psi\rangle\,, \quad \sum_i \hat{P}_i = \hat{I} \tag{17.4}$$

2. 投影测量后系统的量子态：

$$|\psi'\rangle = \frac{\hat{P}_i\,|\psi\rangle}{\sqrt{\langle\psi|\,\hat{P}_i\,|\psi\rangle}} \tag{17.5}$$

3. 投影测量后的密度矩阵：选择和非选择

$$\boldsymbol{\rho}_i' = \frac{\hat{P}_i \boldsymbol{\rho} \hat{P}_i^\dagger}{\mathrm{tr}(\hat{P}_i \boldsymbol{\rho})}, \quad \boldsymbol{\rho}' = \hat{P}_i \boldsymbol{\rho} \hat{P}_i^\dagger \tag{17.6}$$

17.1.3 广义测量 POVM

1. POVM 算符：

$$\hat{E}_i = \hat{M}_i^\dagger \hat{M}_i, \quad \sum_i \hat{E}_i = 1 \tag{17.7}$$

2. 广义测量结果 m_i 的概率：

$$p_i = \langle\psi|\hat{E}_i|\psi\rangle \tag{17.8}$$

17.2 量子间接测量

1. 客体和探测体相互作用演化算符：

$$\hat{U} = \hat{U}(\tau,0) = \hat{P}\exp\left(-\mathrm{i}\int_0^\tau \mathrm{d}t \hat{V}_I(t)\right) \tag{17.9}$$

2. 测量后系统的状态：

$$\boldsymbol{\rho}(\tau) = \hat{U}\boldsymbol{\rho}(0)\hat{U}^\dagger = \hat{U}(\boldsymbol{\rho}_O \otimes \boldsymbol{\rho}_P)\hat{U}^\dagger \tag{17.10}$$

3. 测量结果 m_i 的概率：

$$p_i = \mathrm{tr}\left(|i\rangle\langle i|\,\boldsymbol{\rho}(\tau)\right) = \mathrm{tr}\left(\hat{U}^\dagger\,|i\rangle\langle i|\,\hat{U}(\boldsymbol{\rho}_O \otimes \boldsymbol{\rho}_P)\right) \tag{17.11}$$

4. 测量后客体的状态：

$$\boldsymbol{\rho}_i' = p_i^{-1}\,\langle i|\,\hat{U}(\boldsymbol{\rho}_O \otimes \boldsymbol{\rho}_P)\hat{U}^\dagger\,|i\rangle \tag{17.12}$$

5. 测量算符的形式：

$$\boldsymbol{\rho}_P = |\phi\rangle\langle\phi| \Rightarrow \hat{M}_i = \langle i|\hat{U}|\phi\rangle \tag{17.13}$$

17.3 量子测量中的纠缠和熵

1. 探测粒子和被测系统的 Hamilton 量:

$$\hat{H} = \hat{H}_0 + \frac{\hat{p}^2}{2m} + \lambda \hat{A} \hat{p} \tag{17.14}$$

2. 探测粒子和被测系统的相互作用演化算符:

$$\hat{U}(t) = \mathrm{e}^{-\mathrm{i}\lambda t \hat{A} \hat{p}} \tag{17.15}$$

3. 耦合系统演化为纠缠态:

$$\hat{U}(t) \sum_a c_a |a\rangle |\psi(x)\rangle = \mathrm{e}^{-\lambda a t \hat{p}} \sum_a c_a |a\rangle |\psi(x)\rangle = \sum_a c_a |a\rangle |\psi(x - \lambda a t)\rangle \tag{17.16}$$

4. 非选择投影测量不使 von Neumann 熵减小:

$$\Delta S = S(\boldsymbol{\rho}') - S(\rho) = S\left(\sum_i \boldsymbol{\rho}'_i\right) - S(\boldsymbol{\rho}) \geqslant 0 \tag{17.17}$$

18 相干态

18.1 相干态

18.1.1 谐振子相干态

1. 谐振子初始波函数:

$$\psi(x,0)=\psi_0(x-x_0)=\hat{D}(x_0)\psi_0(x)=\langle x|\hat{D}(x_0)|0\rangle \tag{18.1}$$

2. 谐振子平移算符:

$$\hat{D}(x_0)=\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{p}_x x_0}=\mathrm{e}^{\alpha(\hat{a}^\dagger-\hat{a})},\quad \alpha=\sqrt{\frac{m\omega}{2\hbar}}x_0 \tag{18.2}$$

3. 谐振子相干态:

$$|\alpha\rangle=\mathrm{e}^{\alpha(\hat{a}^\dagger-\hat{a})}|0\rangle=\mathrm{e}^{-\frac{1}{2}|\alpha|^2}\sum_n\frac{\alpha^n}{\sqrt{n!}}|n\rangle \tag{18.3}$$

18.1.2 相干态

1. 相干态:

$$|\alpha\rangle=\mathrm{e}^{-\frac{1}{2}|\alpha|^2}\sum_n\frac{\alpha^n}{\sqrt{n!}}|n\rangle \tag{18.4}$$

2. 相干态是湮灭算符的本征态:

$$\hat{a}|\alpha\rangle=\alpha|\alpha\rangle \tag{18.5}$$

3. 相干态是平移后的真空态:

$$|\alpha\rangle=\hat{D}(\alpha)|0\rangle=\mathrm{e}^{\alpha\hat{a}^\dagger-\alpha^*\hat{a}}|0\rangle=\mathrm{e}^{-\frac{1}{2}|\alpha|^2}\mathrm{e}^{\alpha\hat{a}^\dagger}|0\rangle \tag{18.6}$$

4. 平移算符:

$$\hat{D}^\dagger(\alpha)=\hat{D}^{-1}(\alpha)=\hat{D}(-\alpha) \tag{18.7}$$

$$\hat{D}^\dagger(\alpha)\hat{O}(\hat{a},\hat{a}^\dagger)\hat{D}(\alpha)=\hat{O}(\hat{a}+\alpha,\hat{a}^\dagger+\alpha^*) \tag{18.8}$$

$$\hat{D}(\alpha)\hat{D}(\beta)=\mathrm{e}^{\frac{1}{2}(\alpha\beta^*-\alpha^*\beta)}\hat{D}(\alpha+\beta) \tag{18.9}$$

$$\hat{D}(\alpha)|\beta\rangle=\mathrm{e}^{\frac{1}{2}(\alpha\beta^*-\alpha^*\beta)}|\alpha+\beta\rangle \tag{18.10}$$

$$\langle\alpha|\hat{D}(\gamma)|\beta\rangle=\mathrm{e}^{\gamma\alpha^*-\gamma^*\beta-\frac{1}{2}|\gamma|^2}\langle\alpha|\beta\rangle \tag{18.11}$$

5. 相干态的等式:

$$\hat{a}^\dagger|\alpha\rangle\langle\alpha|=\left(\alpha^*+\frac{\partial}{\partial\alpha}\right)|\alpha\rangle\langle\alpha|,\quad |\alpha\rangle\langle\alpha|\hat{a}=\left(\alpha+\frac{\partial}{\partial\alpha^*}\right)|\alpha\rangle\langle\alpha| \tag{18.12}$$

18.1.3 相干态的性质

1. 粒子数呈 Possion 分布:

$$\langle n\rangle=\langle\alpha|\hat{n}|\alpha\rangle=\langle\alpha|\hat{a}^\dagger\hat{a}|\alpha\rangle=|\alpha|^2 \tag{18.13}$$

$$P_n(\alpha)=|\langle n|\alpha\rangle|^2=\frac{|\alpha|^{2n}}{n!}\mathrm{e}^{-|\alpha|^2}=\frac{\langle n\rangle^n}{n!}\mathrm{e}^{-\langle n\rangle} \tag{18.14}$$

2. 最小不确定性:

$$\langle x\rangle=\sqrt{\frac{\hbar}{2m\omega}}(\alpha^*+\alpha),\quad \langle p\rangle=\mathrm{i}\sqrt{\frac{m\hbar\omega}{2}}(\alpha^*-\alpha) \tag{18.15}$$

$$\langle x^2\rangle=\frac{\hbar}{2m\omega}\left(1+(\alpha^*+\alpha)^2\right),\quad \langle p^2\rangle=\frac{m\hbar\omega}{2}\left(1-(\alpha^*-\alpha)^2\right) \tag{18.16}$$

$$(\Delta x)^2=\langle x^2\rangle-\langle x\rangle^2=\frac{\hbar}{2m\omega},\quad (\Delta p)^2=\langle p^2\rangle-\langle p\rangle^2=\frac{m\omega\hbar}{2} \tag{18.17}$$

$$\Delta x\Delta p=\frac{\hbar}{2} \tag{18.18}$$

3. 非正交性:

$$\langle\beta|\alpha\rangle = \mathrm{e}^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)}\sum_n \frac{(\beta^*\alpha)^n}{n!} = \mathrm{e}^{-\frac{1}{2}(|\alpha|^2+|\beta|^2-2\beta^*\alpha)} \tag{18.19}$$

$$|\langle\beta|\alpha\rangle|^2 = \mathrm{e}^{-|\alpha-\beta|^2} \tag{18.20}$$

4. 完备性:

$$\frac{1}{\pi}\int |\alpha\rangle\langle\alpha|\,\mathrm{d}^2\alpha = \frac{1}{\pi}\sum_{mn}\frac{|m\rangle\langle n|}{\sqrt{m!n!}}\int \mathrm{e}^{-|\alpha|^2}\alpha^{*m}\alpha^n\mathrm{d}^2\alpha \tag{18.21}$$

$$= \frac{1}{\pi}\sum_{mn}\frac{|m\rangle\langle n|}{\sqrt{m!n!}}\int_0^{+\infty}\mathrm{e}^{-|\alpha|^2}|\alpha|^{m+n+1}\mathrm{d}|\alpha|\int_0^{2\pi}\mathrm{e}^{\mathrm{i}(m-n)\theta}\mathrm{d}\theta \tag{18.22}$$

$$= \frac{1}{\pi}\sum_{mn}\frac{|m\rangle\langle n|}{\sqrt{m!n!}}\cdot\frac{n!}{2}\cdot 2\pi\delta_{mn} = \sum_n |n\rangle\langle n| = \hat{I} \tag{18.23}$$

5. 超完备性:

$$|\alpha\rangle = \frac{1}{\pi}\int \mathrm{d}^2\beta\,|\beta\rangle\langle\beta|\alpha\rangle = \frac{1}{\pi}\int \mathrm{d}^2\beta\,|\beta\rangle\,\mathrm{e}^{-\frac{1}{2}(|\alpha|^2+|\beta|^2-2\beta^*\alpha)} \tag{18.24}$$

18.1.4 相干态表象

1. 相干态表象中的量子态:

$$|\psi\rangle = \frac{1}{\pi}\int \mathrm{d}^2\alpha\,|\alpha\rangle\langle\alpha|\psi\rangle\,, \quad \langle\alpha|\psi\rangle = \mathrm{e}^{-\frac{1}{2}|\alpha|^2}\sum_n c_n\frac{(\alpha^*)^n}{\sqrt{n!}} \tag{18.25}$$

2. 相干态表象中力学量的矩阵元:

$$\hat{O} = \sum_{mn}|m\rangle\langle m|\hat{O}|n\rangle\langle n| = \sum_{mn}O_{mn}\frac{1}{\sqrt{m!n!}}(\hat{a}^\dagger)^m|0\rangle\langle 0|\hat{a}^n \tag{18.26}$$

$$\langle\alpha|\hat{O}|\beta\rangle = \sum_{mn}O_{mn}\frac{1}{\sqrt{m!n!}}(\alpha^*)^m\beta^n\mathrm{e}^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)} = O(\alpha^*,\beta)\mathrm{e}^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)} \tag{18.27}$$

整函数算符:

$$O(\alpha^*,\beta) = \sum_{mn}O_{mn}\frac{1}{\sqrt{m!n!}}(\alpha^*)^m\beta^n \tag{18.28}$$

$$\hat{O} = \hat{O}_1\hat{O}_2 \Rightarrow O(\alpha^*,\beta) = \frac{1}{\pi}\int \mathrm{d}^2\gamma O_1(\alpha^*,\gamma)O_2(\gamma^*,\beta) \tag{18.29}$$

3. 相干态表象中的力学量:

$$\hat{O} = \frac{1}{\pi^2}\int \mathrm{d}^2\alpha\mathrm{d}^2\beta\,|\alpha\rangle\langle\alpha|\hat{O}|\beta\rangle\langle\beta| = \frac{1}{\pi^2}\int \mathrm{d}^2\alpha\mathrm{d}^2\beta\hat{O}(\alpha^*,\beta)\mathrm{e}^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)}|\alpha\rangle\langle\beta| \tag{18.30}$$

18.1.5 相干态的涨落

1. 场的正交分量算符:

$$\hat{X}_1 = \frac{1}{2}(\hat{a}+\hat{a}^\dagger), \quad \hat{X}_2 = \frac{1}{2\mathrm{i}}(\hat{a}-\hat{a}^\dagger) \tag{18.31}$$

2. 相干态的涨落:

$$\langle X_1\rangle = \frac{1}{2}(\alpha+\alpha^*), \quad \langle X_2\rangle = \frac{1}{2\mathrm{i}}(\alpha-\alpha^*) \tag{18.32}$$

$$\langle X_1^2\rangle = \frac{1}{4}+\langle X_1\rangle^2\,, \quad \langle X_2^2\rangle = \frac{1}{4}+\langle X_2\rangle^2 \tag{18.33}$$

$$(\Delta X_1)^2 = \langle X_1^2\rangle - \langle X_1\rangle^2 = \frac{1}{4}, \quad (\Delta X_2)^2 = \langle X_2^2\rangle - \langle X_2\rangle^2 = \frac{1}{4} \tag{18.34}$$

18.1.6 相干态的产生和演化

1. 相干态的自由演化：

$$\hat{H}_0 = \hbar\omega\hat{a}^\dagger\hat{a} \tag{18.35}$$

$$|\alpha(t)\rangle = \mathrm{e}^{-\mathrm{i}\omega\hat{a}^\dagger\hat{a}t}|\alpha_0\rangle = \mathrm{e}^{-\frac{1}{2}|\alpha|^2}\sum_n \frac{(\alpha_0\mathrm{e}^{-\mathrm{i}\omega t})^n}{\sqrt{n!}}|n\rangle = |\alpha_0\mathrm{e}^{-\mathrm{i}\omega t}\rangle \tag{18.36}$$

2. 经典源驱动谐振子的时间演化：

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \hbar\omega\hat{a}^\dagger\hat{a} + \hbar g(t)(\hat{a}^\dagger + \hat{a}) \tag{18.37}$$

$$\frac{\partial|\widetilde{\psi}(t)\rangle}{\partial t} = -\mathrm{i}g(t)(\hat{a}^\dagger\mathrm{e}^{\mathrm{i}\omega t} + \hat{a}\mathrm{e}^{-\mathrm{i}\omega t})|\widetilde{\psi}(t)\rangle, \quad |\widetilde{\psi}(t)\rangle = \mathrm{e}^{\mathrm{i}\omega\hat{a}^\dagger\hat{a}t}|\psi(t)\rangle \tag{18.38}$$

$$|\widetilde{\psi}(t)\rangle = \hat{P}\exp\left(-\mathrm{i}\int_0^t g(\tau)(\hat{a}^\dagger\mathrm{e}^{\mathrm{i}\omega\tau} + \hat{a}\mathrm{e}^{-\mathrm{i}\omega\tau})\mathrm{d}\tau\right) \tag{18.39}$$

3. 波函数：

$$|\psi(t)\rangle = \exp\left(\hat{a}^\dagger\alpha(t) - \hat{a}\alpha^*(t) + \mathrm{i}F(t)\right)\mathrm{e}^{-\mathrm{i}\omega\hat{a}^\dagger\hat{a}t}|\psi(0)\rangle \tag{18.40}$$

$$\alpha(t) = -\mathrm{i}\int_0^t \mathrm{d}\tau\mathrm{e}^{\mathrm{i}\omega(t-\tau)}g(\tau), \quad F(t) = \frac{\mathrm{i}}{2}\int_0^t\mathrm{d}\tau\int_0^t\mathrm{d}\tau'\mathrm{sgn}(\tau-\tau')g(\tau)g(\tau')\mathrm{e}^{\mathrm{i}\omega(\tau-\tau')} \tag{18.41}$$

初始态为真空态：$|\psi(0)\rangle = |0\rangle$

$$|\psi(t)\rangle = \exp(\mathrm{i}F(t))|\alpha(t)\rangle \tag{18.42}$$

初始态为相干态：$|\psi(0)\rangle = |\alpha_0\rangle$

$$|\psi(t)\rangle = \exp\left[\mathrm{i}F(t) + \frac{1}{2}(\alpha(t)\alpha_0\mathrm{e}^{\mathrm{i}\omega t} - \alpha^*(t)\alpha_0\mathrm{e}^{-\mathrm{i}\omega t})\right]|\alpha(t) + \alpha_0\mathrm{e}^{-\mathrm{i}\omega t}\rangle \tag{18.43}$$

$$g(t) = 0 \Rightarrow |\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}\omega\hat{a}^\dagger\hat{a}t}|\alpha_0\rangle = |\alpha_0\mathrm{e}^{-\mathrm{i}\omega t}\rangle \tag{18.44}$$

18.2 压缩态

18.2.1 压缩态真空态

1. 压缩算符：

$$\hat{S}(\xi) = \exp\left(\frac{\xi^*}{2}\hat{a}^2 - \frac{\xi}{2}\hat{a}^{\dagger 2}\right), \quad \xi = r\mathrm{e}^{\mathrm{i}\theta} \tag{18.45}$$

$$\hat{S}^\dagger(\xi) = \hat{S}(-\xi) = \hat{S}^{-1}(\xi) \tag{18.46}$$

$$\hat{S}(\xi) = \hat{R}\left(-\frac{\theta}{2}\right)\hat{S}(r)\hat{R}\left(\frac{\theta}{2}\right) = \exp\left(\frac{\mathrm{i}}{2}\theta\hat{a}^\dagger\hat{a}\right)\exp\left(\frac{r}{2}(\hat{a}^2 - \hat{a}^{\dagger 2})\right)\exp\left(-\frac{\mathrm{i}}{2}\theta\hat{a}^\dagger\hat{a}\right) \tag{18.47}$$

$$\hat{S}(\xi) = \exp\left(-\frac{1}{2}\hat{a}^{\dagger 2}\mathrm{e}^{\mathrm{i}\theta}\tanh r\right)\exp\left(-\frac{1}{2}(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger)\ln\cosh r\right)\exp\left(\frac{1}{2}\hat{a}^2\mathrm{e}^{-\mathrm{i}\theta}\tanh r\right) \tag{18.48}$$

2. 压缩真空态：

$$|0,\xi\rangle = \hat{S}(\xi)|0\rangle = \hat{R}\left(-\frac{\theta}{2}\right)\hat{S}(r)\hat{R}\left(\frac{\theta}{2}\right)|0\rangle = \sqrt{\mathrm{sech} r}\sum_{n=0}^{+\infty}\frac{\sqrt{(2n)!}}{n!2^n}(-\mathrm{e}^{\mathrm{i}\theta}\tanh r)^n|2n\rangle \tag{18.49}$$

$$\langle 0,\xi|0,\xi'\rangle = \langle 0|\hat{S}(-\xi)\hat{S}(\xi')|0\rangle = \left(\frac{\mathrm{sech} r\,\mathrm{sech} r'}{1 - \mathrm{e}^{\mathrm{i}(\theta-\theta')}\tanh r\tanh r'}\right)^{\frac{1}{2}} = \mathrm{sech}^{\frac{1}{2}}(r - r'),\ \theta = \theta' \tag{18.50}$$

3. 压缩真空态的平均值：

$$\langle\hat{a}\rangle = \langle\hat{a}^\dagger\rangle^* = 0, \quad \langle\hat{a}^2\rangle = \langle(\hat{a}^\dagger)^2\rangle^* = -\cosh r\sinh r\mathrm{e}^{\mathrm{i}\theta}, \quad \langle\hat{a}^\dagger\hat{a}\rangle = \sinh^2 r \tag{18.51}$$

18.2.2 压缩态

1. 压缩态：

$$|\alpha,\xi\rangle=\hat{S}(\xi)\,|\alpha\rangle=\hat{S}(\xi)\hat{D}(\alpha)\,|0\rangle \tag{18.52}$$

2. 准光子的产生湮灭算符：Bogoliubov 变换

$$\hat{b}=\hat{S}^{\dagger}(\xi)\hat{a}\hat{S}(\xi)=\cosh r\hat{a}-\mathrm{e}^{\mathrm{i}\theta}\sinh r\hat{a}^{\dagger} \tag{18.53}$$

$$\hat{b}^{\dagger}=\hat{S}^{\dagger}(\xi)\hat{a}^{\dagger}\hat{S}(\xi)=\cosh r\hat{a}^{\dagger}-\mathrm{e}^{-\mathrm{i}\theta}\sinh r\hat{a} \tag{18.54}$$

$$[\hat{b},\hat{b}^{\dagger}]=[\hat{a},\hat{a}^{\dagger}]=1 \tag{18.55}$$

3. 准光子的粒子数算符：

$$\hat{n}_g=\hat{b}^{\dagger}\hat{b}=\hat{S}^{\dagger}(\xi)\hat{a}^{\dagger}\hat{a}\hat{S}(\xi) \tag{18.56}$$

$$\hat{n}_g\,|n_g\rangle=n_g\,|n_g\rangle\,,\quad \hat{n}_g\,|0,\xi\rangle=0,\quad |n_g\rangle=\hat{S}^{\dagger}(\xi)\,|n\rangle \tag{18.57}$$

4. 压缩态是准光子空间中的相干态：

$$\hat{a}=\cosh r\hat{b}+\mathrm{e}^{\mathrm{i}\theta}\sinh r\hat{b}^{\dagger},\quad \hat{a}^{\dagger}=\cosh r\hat{b}^{\dagger}+\mathrm{e}^{-\mathrm{i}\theta}\sinh r\hat{b} \tag{18.58}$$

$$|\alpha,\xi\rangle=\hat{S}(\xi)\mathrm{e}^{\alpha\hat{a}^{\dagger}-\alpha^*\hat{a}}\,|0\rangle=\hat{S}(\xi)\mathrm{e}^{\beta\hat{b}^{\dagger}-\beta^*\hat{b}}\,|0\rangle=\hat{S}(\xi)\hat{D}_g(\beta)\,|0\rangle\,,\quad \beta=\alpha\cosh r-\alpha^*\mathrm{e}^{\mathrm{i}\theta}\sinh r \tag{18.59}$$

$$\hat{b}\,|\alpha,\xi\rangle=(\alpha\cosh 2r-\alpha^*\sinh 2r)\,|\alpha,\xi\rangle\,,\quad \hat{b}\,|0,\xi\rangle=0 \tag{18.60}$$

5. 压缩态的平均值：

$$\langle\hat{a}\rangle=\langle\hat{a}^{\dagger}\rangle^*=\alpha\cosh r-\alpha^*\mathrm{e}^{\mathrm{i}\theta}\sinh r \tag{18.61}$$

$$\langle\hat{a}^2\rangle=\langle(\hat{a}^{\dagger})^2\rangle^*=\alpha^2\cosh^2 r+(\alpha^*)^2\mathrm{e}^{2\mathrm{i}\theta}\sinh^2 r-(2|\alpha|^2+1)\mathrm{e}^{\mathrm{i}\theta}\cosh r\sinh r \tag{18.62}$$

$$\langle\hat{a}^{\dagger}\hat{a}\rangle=|\alpha|^2(\cosh^2 r+\sinh^2 r)-(\alpha^*)^2\mathrm{e}^{\mathrm{i}\theta}\sinh r\cosh r-\alpha^2\mathrm{e}^{-\mathrm{i}\theta}\sinh r\cosh r+\sinh^2 r \tag{18.63}$$

18.2.3 压缩态的涨落

1. 压缩态主轴的正交分量算符：

$$\hat{Y}_1=\frac{1}{2}(\hat{a}\mathrm{e}^{-\mathrm{i}\theta/2}+\hat{a}^{\dagger}\mathrm{e}^{\mathrm{i}\theta/2})=\hat{X}_1\cos\frac{\theta}{2}+\hat{X}_2\sin\frac{\theta}{2} \tag{18.64}$$

$$\hat{Y}_2=\frac{1}{2\mathrm{i}}(\hat{a}\mathrm{e}^{-\mathrm{i}\theta/2}-\hat{a}^{\dagger}\mathrm{e}^{\mathrm{i}\theta/2})=\hat{X}_2\cos\frac{\theta}{2}-\hat{X}_1\sin\frac{\theta}{2} \tag{18.65}$$

2. 压缩态的涨落：

$$\langle Y_1\rangle=\frac{1}{2}\mathrm{e}^{-r}(\alpha\mathrm{e}^{-\mathrm{i}\theta/2}+\alpha^*\mathrm{e}^{\mathrm{i}\theta/2}),\quad \langle Y_2\rangle=\frac{1}{2\mathrm{i}}\mathrm{e}^{r}(\alpha\mathrm{e}^{-\mathrm{i}\theta/2}-\alpha^*\mathrm{e}^{\mathrm{i}\theta/2}) \tag{18.66}$$

$$\langle Y_1^2\rangle=\frac{1}{4}\mathrm{e}^{-2r}+\langle Y_1\rangle^2\,,\quad \langle Y_2^2\rangle=\frac{1}{4}\mathrm{e}^{2r}+\langle Y_2\rangle^2 \tag{18.67}$$

$$(\Delta Y_1)^2=\langle Y_1^2\rangle-\langle Y_1\rangle^2=\frac{1}{4}\mathrm{e}^{-2r},\quad (\Delta Y_2)^2=\langle Y_2^2\rangle-\langle Y_2\rangle^2=\frac{1}{4}\mathrm{e}^{2r} \tag{18.68}$$

18.2.4 压缩态的粒子数分布

1. 粒子数表象中的压缩态：

$$\langle n|\beta,\xi\rangle=\frac{(\mathrm{e}^{\mathrm{i}\theta}\tanh r)^{\frac{n}{2}}}{2^{n/2}\sqrt{n!\cosh r}}\exp\left[-\frac{1}{2}\left(|\beta|^2-\mathrm{e}^{-\mathrm{i}\theta}\beta^2\tanh r\right)\right]H_n\left(\frac{\beta\mathrm{e}^{-\mathrm{i}\theta/2}}{\sqrt{2\cosh r\sinh r}}\right) \tag{18.69}$$

2. 压缩态的粒子数涨落：

$$\langle n\rangle=|\alpha|^2+\sinh^2 r \tag{18.70}$$

$$\langle n^2\rangle=(|\alpha|^2+\sinh^2 r)^2+2\sinh^2 r\cosh^2 r+|\alpha\cosh r-\alpha\mathrm{e}^{\mathrm{i}\theta}\sinh r|^2 \tag{18.71}$$

$$(\Delta n)^2=\langle n^2\rangle-\langle n\rangle^2=|\alpha|^2\left[\mathrm{e}^{-2r}\cos^2\left(\frac{\theta}{2}-\phi\right)+\mathrm{e}^{2r}\sin^2\left(\frac{\theta}{2}-\phi\right)\right]+2\sinh^2 r\cosh^2 r \tag{18.72}$$

$$\mathcal{M}=\frac{(\Delta n)^2-\langle n\rangle}{\langle n\rangle} \tag{18.73}$$

18.3　多模压缩态

18.3.1　双模压缩态

1. 双模压缩算符：

$$\hat{S}(\xi) = \exp\left(\xi^* \hat{a}_{\omega+\omega'} \hat{a}_{\omega-\omega'} - \xi \hat{a}^\dagger_{\omega+\omega'} \hat{a}^\dagger_{\omega-\omega'}\right), \quad \xi = r\mathrm{e}^{\mathrm{i}\theta} \tag{18.74}$$

$$\hat{S}^\dagger(\xi) = \hat{S}(-\xi) = \hat{S}^{-1}(\xi) \tag{18.75}$$

$$\hat{S}(\xi)\hat{a}_{\omega\pm\omega'}\hat{S}(\xi) = \cosh r \hat{a}_{\omega\pm\omega'} - \mathrm{e}^{\mathrm{i}\theta} \sinh r \hat{a}^\dagger_{\omega\mp\omega'} \tag{18.76}$$

$$\hat{S}(\xi)\hat{a}^\dagger_{\omega\pm\omega'}\hat{S}(\xi) = \cosh r \hat{a}^\dagger_{\omega\pm\omega'} - \mathrm{e}^{-\mathrm{i}\theta} \sinh r \hat{a}_{\omega\mp\omega'} \tag{18.77}$$

2. 双模压缩真空态：

$$|0,0,\xi\rangle = \hat{S}(\xi)\,|0,0\rangle = \frac{1}{\cosh r} \sum_{n=0}^{+\infty} \left(-\mathrm{e}^{\mathrm{i}\theta} \tanh r\right)^n |n,n\rangle \tag{18.78}$$

3. 双模压缩真空态的平均值：

$$\langle \hat{a}^\dagger_{\omega\pm\omega'} \hat{a}_{\omega\pm\omega'} \rangle = \sinh^2 r, \quad \langle \hat{a}_{\omega\pm\omega'} \hat{a}_{\omega\mp\omega'} \rangle = -\sinh r \cosh r \mathrm{e}^{\mathrm{i}\theta} \tag{18.79}$$

$$\langle \hat{a}^\dagger_{\omega\pm\omega'} \hat{a}_{\omega\mp\omega'} \rangle = \langle \hat{a}^2_{\omega\pm\omega'} \rangle = \langle \hat{a}_{\omega\pm\omega'} \rangle = 0 \tag{18.80}$$

4. 双模压缩真空态是两个压缩真空态的直积：

$$\hat{c} = \frac{1}{\sqrt{2}}(\hat{a}_{\omega+\omega'} + \mathrm{e}^{\mathrm{i}\delta} \hat{a}_{\omega-\omega'}), \quad \hat{d} = \frac{1}{\sqrt{2}}(\hat{a}_{\omega+\omega'} - \mathrm{e}^{-\mathrm{i}\delta} \hat{a}_{\omega-\omega'}) \tag{18.81}$$

$$\hat{S}(\xi) = \exp\left(-\frac{1}{2}\xi(\hat{c}^{\dagger 2}\mathrm{e}^{\mathrm{i}\delta} - \hat{d}^2 \mathrm{e}^{-\mathrm{i}\delta}) + \frac{1}{2}\xi^*(\hat{c}^{\dagger 2}\mathrm{e}^{-\mathrm{i}\delta} - \hat{d}^2 \mathrm{e}^{\mathrm{i}\delta})\right) = \hat{S}_c(\xi \mathrm{e}^{\mathrm{i}\delta}) \hat{S}_d(-\xi \mathrm{e}^{-\mathrm{i}\delta}) \tag{18.82}$$

5. 双模压缩态：

$$|\alpha,\beta,\xi\rangle = \hat{S}(\xi)\,|\alpha,\beta\rangle = \hat{S}(\xi)\hat{D}_{\omega+\omega'}(\alpha)\hat{D}_{\omega-\omega'}(\beta)\,|0,0\rangle \tag{18.83}$$

18.3.2　多模压缩态

1. 多模压缩算符：

$$S(\xi(\omega)) = \int \frac{\mathrm{d}\omega'}{2\pi} \exp\left(\xi^*(\omega')\hat{a}_{\omega+\omega'}\hat{a}_{\omega-\omega'} - \xi(\omega')\hat{a}^\dagger_{\omega+\omega'}\hat{a}^\dagger_{\omega-\omega'}\right) \tag{18.84}$$

2. 多模压缩真空态：

$$\langle 0(\omega), \xi(\omega)\rangle = S(\xi(\omega))\,|0(\omega)\rangle \tag{18.85}$$

3. 多模压缩态：

$$|\alpha(\omega), \xi(\omega)\rangle = S(\xi(\omega))\,|\alpha(\omega)\rangle = S(\xi(\omega))D(\alpha(\omega))\,|0(\omega)\rangle \tag{18.86}$$

18.4　奇偶态

1. 奇偶态：

$$|\alpha\rangle_o = N_o(|\alpha\rangle - |-\alpha\rangle) = (\sinh|\alpha|^2)^{-\frac{1}{2}} \sum_{n=0}^{+\infty} \frac{\alpha^{2n+1}}{\sqrt{(2n+1)!}} |2n+1\rangle \tag{18.87}$$

$$|\alpha\rangle_e = N_e(|\alpha\rangle + |-\alpha\rangle) = (\cosh|\alpha|^2)^{-\frac{1}{2}} \sum_{n=0}^{+\infty} \frac{\alpha^{2n}}{\sqrt{(2n)!}} |2n\rangle \tag{18.88}$$

$$|\alpha\rangle = \mathrm{e}^{-\frac{1}{2}|\alpha|^2} \left[(\sinh|\alpha|^2)^{\frac{1}{2}}\,|\alpha\rangle_o + (\cosh|\alpha|^2)^{\frac{1}{2}}\,|\alpha\rangle_e\right] \tag{18.89}$$

2. 奇偶态是湮灭算符平方的本征态：

$$\hat{a}^2 \left|\alpha\right\rangle_{o/e} = \hat{a}^2 N_{o/e}(\left|\alpha\right\rangle \mp \left|-\alpha\right\rangle) = \alpha^2 \left|\alpha\right\rangle_{o/e} \tag{18.90}$$

$$\hat{a} \left|\alpha\right\rangle_o = \alpha \coth^{\frac{1}{2}} |\alpha|^2 \left|\alpha\right\rangle_e, \quad \hat{a} \left|\alpha\right\rangle_e = \alpha \tanh^{\frac{1}{2}} |\alpha|^2 \left|\alpha\right\rangle_o \tag{18.91}$$

3. 非正交性：

$${}_o\langle\alpha|\alpha'\rangle_o = (\sinh|\alpha|^2 \sinh|\alpha'|^2)^{-\frac{1}{2}} \sinh(\alpha^*\alpha') \tag{18.92}$$

$${}_o\langle\alpha|\alpha'\rangle_o = (\cosh|\alpha|^2 \cosh|\alpha'|^2)^{-\frac{1}{2}} \cosh(\alpha^*\alpha') \tag{18.93}$$

4. 完备性：

$$1 = \frac{1}{\pi}\int \mathrm{e}^{-|\alpha|^2} \left[\sinh|\alpha|^2 \left|\alpha\right\rangle_{oo} \langle\alpha| + \cosh|\alpha|^2 \left|\alpha\right\rangle_{ee} \langle\alpha|\right] \mathrm{d}\alpha^2 = \mathit{\Pi}_o + \mathit{\Pi}_e \tag{18.94}$$

19 量子分布理论

19.1 Glauber-Sudarshan P 表示

1. 正规排列的算符:

$$\hat{O}_N(\hat{a},\hat{a}^\dagger)=\sum_n\sum_m c_{nm}(\hat{a}^\dagger)^n\hat{a}^m \tag{19.1}$$

$$\begin{aligned}\langle O_N(\hat{a},\hat{a}^\dagger)\rangle&=\mathrm{tr}[\hat{\rho}\hat{O}_N(\hat{a},\hat{a}^\dagger)]=\sum_n\sum_m c_{nm}\mathrm{tr}[\hat{\rho}(\hat{a}^\dagger)^n\hat{a}^m]\\&=\sum_n\sum_m c_{nm}\mathrm{tr}\left[\frac{1}{\pi^2}\int\mathrm{d}\alpha^2\mathrm{d}\beta^2\langle\alpha|\hat{\rho}|\beta\rangle\langle\beta|(\hat{a}^\dagger)^n\hat{a}^m|\alpha\rangle\right]\\&=\int\mathrm{d}^2\alpha\,\frac{1}{\pi^2}\langle\alpha|\hat{\rho}|\alpha\rangle\sum_n\sum_m c_{nm}(\alpha^*)^n\alpha^m\\&=\int\mathrm{d}^2\alpha\,\mathrm{tr}[\hat{\rho}\delta(\alpha^*-\hat{a}^\dagger)\delta(\alpha-\hat{a})]\sum_n\sum_m c_{nm}(\alpha^*)^n\alpha^m\\&=\int\mathrm{d}^2\alpha\,P(\alpha,\alpha^*)\hat{O}_N(\alpha,\alpha^*)\end{aligned} \tag{19.2}$$

2. P 函数:

$$P(\alpha,\alpha^*)=\mathrm{tr}[\rho\delta(\alpha^*-\hat{a}^\dagger)\delta(\alpha-\hat{a})] \tag{19.3}$$

$$\delta(\alpha^*-\hat{a}^\dagger)\delta(\alpha-\hat{a})=\frac{1}{\pi^2}\int\mathrm{d}^2\beta\,e^{-\beta(\alpha^*-\hat{a}^\dagger)}e^{\beta^*(\alpha-\hat{a})}=\frac{1}{\pi^2}\int\mathrm{d}^2\beta\,e^{-\mathrm{i}\beta(\alpha^*-\hat{a}^\dagger)}e^{-\mathrm{i}\beta^*(\alpha-\hat{a})} \tag{19.4}$$

$$\int\mathrm{d}^2\alpha\,P(\alpha,\alpha^*)=1 \tag{19.5}$$

$$\hat{\rho}=\int\mathrm{d}^2\alpha\,P(\alpha,\alpha^*)|\alpha\rangle\langle\alpha| \tag{19.6}$$

3. P 函数的计算:

$$\alpha=x_\alpha+\mathrm{i}y_\alpha,\ \beta=x_\beta+\mathrm{i}y_\beta\ \Rightarrow\ \mathrm{d}^2\alpha=\mathrm{d}x_\alpha\mathrm{d}y_\alpha,\ \beta\alpha^*-\beta^*\alpha=2\mathrm{i}(y_\beta x_\alpha-x_\beta y_\alpha) \tag{19.7}$$

$$\begin{aligned}\langle-\beta|\hat{\rho}|\beta\rangle\,\mathrm{e}^{|\beta|^2}&=\mathrm{e}^{|\beta|^2}\int\mathrm{d}^2\alpha P(\alpha,\alpha^*)\,\langle-\beta|\alpha\rangle\,\langle\alpha|\beta\rangle=\int\mathrm{d}^2\alpha\,\left[P(\alpha,\alpha^*)\mathrm{e}^{-|\alpha|^2}\right]\mathrm{e}^{\beta\alpha^*-\beta^*\alpha}\\&=\int\mathrm{d}x_\alpha\mathrm{d}y_\alpha\,P(x_\alpha,y_\alpha)\mathrm{e}^{-(x_\alpha^2+y_\alpha^2)}\mathrm{e}^{2\mathrm{i}(y_\beta x_\alpha-x_\beta y_\alpha)}\end{aligned} \tag{19.8}$$

$$\begin{aligned}P(\alpha,\alpha^*)&=\frac{\mathrm{e}^{(x_\alpha^2+y_\alpha^2)}}{\pi^2}\int\mathrm{d}x_\beta\mathrm{d}y_\beta\,\langle-\beta|\hat{\rho}|\beta\rangle\,\mathrm{e}^{x_\beta^2+y_\beta^2}\mathrm{e}^{2\mathrm{i}(y_\alpha x_\beta-x_\alpha y_\beta)}\\&=\frac{\mathrm{e}^{|\alpha|^2}}{\pi^2}\int\mathrm{d}^2\beta\,\langle-\beta|\hat{\rho}|\beta\rangle\,\mathrm{e}^{|\beta|^2}\mathrm{e}^{-\beta\alpha^*+\beta^*\alpha}\end{aligned} \tag{19.9}$$

4. P 函数的例子:

(1) 热场态:

$$\hat{\rho}=\sum_n\frac{\langle n\rangle^n}{(1+\langle n\rangle)^{n+1}}\,|n\rangle\,\langle n|\,,\quad\rho_{nn}=\langle n|\hat{\rho}|n\rangle=\frac{\langle n\rangle^n}{(1+\langle n\rangle)^{n+1}} \tag{19.10}$$

$$\begin{aligned}\langle-\beta|\hat{\rho}|\beta\rangle&=\sum_n\frac{\langle n\rangle^n}{(1+\langle n\rangle)^{n+1}}\,\langle-\beta|n\rangle\,\langle n|\beta\rangle=\frac{\mathrm{e}^{-|\beta|^2}}{1+\langle n\rangle}\sum_n\frac{(-|\beta|^2)^n}{n!}\left(\frac{\langle n\rangle}{1+\langle n\rangle}\right)^n\\&=\frac{\mathrm{e}^{-|\beta|^2}}{1+\langle n\rangle}\exp\left(-\frac{|\beta|^2}{1+\langle n\rangle^{-1}}\right)\end{aligned} \tag{19.11}$$

$$P(\alpha,\alpha^*)=\frac{\mathrm{e}^{|\alpha|^2}}{\pi^2(1+\langle n\rangle)}\int\mathrm{d}^2\beta\,\exp\left(-\frac{|\beta|^2}{1+\langle n\rangle}\right)\mathrm{e}^{-\beta\alpha^*+\alpha\beta^*}=\frac{1}{\pi\,\langle n\rangle}\exp\left(-\frac{|\alpha|^2}{\langle n\rangle}\right) \tag{19.12}$$

(2) 相干态:

$$\hat{\rho} = |\alpha_0\rangle\langle\alpha_0| \tag{19.13}$$

$$\langle -\beta|\hat{\rho}|\beta\rangle = \langle -\beta|\alpha_0\rangle\langle\alpha_0|\beta\rangle = \mathrm{e}^{-|\alpha_0|^2-|\beta|^2-\alpha_0\beta^*+\beta\alpha_0^*} \tag{19.14}$$

$$P(\alpha,\alpha^*) = \frac{1}{\pi^2}\mathrm{e}^{|\alpha|^2-|\alpha_0|^2}\int \mathrm{d}^2\beta\,\mathrm{e}^{-\beta(\alpha^*-\alpha_0^*)+\beta^*(\alpha-\alpha_0)} = \delta^2(\alpha-\alpha_0) \tag{19.15}$$

(3) 粒子数态:

$$\hat{\rho} = |n\rangle\langle n| \tag{19.16}$$

$$\langle -\beta|\hat{\rho}|\beta\rangle = \langle -\beta|n\rangle\langle n|\beta\rangle = \mathrm{e}^{-|\beta|^2}\frac{(-1)^n|\beta|^{2n}}{n!} \tag{19.17}$$

$$\begin{aligned} P(\alpha,\alpha^*) &= \frac{(-1)^n\mathrm{e}^{|\alpha|^2}}{\pi^2 n!}\int \mathrm{d}^2\beta\,|\beta|^{2n}\mathrm{e}^{-\beta\alpha^*+\beta^*\alpha} \\ &= \frac{\mathrm{e}^{|\alpha|^2}}{\pi^2 n!}\frac{\partial^{2n}}{\partial\alpha^n\partial\alpha^{*n}}\int \mathrm{d}^2\beta\,\mathrm{e}^{-\beta\alpha^*+\beta^*\alpha} = \frac{\mathrm{e}^{|\alpha|^2}}{n!}\frac{\partial^{2n}}{\partial\alpha^n\partial\alpha^{*n}}\delta^2(\alpha) \end{aligned} \tag{19.18}$$

$n>0$，P 函数不是非负定的，故粒子数态无良好定义的 P 表示

19.2 Husimi Q 表示

1. 反正规排列的算符:

$$\hat{O}_A(\hat{a},\hat{a}^\dagger) = \sum_n\sum_m d_{nm}\hat{a}^n(\hat{a}^\dagger)^m \tag{19.19}$$

$$\begin{aligned} \langle O_A(\hat{a},\hat{a}^\dagger)\rangle = \mathrm{tr}[\hat{\rho}O_A(\hat{a},\hat{a}^\dagger)] &= \sum_n\sum_m d_{nm}\mathrm{tr}[\hat{\rho}\hat{a}^n(\hat{a}^\dagger)^m] \\ &= \sum_n\sum_m d_{nm}\mathrm{tr}\left[\frac{1}{\pi}\int \mathrm{d}^2\alpha\,\hat{\rho}\hat{a}^n|\alpha\rangle\langle\alpha|(\hat{a}^\dagger)^m\right] \\ &= \int \mathrm{d}^2\alpha\,\frac{1}{\pi}\langle\alpha|\hat{\rho}|\alpha\rangle\sum_n\sum_m d_{nm}\alpha^n(\alpha^*)^m \\ &= \int \mathrm{d}^2\alpha\,\mathrm{tr}[\hat{\rho}\delta(\alpha-\hat{a})\delta(\alpha^*-\hat{a}^\dagger)]\sum_n\sum_m d_{nm}\alpha^n(\alpha^*)^m \\ &= \int \mathrm{d}^2\alpha\,Q(\alpha,\alpha^*)\hat{O}_A(\alpha,\alpha^*) \end{aligned} \tag{19.20}$$

2. Q 函数:

$$Q(\alpha,\alpha^*) = \mathrm{tr}[\hat{\rho}\delta(\alpha-\hat{a})\delta(\alpha^*-\hat{a}^\dagger)] \tag{19.21}$$

$$\delta(\alpha-\hat{a})\delta(\alpha^*-\hat{a}^\dagger) = \frac{1}{\pi^2}\int \mathrm{d}^2\beta\,e^{-\beta(\alpha-\hat{a})}e^{\beta^*(\alpha^*-\hat{a}^\dagger)} = \frac{1}{\pi^2}\int \mathrm{d}^2\beta\,e^{-\mathrm{i}\beta(\alpha-\hat{a})}e^{-\mathrm{i}\beta^*(\alpha^*-\hat{a}^\dagger)} \tag{19.22}$$

$$\int \mathrm{d}^2\alpha Q(\alpha.\alpha^*) = 1 \tag{19.23}$$

$$0 < Q(\alpha,\alpha^*) = \frac{1}{\pi}\sum_i P_i\,|\langle\psi_i|\alpha\rangle|^2 \leqslant \frac{1}{\pi}\sum_i P_i = \frac{1}{\pi} \tag{19.24}$$

3. Q 函数的计算:

$$Q(\alpha,\alpha^*) = \frac{1}{\pi}\mathrm{tr}\left[\int \mathrm{d}^2\alpha'\,\hat{\rho}\delta(\alpha-\hat{a})|\alpha'\rangle\langle\alpha'|\delta(\alpha^*-\hat{a}^\dagger)\right] = \frac{1}{\pi}\langle\alpha|\hat{\rho}|\alpha\rangle \tag{19.25}$$

4. Q 函数的例子:

(1) 热场态:

$$\hat{\rho} = \sum_n \frac{\langle n\rangle^n}{(1+\langle n\rangle)^{n+1}}|n\rangle\langle n| \tag{19.26}$$

$$Q(\alpha,\alpha^*) = \frac{1}{\pi}\sum_n \frac{\langle n\rangle^n}{(1+\langle n\rangle)^{n+1}}|\langle\alpha|n\rangle|^2 = \frac{1}{\pi}\frac{1}{1+\langle n\rangle}\exp\left(-\frac{|\alpha|^2}{1+\langle n\rangle}\right) \tag{19.27}$$

(2) 相干态:

$$\hat{\rho} = |\alpha_0\rangle\langle\alpha_0| \tag{19.28}$$

$$Q(\alpha,\alpha^*) = \frac{1}{\pi}|\langle\alpha|\alpha_0\rangle|^2 = \frac{1}{\pi}\mathrm{e}^{-|\alpha-\alpha_0|^2} \tag{19.29}$$

(3) 粒子数态:

$$\hat{\rho} = |n\rangle\langle n| \tag{19.30}$$

$$Q(\alpha,\alpha^*) = \frac{1}{\pi}|\langle\alpha|n\rangle|^2 = \frac{1}{\pi}\frac{|\alpha|^{2n}}{n!}\mathrm{e}^{-|\alpha|^2} \tag{19.31}$$

(4) 压缩态:

$$\hat{\rho} = |\beta,\xi\rangle\langle\beta,\xi| \tag{19.32}$$

$$\begin{aligned}
\langle\alpha|\beta,\xi\rangle &= \frac{1}{\alpha^*}\langle\alpha|\hat{a}^\dagger\hat{S}(\xi)|\beta\rangle = \frac{1}{\alpha^*}\langle\alpha|\hat{S}(\xi)S^\dagger(\xi)\hat{a}^\dagger\hat{S}(\xi)|\beta\rangle \\
&= \frac{1}{\alpha^*}\langle\alpha|\hat{S}(\xi)\left(\hat{a}^\dagger\cosh r - \hat{a}\mathrm{e}^{-\mathrm{i}\theta}\sinh r\right)|\beta\rangle \\
&= \frac{1}{\alpha^*}\left[\cosh r\left(\frac{\partial}{\partial\beta}+\frac{1}{2}\beta^*\right) - \mathrm{e}^{-\mathrm{i}\theta}\beta\sinh r\right]\langle\alpha|\hat{S}(\xi)|\beta\rangle
\end{aligned}$$

$$\Rightarrow \left[\cosh r\frac{\partial}{\partial\beta} - \beta\mathrm{e}^{-\mathrm{i}\theta}\mathrm{sech}r + \left(\frac{1}{2}\beta^*\cosh r - \alpha^*\right)\right]\langle\alpha|S(\xi)|\beta\rangle = 0 \tag{19.33}$$

$$\Rightarrow \langle\alpha|\hat{S}(\xi)|\beta\rangle = K(\alpha,\alpha^*,\beta^*,r,\theta)\exp\left(-\frac{1}{2}|\beta|^2 + \alpha^*\beta\mathrm{sech}r + \frac{1}{2}\mathrm{e}^{-\mathrm{i}\theta}\beta^2\tanh r\right) \tag{19.34}$$

$$\langle\alpha|\hat{S}(\xi)|\beta\rangle^* = \langle\beta|\hat{S}^\dagger(\xi)|\alpha\rangle = \langle\beta|\hat{S}(-\xi)|\alpha\rangle$$

$$\Rightarrow K^*\exp\left(-\frac{1}{2}|\beta|^2 + \frac{1}{2}\mathrm{e}^{\mathrm{i}\theta}(\beta^*)^2\tanh r\right) = K\exp\left(-\frac{1}{2}|\alpha|^2 - \frac{1}{2}\mathrm{e}^{-\mathrm{i}\theta}\alpha^2\tanh r\right) \tag{19.35}$$

$$\Rightarrow K = (\mathrm{sech}r)^{\frac{1}{2}}\exp\left(-\frac{1}{2}|\alpha|^2 - \frac{1}{2}\mathrm{e}^{\mathrm{i}\theta}(\alpha^*)^2\tanh r\right) \tag{19.36}$$

$$\Rightarrow \langle\alpha|\beta,\xi\rangle = (\mathrm{sech}r)^{\frac{1}{2}}\exp\left\{-\frac{1}{2}(|\alpha|^2+|\beta|^2) + \alpha^*\beta\mathrm{sech}r - \frac{1}{2}\left[\mathrm{e}^{\mathrm{i}\theta}(\alpha^*)^2 - \mathrm{e}^{-\mathrm{i}\theta}\beta^2\right]\tanh r\right\} \tag{19.37}$$

$$Q(\alpha,\alpha^*) = \frac{1}{\pi}|\langle\alpha|\beta,\xi\rangle|^2$$

$$= \frac{\mathrm{sech}r}{\pi}\exp\left\{-\left(|\alpha|^2+|\beta|^2\right) + (\alpha\beta^*+\beta\alpha^*)\mathrm{sech}r - \frac{1}{2}\left[\mathrm{e}^{\mathrm{i}\theta}(\alpha^{*2}-\beta^2) + \mathrm{e}^{-\mathrm{i}\theta}(\alpha^2-\beta^{*2})\right]\tanh r\right\} \tag{19.38}$$

19.3 Wigner-Weyl W 表示

1. 对称排列的算符:

$$\frac{1}{2}\langle\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\rangle = \int \mathrm{d}^2\alpha\, W(\alpha,\alpha^*)\alpha\alpha^* \tag{19.39}$$

2. 三种分布函数:

$$P(\alpha,\alpha^*) = \frac{1}{\pi^2}\int \mathrm{d}^2\beta\,\mathrm{e}^{-\mathrm{i}\beta\alpha^*-\mathrm{i}\beta^*\alpha}C^{(n)}(\beta,\beta^*), \quad C^{(n)}(\beta,\beta^*) = \mathrm{tr}\left(\mathrm{e}^{i\beta\hat{a}^\dagger}\mathrm{e}^{i\beta^*\hat{a}}\hat{\rho}\right) \tag{19.40}$$

$$Q(\alpha,\alpha^*) = \frac{1}{\pi^2}\int \mathrm{d}^2\beta\,\mathrm{e}^{-\mathrm{i}\beta\alpha^*-\mathrm{i}\beta^*\alpha}C^{(a)}(\beta,\beta^*), \quad C^{(a)}(\beta,\beta^*) = \mathrm{tr}\left(\mathrm{e}^{\mathrm{i}\beta^*\hat{a}}\mathrm{e}^{\mathrm{i}\beta\hat{a}^\dagger}\hat{\rho}\right) \tag{19.41}$$

$$W(\alpha,\alpha^*) = \frac{1}{\pi^2}\int \mathrm{d}^2\beta\,\mathrm{e}^{-\mathrm{i}\beta\alpha^*-\mathrm{i}\beta^*\alpha}C^{(s)}(\beta,\beta^*), \quad C^{(s)}(\beta,\beta^*) = \mathrm{tr}\left(\mathrm{e}^{\mathrm{i}\beta\hat{a}^\dagger+\mathrm{i}\beta^*\hat{a}}\hat{\rho}\right) \tag{19.42}$$

3. Wigner 函数:

$$W(x,p) = \frac{1}{\pi\hbar}\int_{-\infty}^{+\infty}\langle x-x'|\hat{\rho}|x+x'\rangle\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}2px'}\mathrm{d}x' = \frac{1}{\pi\hbar}\int_{-\infty}^{+\infty}\langle p-p'|\hat{\rho}|p+p'\rangle\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}2xp'}\mathrm{d}p' \tag{19.43}$$

4. Wigner 函数的计算:

$$W(\alpha,\alpha^*) = \frac{2}{\pi^2}\mathrm{e}^{2|\alpha|^2}\int \mathrm{d}^2\beta\,\langle-\beta|\hat{\rho}|\beta\rangle\,\mathrm{e}^{-2(\beta\alpha^*-\beta^*\alpha)} \tag{19.44}$$

19.4 三种分布函数的关系

1. 密度算符的广义表示：

$$\hat{\rho} = \pi \int \mathrm{d}^2\alpha \, F^{(\Omega)}(\alpha, \alpha^*) \Delta^{(\Omega)}(\alpha - \hat{a}, \alpha^* - \hat{a}^\dagger) \tag{19.45}$$

$$\Delta^{(\Omega)}(\alpha - \hat{a}, \alpha^* - \hat{a}^\dagger) = \frac{1}{\pi^2} \int \mathrm{d}^2\beta \, \exp\Big[\Omega(\beta, \beta^*)\Big] \exp\Big[- \beta(\alpha^* - \hat{a}^\dagger) + \beta^*(\alpha - \hat{a})\Big] \tag{19.46}$$

(1) P 表示：

$$\Omega(\beta, \beta^*) = -\frac{|\beta|^2}{2}, \quad F^{(\Omega)}(\alpha, \alpha^*) = P(\alpha, \alpha^*) \tag{19.47}$$

(2) Q 表示：

$$\Omega(\beta, \beta^*) = \frac{|\beta|^2}{2}, \quad F^{(\Omega)}(\alpha, \alpha^*) = Q(\alpha, \alpha^*) \tag{19.48}$$

(3) W 表示：

$$\Omega(\beta, \beta^*) = 0, \quad F^{(\Omega)}(\alpha, \alpha^*) = W(\alpha, \alpha^*) \tag{19.49}$$

2. 三种分布函数的关系：

$$Q(\alpha, \alpha^*) = \frac{1}{\pi} \int \mathrm{d}^2\alpha' \, P(\alpha', \alpha'^*) \mathrm{e}^{-|\alpha - \alpha'|^2}, \quad P(\alpha, \alpha^*) = \exp\left(-\frac{\partial^2}{\partial\alpha^*\partial\alpha}\right) Q(\alpha, \alpha^*) \tag{19.50}$$

$$W(\alpha, \alpha^*) = \frac{2}{\pi} \int \mathrm{d}^2\alpha' \, P(\alpha', \alpha'^*) \mathrm{e}^{-2|\alpha - \alpha'|^2}, \quad P(\alpha, \alpha^*) = \exp\left(-\frac{1}{2} \frac{\partial^2}{\partial\alpha^*\partial\alpha}\right) W(\alpha, \alpha^*) \tag{19.51}$$

20 电磁场量子化

20.1 谐振腔内的电磁场量子化

1. 电磁场在腔内本征模式展开：

$$\nabla^2 \boldsymbol{u}_l(\boldsymbol{r}) + k_l^2 \boldsymbol{u}_l(\boldsymbol{r}) = 0 \tag{20.1}$$

$$\frac{\mathrm{d}^2 p_l(t)}{\mathrm{d}t^2} + \omega_l^2 p_l(t) = 0, \quad \frac{\mathrm{d}^2 q_l(t)}{\mathrm{d}t^2} + \omega_l^2 q_l(t) = 0 \tag{20.2}$$

$$\boldsymbol{E}(\boldsymbol{r},t) = \frac{1}{\sqrt{\varepsilon_0}} \sum_l p_l(t)\boldsymbol{u}_l(\boldsymbol{r}), \quad \boldsymbol{H}(\boldsymbol{r},t) = \frac{1}{\sqrt{\mu_0}} \sum_l q_l(t) \nabla \times \boldsymbol{u}_l(\boldsymbol{r}) \tag{20.3}$$

2. 电磁场 Hamilton 量：

$$H_{EM} = \frac{1}{2}\int_V \left(\varepsilon_0 \boldsymbol{E}^2 + \mu_0 \boldsymbol{H}^2\right) \mathrm{d}V = \sum_l \frac{1}{2}\left(p_l^2(t) + \omega_l^2 q_l^2(t)\right) = \sum_l H_l \tag{20.4}$$

3. 电磁场产生湮灭算符：

$$\hat{a}_l(t) = \frac{1}{\sqrt{2\hbar\omega_l}}(\omega_l \hat{q}_l(t) + \mathrm{i}\hat{p}_l(t)), \quad \hat{a}_l^\dagger(t) = \frac{1}{\sqrt{2\hbar\omega_l}}(\omega_l \hat{q}_l(t) - \mathrm{i}\hat{p}_l(t)) \tag{20.5}$$

$$\hat{H}_{EM} = \frac{1}{2}\sum_l \hbar\omega_l \left(\hat{a}_l^\dagger \hat{a}_l + \hat{a}_l \hat{a}_l^\dagger\right) = \sum_l \hbar\omega_l \left(\hat{a}_l^\dagger \hat{a}_l + \frac{1}{2}\right) \tag{20.6}$$

4. 电磁场量子化：

$$\hat{\boldsymbol{A}}(\boldsymbol{r},t) = \sum_l \sqrt{\frac{\hbar}{2\varepsilon_0\omega_l}} (\hat{a}_l^\dagger(t) + \hat{a}_l(t)) \boldsymbol{u}_l(\boldsymbol{r}) \tag{20.7}$$

$$\hat{\boldsymbol{E}}(\boldsymbol{r},t) = -\mathrm{i}\sum_l \sqrt{\frac{\hbar\omega_l}{2\varepsilon_0}} (\hat{a}_l^\dagger(t) - \hat{a}_l(t)) \boldsymbol{u}_l(\boldsymbol{r}) \tag{20.8}$$

$$\hat{\boldsymbol{H}}(\boldsymbol{r},t) = \sum_l \sqrt{\frac{\hbar\omega_l}{2\mu_0}} (\hat{a}_l^\dagger(t) + \hat{a}_l(t)) \nabla \times \boldsymbol{u}_l(\boldsymbol{r}) \tag{20.9}$$

20.2 自由空间的电磁场量子化

1. 磁矢势的行波解：

$$\boldsymbol{A}(\boldsymbol{r},t) = \frac{1}{\sqrt{V}} \sum_{k\sigma} \boldsymbol{e}_\sigma \left(A_{k\sigma} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r} - \omega_k t)} + A_{k\sigma}^\dagger \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r} - \omega_k t)}\right) \tag{20.10}$$

2. 电磁场产生湮灭算符：

$$\hat{a}_{k\sigma}(t) = \hat{a}_{k\sigma} \mathrm{e}^{-\mathrm{i}\omega_k t} = \sqrt{\frac{2\varepsilon_0\omega_k}{\hbar}} A_{k\sigma} \mathrm{e}^{-\mathrm{i}\omega_k t} \tag{20.11}$$

$$\hat{H}_{EM} = \sum_{k\sigma} \hbar\omega_k \left(\hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} + \frac{1}{2}\right) \tag{20.12}$$

3. 电磁场量子化：

$$\hat{\boldsymbol{A}}(\boldsymbol{r},t) = \sum_{k\sigma} \boldsymbol{e}_\sigma \sqrt{\frac{\hbar}{2\varepsilon_0\omega_k V}} \left(\hat{a}_{k\sigma} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r} - \omega_k t)} + \hat{a}_{k\sigma}^\dagger \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r} - \omega_k t)}\right) \tag{20.13}$$

$$\hat{\boldsymbol{E}}(\boldsymbol{r},t) = \mathrm{i}\sum_{k\sigma} \boldsymbol{e}_\sigma \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0 V}} \left(\hat{a}_{k\sigma} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r} - \omega_k t)} - \hat{a}_{k\sigma}^\dagger \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r} - \omega_k t)}\right) \tag{20.14}$$

$$\hat{\boldsymbol{H}}(\boldsymbol{r},t) = \mathrm{i}\sum_{k\sigma} \frac{c\boldsymbol{k} \times \boldsymbol{e}_\sigma}{\omega_k} \sqrt{\frac{\hbar\omega_k}{2\mu_0 V}} \left(\hat{a}_{k\sigma} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r} - \omega_k t)} - \hat{a}_{k\sigma}^\dagger \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r} - \omega_k t)}\right) \tag{20.15}$$

$$\hat{\boldsymbol{P}} = \frac{1}{c^2}\int_V \hat{\boldsymbol{E}} \times \hat{\boldsymbol{H}} \mathrm{d}V = \frac{1}{2}\sum_{k\sigma} \hbar\boldsymbol{k} (\hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} + \hat{a}_{k\sigma} \hat{a}_{k\sigma}^\dagger) \tag{20.16}$$

21 光场相干性及其干涉

21.1 量子相关函数

1. 电场算符:

$$\hat{E}(\boldsymbol{r},t)=\hat{E}^{+}(\boldsymbol{r},t)+\hat{E}^{-}(\boldsymbol{r},t) \tag{21.1}$$

$$\hat{E}^{+}(\boldsymbol{r},t)=\sum_{k\sigma}\boldsymbol{e}_{\sigma}\mathcal{E}_{k}\hat{a}_{k\sigma}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{k}t)},\quad \hat{E}^{-}(\boldsymbol{r},t)=(\hat{E}^{+}(\boldsymbol{r},t))^{\dagger} \tag{21.2}$$

2. 电磁场吸收一、二个光子的总跃迁概率:

$$w_1(\boldsymbol{r},t)=\sum_{f}|\langle f|\hat{E}^{+}(\boldsymbol{r},t)|i\rangle|^2=\langle i|\hat{E}^{-}(\boldsymbol{r},t)\hat{E}^{+}(\boldsymbol{r},t)|i\rangle \tag{21.3}$$

$$w_2(\boldsymbol{r}_1,\boldsymbol{r}_2;t_1,t_2)=\langle i|\hat{E}^{-}(\boldsymbol{r}_2,t_2)\hat{E}^{-}(\boldsymbol{r}_2,t_2)\hat{E}^{+}(\boldsymbol{r}_1,t_1)\hat{E}^{+}(\boldsymbol{r}_1,t_1)|i\rangle \tag{21.4}$$

3. 一、二阶相关函数:

$$G^{(1)}(\boldsymbol{r}_1,\boldsymbol{r}_2;t_1,t_2)=\langle\hat{E}^{-}(\boldsymbol{r}_1,t_1)\hat{E}^{+}(\boldsymbol{r}_2,t_2)\rangle \tag{21.5}$$

$$G^{(2)}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3,\boldsymbol{r}_4;t_1,t_2,t_3,t_4)=\langle\hat{E}^{-}(\boldsymbol{r}_1,t_1)\hat{E}^{-}(\boldsymbol{r}_2,t_2)\hat{E}^{+}(\boldsymbol{r}_3,t_3)\hat{E}^{+}(\boldsymbol{r}_4,t_4)\rangle \tag{21.6}$$

4. 一、二阶相干度:

$$g^{(1)}(\boldsymbol{r}_1,\boldsymbol{r}_2;t_1,t_2)=\frac{\langle\hat{E}^{-}(\boldsymbol{r}_1,t_1)\hat{E}^{+}(\boldsymbol{r}_2,t_2)\rangle}{\sqrt{\langle\hat{E}^{-}(\boldsymbol{r}_1,t_1)\hat{E}^{+}(\boldsymbol{r}_1,t_1)\rangle\langle\hat{E}^{-}(\boldsymbol{r}_2,t_2)\hat{E}^{+}(\boldsymbol{r}_2,t_2)\rangle}} \tag{21.7}$$

$$g^{(2)}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_2,\boldsymbol{r}_1;t_1,t_2,t_2,t_1)=\frac{\langle\hat{E}^{-}(\boldsymbol{r}_1,t_1)\hat{E}^{-}(\boldsymbol{r}_2,t_2)\hat{E}^{+}(\boldsymbol{r}_2,t_2)\hat{E}^{+}(\boldsymbol{r}_1,t_1)\rangle}{\langle\hat{E}^{-}(\boldsymbol{r}_1,t_1)\hat{E}^{+}(\boldsymbol{r}_1,t_1)\rangle\langle\hat{E}^{-}(\boldsymbol{r}_2,t_2)\hat{E}^{+}(\boldsymbol{r}_2,t_2)\rangle} \tag{21.8}$$

5. 单模情形下，在空间固定位置处:

$$g^{(1)}(\tau)=\frac{\langle\hat{a}^{\dagger}(t+\tau)\hat{a}(t)\rangle}{\langle\hat{a}^{\dagger}\hat{a}\rangle},\quad g^{(2)}(\tau)=\frac{\langle\hat{a}^{\dagger}(t)\hat{a}^{\dagger}(t+\tau)\hat{a}(t+\tau)\hat{a}(t)\rangle}{\langle\hat{a}^{\dagger}\hat{a}\rangle^2} \tag{21.9}$$

21.2 经典场-场干涉

21.2.1 Michelson 干涉仪和引力波探测

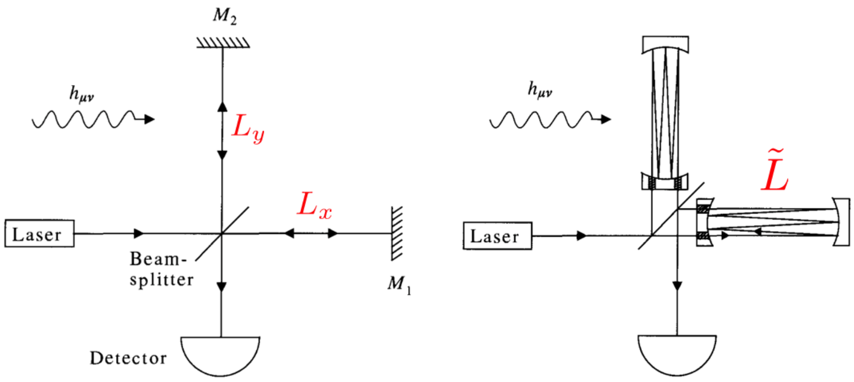

图 1: Michelson interferometer

1. 长度变化:

$$L_x=L(1+h_0\cos\omega_g t),\quad L_y=L \tag{21.10}$$

2. 相移:

$$\Delta\theta^{(p)}=\frac{\omega}{c}\widetilde{L}h_0,\quad \Delta\theta_n\sim\frac{1}{\sqrt{\langle n\rangle}}=\sqrt{\frac{\hbar\omega}{Pt_m}} \tag{21.11}$$

3. 最小可测引力波振幅:

$$h_{\min}^{(p)}\sim\frac{c}{\nu\widetilde{L}}\sqrt{\frac{\hbar\omega}{Pt_m}}=\frac{\varrho}{\nu}\sqrt{\frac{\hbar\omega}{Pt_m}} \tag{21.12}$$

21.2.2 Sagnac 环形干涉仪

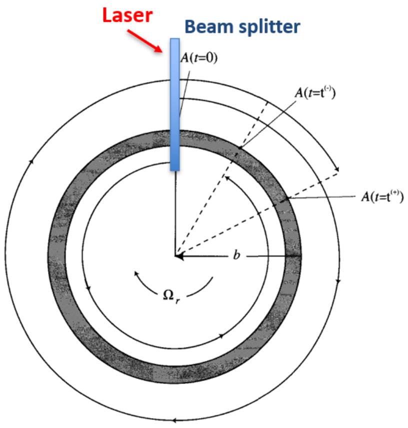

图 2: The Sagnac ring interferometer

1. 接收时间：

$$t^+ = \frac{2\pi b + b\Omega_r t^+}{c} = \frac{2\pi b}{c}\left(1 - \frac{b\Omega_r}{c}\right)^{-1} \tag{21.13}$$

$$t^- = \frac{2\pi b + b\Omega_r t^-}{c} = \frac{2\pi b}{c}\left(1 + \frac{b\Omega_r}{c}\right)^{-1} \tag{21.14}$$

2. 时间差：

$$\Delta t = t^+ - t^- = \frac{4\pi b^2\Omega_r}{c^2 - b^2\Omega_r^2} \approx \frac{4\pi b^2\Omega_r}{c^2} \tag{21.15}$$

3. 光程差：

$$\Delta L = c\Delta t = \frac{4\pi b^2\Omega_r}{c} = \frac{2bL\Omega_r}{c}, \quad L = 2\pi b \tag{21.16}$$

21.2.3 Michelson 星光干涉仪

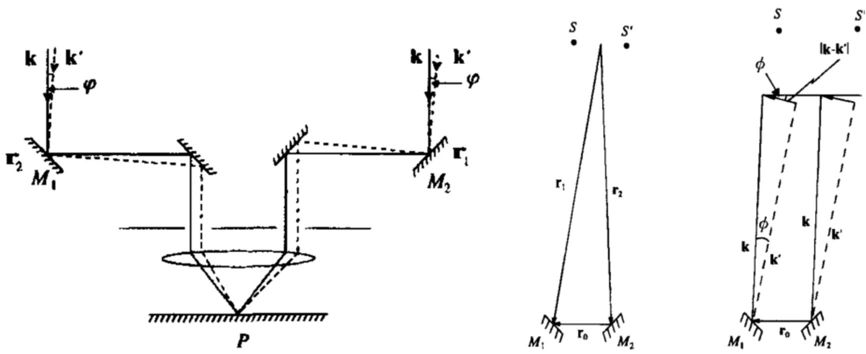

图 3: Michelson stellar interferometer

1. 接收的光场：

$$\hat{E}^+(\boldsymbol{r},t) = \hat{E}_k^+(\boldsymbol{r}_1,t) + \hat{E}_k^+(\boldsymbol{r}_2,t) + \hat{E}_{k'}(\boldsymbol{r}_1,t) + \hat{E}_{k'}(\boldsymbol{r}_2,t), \quad \hat{\xi}_k = \boldsymbol{e}_\sigma \mathcal{E}_k \hat{a}_{k\sigma} \tag{21.17}$$

2. 接收的光强：

$$\begin{aligned} I &= K\langle \hat{E}^-(\boldsymbol{r},t)\hat{E}^+(\boldsymbol{r},t)\rangle = K\left\langle \left|\hat{\xi}_k\left(e^{i\boldsymbol{k}\cdot\boldsymbol{r}_1} + e^{i\boldsymbol{k}\cdot\boldsymbol{r}_2}\right) + \hat{\xi}_{k'}\left(e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_1} + e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_2}\right)\right|^2 \right\rangle \\ &= K\left\langle 2\left(|\hat{\xi}_k|^2 + |\hat{\xi}_{k'}|^2\right) + |\hat{\xi}_k|^2\left(e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)} + c.c.\right) + |\hat{\xi}_{k'}|^2\left(e^{i\boldsymbol{k}'\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)} + c.c.\right)\right\rangle \\ &= 2KI_0\left[2 + \cos\left(\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)\right) + \cos\left(\boldsymbol{k}'\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)\right)\right] \\ &\approx 4KI_0\left[1 + \cos\frac{(\boldsymbol{k}+\boldsymbol{k}')\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}{2}\cos\frac{\pi r_0\varphi}{\lambda}\right] \end{aligned} \tag{21.18}$$

21.2.4 Young's 双缝干涉

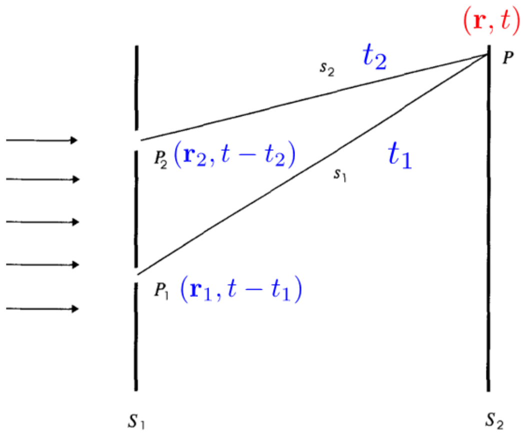

图 4: Young's double-slit experiment

1. 干涉屏上的光场分布:

$$\hat{E}^+(\boldsymbol{r},t) = K_1\hat{E}^+(\boldsymbol{r}_1,t-t_1) + K_2\hat{E}^+(\boldsymbol{r}_2,t-t_2), \quad s_i = ct_i \tag{21.19}$$

2. 干涉屏上的光强分布:

$$\begin{aligned}
\langle I(\boldsymbol{r},t)\rangle &= \langle \hat{E}^-(\boldsymbol{r},t)\hat{E}^+(\boldsymbol{r},t)\rangle \\
&= |K_1|^2 \langle \hat{E}^-(\boldsymbol{r}_1,t-t_1)\hat{E}^+(\boldsymbol{r}_1,t-t_1)\rangle + |K_2|^2 \langle \hat{E}^-(\boldsymbol{r}_2,t-t_2)\hat{E}^+(\boldsymbol{r}_2,t-t_2)\rangle \\
&+ 2\mathrm{Re}\left[(|K_1^* K_2 \langle \hat{E}^-(\boldsymbol{r}_1,t-t_1)\hat{E}^+(\boldsymbol{r}_2,t-t_2)\rangle\right] \\
&= |K_1|^2 G^{(1)}(\boldsymbol{r}_1,\boldsymbol{r}_1;0) + |K_2|^2 G^{(1)}(\boldsymbol{r}_2,\boldsymbol{r}_2;0) + 2\mathrm{Re}\left[K_1^* K_2 G^{(1)}(\boldsymbol{r}_1,\boldsymbol{r}_2;\tau)\right] \\
&= \langle I_1(\boldsymbol{r},t)\rangle + \langle I_2(\boldsymbol{r},t)\rangle + 2\sqrt{\langle I_1(\boldsymbol{r},t)\rangle \langle I_2(\boldsymbol{r},t)\rangle}\left|g^{(1)}(\boldsymbol{r}_1,\boldsymbol{r}_2;\tau)\right| \cos\left[k(s_1-s_2)+\phi\right]
\end{aligned} \tag{21.20}$$

3. 衬比度:

$$\gamma = \frac{\langle I(\boldsymbol{r},t)\rangle_{\max} - \langle I(\boldsymbol{r},t)\rangle_{\min}}{\langle I(\boldsymbol{r},t)\rangle_{\max} + \langle I(\boldsymbol{r},t)\rangle_{\min}} = \frac{2\sqrt{\langle I_1(\boldsymbol{r},t)\rangle \langle I_2(\boldsymbol{r},t)\rangle}}{\langle I_1(\boldsymbol{r},t)\rangle + \langle I_2(\boldsymbol{r},t)\rangle}\left|g^{(1)}(\boldsymbol{r}_1,\boldsymbol{r}_2;\tau)\right| \tag{21.21}$$

21.3 量子光-光干涉

21.3.1 Hanbury-Brown-Twiss 干涉仪

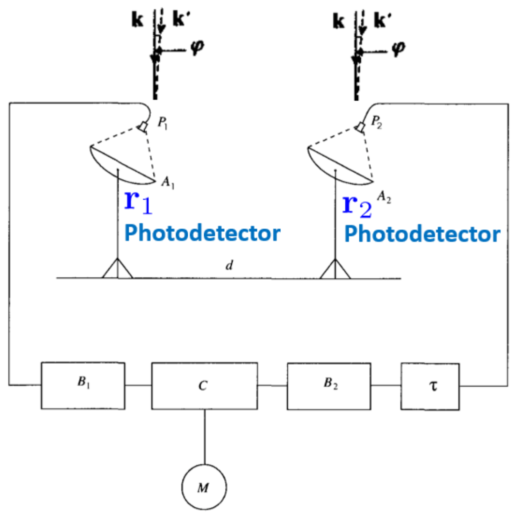

图 5: Hanbury-Brown-Twiss interferometer

1. 接收的光场：

$$\hat{E}^{+}(\boldsymbol{r}_i,t)=\hat{E}_k^{+}(\boldsymbol{r}_i,t)+\hat{E}_{k'}^{+}(\boldsymbol{r}_i,t),\quad \hat{\xi}_k=\boldsymbol{e}_\sigma\mathcal{E}_k\hat{a}_{k\sigma} \tag{21.22}$$

2. 接收的光强：

$$\begin{aligned}I(\boldsymbol{r}_i,t)&=K\langle\hat{E}^{-}(\boldsymbol{r}_i,t)\hat{E}^{+}(\boldsymbol{r}_i,t)\rangle=K\left\langle\left|\hat{\xi}_k\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_1}+\hat{\xi}_{k'}\mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}_1}\right|^2\right\rangle\\&=K\Big\langle|\hat{\xi}_k|^2+|\hat{\xi}_{k'}|^2+\big(\hat{\xi}_k\hat{\xi}_{k'}^{\dagger}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}_i}+c.c.\big)\Big\rangle\end{aligned} \tag{21.23}$$

3. 光强联合计数：

$$\begin{aligned}\langle I(\boldsymbol{r}_1,t)I(\boldsymbol{r}_2,t)\rangle&=K^2\left\langle\Big(|\hat{\xi}_k|^2+|\hat{\xi}_{k'}|^2+\big(\hat{\xi}_k\hat{\xi}_{k'}^{*}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}_1}+c.c.\big)\Big)\Big(|\hat{\xi}_k|^2+|\hat{\xi}_{k'}|^2+\big(\hat{\xi}_k\hat{\xi}_{k'}^{*}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}_2}+c.c.\big)\Big)\right\rangle\\&=K^2\Big[\big(\langle|\hat{\xi}_k|^2\rangle+\langle|\hat{\xi}_{k'}|^2\rangle\big)^2+\langle|\hat{\xi}_k|^2\rangle\langle|\hat{\xi}_{k'}|^2\rangle\big(\mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}+c.c.\big)\Big]\\&=K^2\left[\big(\langle|\hat{\xi}_k|^2\rangle+\langle|\hat{\xi}_{k'}|^2\rangle\big)^2+\langle|\hat{\xi}_k|^2\rangle\langle|\hat{\xi}_{k'}|^2\rangle2\cos\left(\frac{2\pi\varphi r_0}{\lambda}\right)\right]\end{aligned} \tag{21.24}$$

4. 二阶相关函数：

$$\begin{aligned}G^{(2)}(\boldsymbol{r}_1,\boldsymbol{r}_2;t,t)&=\langle\hat{E}^{(-)}(\boldsymbol{r}_1,t)\hat{E}^{(-)}(\boldsymbol{r}_2,t)\hat{E}^{(+)}(\boldsymbol{r}_2,t)\hat{E}^{(+)}(\boldsymbol{r}_1,t)\rangle\\&=\mathcal{E}_k^4\Big\langle\big(\hat{a}_k^{\dagger}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_1}+\hat{a}_{k'}^{\dagger}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}_1}\big)\big(\hat{a}_k^{\dagger}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_2}+\hat{a}_{k'}^{\dagger}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}_2}\big)\\&\times\big(\hat{a}_k\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_2}+\hat{a}_{k'}\mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}_2}\big)\big(\hat{a}_k\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_1}+\hat{a}_{k'}\mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}_1}\big)\Big\rangle\\&=\mathcal{E}_k^4\Big\langle\hat{a}_k^{\dagger}\hat{a}_k^{\dagger}\hat{a}_k\hat{a}_k+\hat{a}_{k'}^{\dagger}\hat{a}_{k'}^{\dagger}\hat{a}_{k'}\hat{a}_{k'}\\&+\hat{a}_k^{\dagger}\hat{a}_{k'}^{\dagger}\hat{a}_k\hat{a}_{k'}\Big(1+\mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}\Big)+\hat{a}_{k'}^{\dagger}\hat{a}_k^{\dagger}\hat{a}_{k'}\hat{a}_k\Big(1+\mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}\Big)\Big\rangle\\&=2\mathcal{E}_k^4\Big[\langle n^2\rangle-\langle n\rangle+\langle n\rangle^2\Big(1+\cos(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)\Big)\Big]\end{aligned} \tag{21.25}$$

(1) 星光：热场态

$$\langle n^2\rangle=2\langle n\rangle^2+\langle n\rangle \tag{21.26}$$

$$G^{(2)}(\boldsymbol{r}_1,\boldsymbol{r}_2;t,t)=2\mathcal{E}_k^4\Big[2\langle n^2\rangle+\langle n\rangle^2\Big(1+\cos(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)\Big)\Big] \tag{21.27}$$

(2) 激光：相干态

$$\langle n^2\rangle=\langle n\rangle^2+\langle n\rangle \tag{21.28}$$

$$G^{(2)}(\boldsymbol{r}_1,\boldsymbol{r}_2;t,t)=2\mathcal{E}_k^4\Big[\langle n^2\rangle+\langle n\rangle^2\Big(1+\cos(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)\Big)\Big] \tag{21.29}$$

21.3.2 Hong-Ou-Mandel 干涉仪

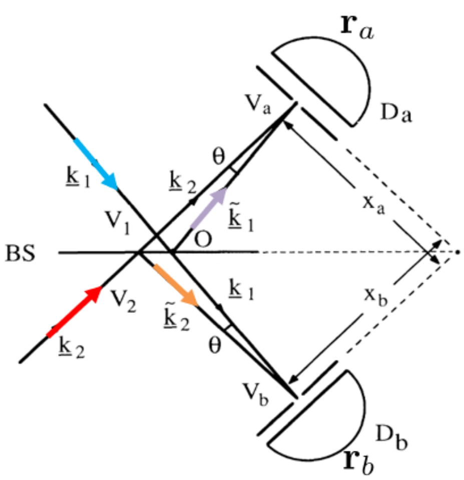

图 6: Hong-Ou-Mandel interferometer

1. 接收的光场：

$$\hat{E}^{+}(\boldsymbol{r}_a)=\frac{1}{2}\mathcal{E}_k\left(\mathrm{i}\hat{a}_1\mathrm{e}^{\mathrm{i}\widetilde{\boldsymbol{k}}_1\cdot\boldsymbol{r}_a}+\hat{a}_2\mathrm{e}^{\mathrm{i}\boldsymbol{k}_2\cdot\boldsymbol{r}_a}\right) \tag{21.30}$$

$$\hat{E}^{+}(\boldsymbol{r}_b)=\frac{1}{2}\mathcal{E}_k\left(\mathrm{i}\hat{a}_1\mathrm{e}^{\mathrm{i}\boldsymbol{k}_1\cdot\boldsymbol{r}_b}+\hat{a}_2\mathrm{e}^{\mathrm{i}\widetilde{\boldsymbol{k}}_2\cdot\boldsymbol{r}_b}\right) \tag{21.31}$$

2. 双光子联合探测概率：

$$\begin{aligned}P(\boldsymbol{r}_a,\boldsymbol{r}_b)&=K_aK_b\left\langle 1,1\right|\hat{E}^{(-)}(\boldsymbol{r}_a)\hat{E}^{(-)}(\boldsymbol{r}_b)\hat{E}^{(+)}(\boldsymbol{r}_b)\hat{E}^{(+)}(\boldsymbol{r}_a)\left|1,1\right\rangle\\&=\frac{1}{2}K_aK_b\mathcal{E}_k^4\left\{1-\cos\left[(\boldsymbol{k}_2-\widetilde{\boldsymbol{k}}_1)\cdot\boldsymbol{r}_a-(\widetilde{\boldsymbol{k}}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}_b\right]\right\}\\&=\frac{1}{2}K_aK_b\mathcal{E}_k^4\left[1-\cos\frac{2\pi(x_a-x_b)}{L}\right]\end{aligned} \tag{21.32}$$

3. 衬比度：

$$\gamma=\frac{P_{\max}(\boldsymbol{r}_a,\boldsymbol{r}_b)-P_{\min}(\boldsymbol{r}_a,\boldsymbol{r}_b)}{P_{\max}(\boldsymbol{r}_a,\boldsymbol{r}_b)+P_{\min}(\boldsymbol{r}_a,\boldsymbol{r}_b)}=1 \tag{21.33}$$

21.4 分束器的量子力学描述

1. 分束器：

$$\begin{pmatrix}\hat{b}_1\\\hat{b}_2\end{pmatrix}=\begin{pmatrix}t&r\\r&t\end{pmatrix}\begin{pmatrix}\hat{a}_1\\\hat{a}_2\end{pmatrix} \tag{21.34}$$

$$|r|^2+|t|^2=1,\quad tr^*+rt^*=0 \tag{21.35}$$

2. 分束器的性质：

(1) 光子数守恒：

$$\hat{b}_1^\dagger\hat{b}_1+\hat{b}_2^\dagger\hat{b}_2=\hat{a}_1^\dagger\hat{a}_1+\hat{a}_2^\dagger\hat{a}_2 \tag{21.36}$$

(2) 经典输入输出关系：

$$\hat{\rho}_{\text{in}}=\hat{\rho}_1\otimes|0\rangle\langle 0| \tag{21.37}$$

$$\langle\hat{b}_1^\dagger\hat{b}_1\rangle=\operatorname{tr}\left(\hat{b}_1^\dagger\hat{b}_1\hat{\rho}_{\text{in}}\right)=|t|^2\operatorname{tr}\left(\hat{a}_1^\dagger\hat{a}_1\hat{\rho}_1\right) \tag{21.38}$$

$$\langle\hat{b}_2^\dagger\hat{b}_2\rangle=\operatorname{tr}\left(\hat{b}_2^\dagger\hat{b}_2\hat{\rho}_{\text{in}}\right)=|r|^2\operatorname{tr}\left(\hat{a}_1^\dagger\hat{a}_1\hat{\rho}_1\right) \tag{21.39}$$

(3) 单光子不可再分：

$$\hat{\rho}_{\text{in}}=|1\rangle\langle 1|\otimes|0\rangle\langle 0| \tag{21.40}$$

$$G^{(2)}(\boldsymbol{r}_1,\boldsymbol{r}_2;t,t)=\langle\hat{b}_1^\dagger\hat{b}_2^\dagger\hat{b}_1\hat{b}_2\rangle=|r|^2|t|^2\left[\langle(\hat{a}_1^\dagger\hat{a}_1)^2\rangle-\langle\hat{a}_1^\dagger\hat{a}_1\rangle\right]=0 \tag{21.41}$$

(4) 双光子干涉：

$$\hat{\rho}_{\text{in}}=|1\rangle\langle 1|\otimes|1\rangle\langle 1| \tag{21.42}$$

$$G^{(2)}(\boldsymbol{r}_1,\boldsymbol{r}_2;t,t)=\langle\hat{b}_1^\dagger\hat{b}_2^\dagger\hat{b}_1\hat{b}_2\rangle=(|t|^2-|r|^2)^2=0 \tag{21.43}$$

21.5 压缩光场的零拍探测

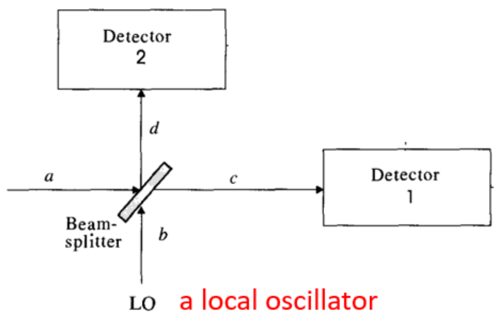

图 7: Detection and measurement of the squeezed state via HD

1. 输出光场：

$$\hat{c}=\sqrt{T}\hat{a}+\mathrm{i}\sqrt{1-T}\hat{b},\quad \hat{d}=\mathrm{i}\sqrt{1-T}\hat{a}+\sqrt{T}\hat{b} \tag{21.44}$$

2. 探测的光子数：

$$\hat{c}^\dagger\hat{c}=T\hat{a}^\dagger\hat{a}+(1-T)\hat{b}^\dagger\hat{b}+\mathrm{i}\sqrt{T(1-T)}\big(\hat{a}^\dagger\hat{b}-\hat{b}^\dagger\hat{a}\big) \tag{21.45}$$

$$\hat{d}^\dagger\hat{d}=(1-T)\hat{a}^\dagger\hat{a}+T\hat{b}^\dagger\hat{b}-\mathrm{i}\sqrt{T(1-T)}\big(\hat{a}^\dagger\hat{b}-\hat{b}^\dagger\hat{a}\big) \tag{21.46}$$

3. 大振幅本地相干光场：

$$\hat{b}\,|\beta_l\rangle=\beta_l\,|\beta_l\rangle\,,\quad \beta_l=|\beta_l|\mathrm{e}^{\mathrm{i}\phi_l} \tag{21.47}$$

4. 普通零拍探测：

$$T\approx 1\gg R \tag{21.48}$$

(1) 探测的光子数：

$$\begin{aligned}\langle\hat{c}^\dagger\hat{c}\rangle&=T\,\langle\hat{a}^\dagger\hat{a}\rangle+(1-T)|\beta_l|^2-2\sqrt{T(1-T)}|\beta_l|\left\langle X\left(\phi_l+\frac{\pi}{2}\right)\right\rangle\\&\approx(1-T)|\beta_l|^2-2\sqrt{T(1-T)}|\beta_l|\left\langle X\left(\phi_l+\frac{\pi}{2}\right)\right\rangle,\quad X(\phi)=\frac{1}{2}\left(\hat{a}\mathrm{e}^{-\mathrm{i}\phi}+\hat{a}^\dagger\mathrm{e}^{\mathrm{i}\phi}\right)\end{aligned} \tag{21.49}$$

(2) 探测的光子数涨落：

$$(\Delta n_c)^2=(1-T)|\beta_l|^2\left\{(1-T)+4T\left[\Delta X\left(\phi_l+\frac{\pi}{2}\right)\right]^2\right\} \tag{21.50}$$

(3) 输入压缩光：

$$\left[\Delta X\left(\phi_l+\frac{\pi}{2}\right)\right]^2<\frac{1}{4}\Rightarrow(\Delta n_c)^2<(1-T)|\beta_l|^2 \tag{21.51}$$

5. 平衡零拍探测：

$$T=R=\frac{1}{2} \tag{21.52}$$

(1) 探测的光子数差：

$$n_{cd}=\hat{c}^\dagger\hat{c}-\hat{d}^\dagger\hat{d}=-\mathrm{i}(\hat{a}^\dagger\hat{b}-\hat{b}^\dagger\hat{a}) \tag{21.53}$$

$$\langle n_{cd}\rangle=-2|\beta_l|\left\langle X\left(\phi_l+\frac{\pi}{2}\right)\right\rangle,\quad X(\phi)=\frac{1}{2}\left(\hat{a}\mathrm{e}^{-\mathrm{i}\phi}+\hat{a}^\dagger\mathrm{e}^{\mathrm{i}\phi}\right) \tag{21.54}$$

(2) 探测的光子数差涨落：

$$(\Delta n_{cd})^2=4|\beta_l|^2\left[\Delta X\left(\phi_l+\frac{\pi}{2}\right)\right]^2 \tag{21.55}$$

21.6 光场相干性的量子理论

1. 二阶相干度的经典理论：

$$g_c^{(2)}(\tau)=\frac{\langle I_1(t)I_2(t+\tau)\rangle}{\langle I_1(t)\rangle\,\langle I_2(t)\rangle} \tag{21.56}$$

$$\langle I_1(t)I_2(t)\rangle\geqslant\langle I_1(t)\rangle\,\langle I_2(t)\rangle\,,\quad \langle I_1(t)I_2(t)\rangle\geqslant\langle I_1(t)I_2(t+\tau)\rangle \tag{21.57}$$

$$g_c^{(2)}(0)\geqslant 1,\quad g_c^{(2)}(0)\geqslant g_c^{(2)}(\tau) \tag{21.58}$$

2. 二阶相干度的量子理论：

$$g^{(2)}(\tau)=\frac{\langle\hat{a}^\dagger(t)\hat{a}^\dagger(t+\tau)\hat{a}(t+\tau)\hat{a}(t)\rangle}{\langle\hat{a}^\dagger(t)\hat{a}(t)\rangle\,\langle\hat{a}^\dagger(t)\hat{a}(t+\tau)\rangle} \tag{21.59}$$

$$g^{(2)}(\tau)=g^{(2)}(0)=1+\frac{\langle(\Delta n)^2\rangle-\langle n\rangle}{\langle n\rangle^2} \tag{21.60}$$

3. 光子的群聚和反群聚效应：

$$g^{(2)}(0)\geqslant g^{(2)}(\tau)\Longleftrightarrow\text{群聚效应} \tag{21.61}$$

$$g^{(2)}(0)<g^{(2)}(\tau)\Longleftrightarrow\text{反群聚效应} \tag{21.62}$$

4. 不同光子数分布的二阶相干度:

(1) 相干态:

$$g^{(2)}(\tau) = g^{(2)}(0) = 1 \tag{21.63}$$

(2) 热场态:

$$g^{(2)}(\tau) = g^{(2)}(0) = 2 \tag{21.64}$$

(3) 粒子数态:

$$g^{(2)}(\tau) = g^{(2)}(0) = \begin{cases} 1 - \dfrac{1}{n} & n \geqslant 2 \\ 0 & n = 0, 1 \end{cases} \tag{21.65}$$

22 经典光场与原子相互作用

22.1 原子光场耦合和电偶极近似

1. 电磁场和带电粒子系统的演化：

$$\hat{H}\psi(\boldsymbol{r},t) = \mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) \tag{22.1}$$

$$\hat{H} = \frac{1}{2m}(\boldsymbol{P} - q\boldsymbol{A}(\boldsymbol{r},t))^2 + e\varphi(\boldsymbol{r},t) + V(\boldsymbol{r}) \tag{22.2}$$

2. Coulomb 规范：

$$\varphi^c(\boldsymbol{r},t) = 0, \quad \nabla\cdot\boldsymbol{A}^c(\boldsymbol{r},t) = 0 \tag{22.3}$$

(1) 系统演化：

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi^c(\boldsymbol{r},t) = \hat{H}^c\psi^c(\boldsymbol{r},t) \tag{22.4}$$

$$\hat{H}^c = \hat{H}_0 + \hat{H}_I^c = \frac{1}{2m}(\boldsymbol{P} - e\boldsymbol{A}(\boldsymbol{r},t))^2 + V(\boldsymbol{r}) \tag{22.5}$$

(2) 电偶极近似：$\boldsymbol{A}^c(\boldsymbol{r},t) \sim \boldsymbol{A}^c(\boldsymbol{r}_0,t)$，平方项不能导致跃迁

$$\hat{H}_I^c = -\frac{e}{m}\boldsymbol{A}^c(\boldsymbol{r},t)\cdot\boldsymbol{P} + \frac{e^2}{2m}(\boldsymbol{A}(\boldsymbol{r},t))^2 \approx -\frac{e}{m}\boldsymbol{A}^c(\boldsymbol{r}_0,t)\cdot\boldsymbol{P} \tag{22.6}$$

(3) 系统波函数在自由能量本征函数展开：

$$\psi^c(\boldsymbol{r},t) = \sum_n a_n(t)\psi_n(\boldsymbol{r}) \Rightarrow \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}a_n(t) = E_n a_n(t) + \sum_n \langle m|\hat{H}_I^c|n\rangle \tag{22.7}$$

(4) 跃迁矩阵元：

$$T_{mn}^c = \langle m|\hat{H}_I^c|n\rangle = \langle m| -\frac{e}{m}\boldsymbol{A}^c(\boldsymbol{r}_0,t)\cdot\boldsymbol{P}|n\rangle \tag{22.8}$$

3. 电场规范：

$$\varLambda(\boldsymbol{r},t) = -\boldsymbol{A}^c(\boldsymbol{r}_0,t)\cdot\boldsymbol{r} \tag{22.9}$$

$$\boldsymbol{A}^e(\boldsymbol{r},t) = \boldsymbol{A}^c(\boldsymbol{r}_0,t) + \nabla\varLambda(\boldsymbol{r},t) = 0, \quad \varphi^e(\boldsymbol{r},t) = -\frac{\partial}{\partial t}\varLambda(\boldsymbol{r},t) = -\boldsymbol{r}\cdot\boldsymbol{E}(\boldsymbol{r}_0,t) \tag{22.10}$$

(1) 系统演化：

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi^e(\boldsymbol{r},t) = \hat{H}^e\psi^e(\boldsymbol{r},t) \tag{22.11}$$

$$\hat{H}^e = \hat{H}_0 + \hat{H}_I^e = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{r}) - \boldsymbol{d}\cdot\boldsymbol{E}(\boldsymbol{r}_0,t) \tag{22.12}$$

(2) 系统量子态在自由能量本征态展开：

$$\psi^c(\boldsymbol{r},t) = \sum_n a_n(t)\psi_n(\boldsymbol{r}) \Rightarrow \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}a_n(t) = E_n a_n(t) + \sum_n \langle m|\hat{H}_I^e|n\rangle \tag{22.13}$$

(3) 跃迁矩阵元：

$$T_{mn}^e = \langle m|\hat{H}_I^e|n\rangle = \langle m| -\boldsymbol{d}\cdot\boldsymbol{E}(\boldsymbol{r}_0,t)|n\rangle \tag{22.14}$$

4. 两种规范的关系：

(1) 波函数的关系：

$$\psi^e(\boldsymbol{r},t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}e\varLambda(\boldsymbol{r},t)}\psi^c(\boldsymbol{r},t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}e\boldsymbol{A}^c(\boldsymbol{r}_0,t)\cdot\boldsymbol{r}}\psi^c(\boldsymbol{r},t) \tag{22.15}$$

(2) 跃迁矩阵元的关系：

$$\boldsymbol{E}(\boldsymbol{r}_0,t) = \boldsymbol{E}_0\cos\omega t, \quad \boldsymbol{A}^c(\boldsymbol{r}_0,t) = \frac{\boldsymbol{E}_0}{\omega}\sin\omega t \tag{22.16}$$

$$T_{mn}^c = \frac{E_m - E_n}{\hbar\omega}T_{mn}^e = \frac{\omega_{mn}}{\omega}T_{mn}^e \tag{22.17}$$

22.2　Rabi 振荡

1. 二能级原子的 Hamilton 量:

$$\hat{H}_0 = \hbar\omega_e \left|e\right\rangle\left\langle e\right| + \hbar\omega_g \left|g\right\rangle\left\langle g\right| = \frac{1}{2}\hbar(\omega_e+\omega_g)\hat{I} + \frac{1}{2}\hbar\omega_{eg}\hat{\sigma}_z \to \frac{1}{2}\hbar\omega_{eg}\hat{\sigma}_z \tag{22.18}$$

$$\hat{H}_I = -(\left|e\right\rangle\left\langle e\right| + \left|g\right\rangle\left\langle g\right|)\boldsymbol{d}(\left|e\right\rangle\left\langle e\right| + \left|g\right\rangle\left\langle g\right|)\cdot\boldsymbol{E}(t) = -(\boldsymbol{d}_{eg}\hat{\sigma}_+ + \boldsymbol{d}_{ge}\hat{\sigma}_-)\cdot\boldsymbol{E}(t) \tag{22.19}$$

2. 经典电场形式:

$$\boldsymbol{E}(t) = \boldsymbol{E}_0\cos\omega t, \quad \varOmega_{eg} = \frac{\boldsymbol{d}_{eg}\cdot\boldsymbol{E}_0}{\hbar}, \quad \varOmega_{ge} = \varOmega_{eg}^* \tag{22.20}$$

$$\hat{H}_I = -\frac{\hbar}{2}\left(\varOmega_{eg}\hat{\sigma}_+\mathrm{e}^{-\mathrm{i}\omega t} + \varOmega_{ge}\hat{\sigma}_-\mathrm{e}^{\mathrm{i}\omega t} + \varOmega_{eg}\hat{\sigma}_+\mathrm{e}^{\mathrm{i}\omega t} + \varOmega_{ge}\hat{\sigma}_-\mathrm{e}^{-\mathrm{i}\omega t}\right) \tag{22.21}$$

22.2.1　概率幅方法

1. 以光场频率 ω 旋转的坐标系中的 Hamilton 量:

$$\widetilde{U}(t) = \mathrm{e}^{\mathrm{i}\frac{1}{2}\omega\hat{\sigma}_z t}, \quad \varDelta = \omega_{eg} - \omega \tag{22.22}$$

$$\widetilde{H}_0 = \mathrm{i}\hbar\frac{\mathrm{d}\widetilde{U}}{\mathrm{d}t}\widetilde{U}^\dagger + \widetilde{U}\hat{H}_0\widetilde{U}^\dagger = -\frac{1}{2}\hbar\omega\hat{\sigma}_z + \frac{1}{2}\hbar\omega_{eg}\hat{\sigma}_z = \frac{1}{2}\hbar\varDelta\hat{\sigma}_z \tag{22.23}$$

$$\widetilde{H}_I = \widetilde{U}\hat{H}_I\widetilde{U}^\dagger = -\frac{\hbar}{2}\left(\varOmega_{eg}\hat{\sigma}_+ + \varOmega_{ge}\hat{\sigma}_- + \varOmega_{eg}\hat{\sigma}_+\mathrm{e}^{\mathrm{i}2\omega t} + \varOmega_{ge}\hat{\sigma}_-\mathrm{e}^{-\mathrm{i}2\omega t}\right) \tag{22.24}$$

$$\widetilde{H} = \frac{1}{2}\hbar\varDelta\hat{\sigma}_z + \frac{1}{2}\hbar\varOmega_R(\mathrm{e}^{\mathrm{i}\phi}\hat{\sigma}_+ + \mathrm{e}^{-\mathrm{i}\phi}\hat{\sigma}_-) \tag{22.25}$$

2. 二能级原子的演化:

$$\widetilde{H}\,|\widetilde{\psi}(t)\rangle = \mathrm{i}\hbar\frac{\partial}{\partial t}|\widetilde{\psi}(t)\rangle \tag{22.26}$$

$$|\widetilde{\psi}(t)\rangle = \widetilde{U}(t)\,|\psi(t)\rangle = C_e(t)\left|e\right\rangle + C_g(t)\left|g\right\rangle \tag{22.27}$$

3. 系数演化方程:

$$\begin{pmatrix}\dot{C}_e(t)\\ \dot{C}_g(t)\end{pmatrix} = -\frac{\mathrm{i}}{2}\begin{pmatrix}\varDelta & -\varOmega_R\mathrm{e}^{\mathrm{i}\phi}\\ -\varOmega_R\mathrm{e}^{-\mathrm{i}\phi} & -\varDelta\end{pmatrix}\begin{pmatrix}C_e(t)\\ C_g(t)\end{pmatrix} \tag{22.28}$$

4. 系数的形式解:

$$\begin{pmatrix}C_e(t)\\ C_g(t)\end{pmatrix} = \begin{pmatrix}\cos\dfrac{\varOmega t}{2} - \mathrm{i}\dfrac{\varDelta}{\varOmega}\sin\dfrac{\varOmega t}{2} & \mathrm{i}\dfrac{\varOmega_R}{\varOmega}\mathrm{e}^{\mathrm{i}\phi}\sin\dfrac{\varOmega t}{2}\\ \mathrm{i}\dfrac{\varOmega_R}{\varOmega}\mathrm{e}^{-\mathrm{i}\phi}\sin\dfrac{\varOmega t}{2} & \cos\dfrac{\varOmega t}{2} + \mathrm{i}\dfrac{\varDelta}{\varOmega}\sin\dfrac{\varOmega t}{2}\end{pmatrix}\begin{pmatrix}C_e(0)\\ C_g(0)\end{pmatrix} \tag{22.29}$$

$$\varOmega_R = |\varOmega_{eg}| = |\varOmega_{ge}|, \quad \varOmega = \sqrt{\varOmega_R^2 + \varDelta^2} \tag{22.30}$$

5. 原子能级布居反转的演化:

$$C_e(0) = 1, \quad C_g(0) = 0 \tag{22.31}$$

$$W(t) = \langle\hat{\sigma}_z\rangle = |C_e(t)|^2 - |C_g(t)|^2 = \frac{\varDelta^2 - \varOmega_R^2}{\varOmega^2}\sin^2\left(\frac{\varOmega t}{2}\right) + \cos^2\left(\frac{\varOmega t}{2}\right) \tag{22.32}$$

6. 共振时产生 Rabi 振荡:

$$W(t) = \cos\varOmega_R t, \quad \varDelta = 0, \quad \varOmega = \varOmega_R \tag{22.33}$$

22.2.2 相互作用绘景方法

1. 相互作用绘景中的 Hamilton 量：

$$\widetilde{U}(t)=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0 t}=\mathrm{e}^{\mathrm{i}\frac{1}{2}\hbar\omega_{eg}\hat{\sigma}_z t} \tag{22.34}$$

$$\widetilde{H}_I=\widetilde{U}\hat{H}_I\widetilde{U}^{\dagger}=-\frac{\hbar}{2}\left(\Omega_{eg}\hat{\sigma}_+\mathrm{e}^{\mathrm{i}\Delta t}+\Omega_{ge}\hat{\sigma}_-\mathrm{e}^{-\mathrm{i}\Delta t}+\Omega_{eg}\hat{\sigma}_+\mathrm{e}^{\mathrm{i}(\omega_{eg}+\omega)t}+\Omega_{ge}\hat{\sigma}_-\mathrm{e}^{-\mathrm{i}(\omega_{eg}+\omega)t}\right) \tag{22.35}$$

$$\widetilde{H}_I=-\frac{1}{2}\hbar\Omega_R(\mathrm{e}^{\mathrm{i}\phi}\hat{\sigma}_++\mathrm{e}^{-\mathrm{i}\phi}\hat{\sigma}_-),\quad \Delta=0 \tag{22.36}$$

$$\widetilde{H}_I^{2n}(t)=\left(\frac{\hbar\Omega_R}{2}\right)^{2n},\quad \widetilde{H}_I^{2n+1}(t)=-\left(\frac{\hbar\Omega_R}{2}\right)^{2n+1}\left(\mathrm{e}^{\mathrm{i}\phi}\hat{\sigma}_++\mathrm{e}^{-\mathrm{i}\phi}\hat{\sigma}_-\right) \tag{22.37}$$

2. 二能级原子的演化：

$$|\widetilde{\psi}(t)\rangle=\hat{U}(t,0)\,|\widetilde{\psi}(0)\rangle \tag{22.38}$$

$$\begin{aligned}\hat{U}(t,0)&=\hat{I}+\frac{1}{\mathrm{i}\hbar}\int_0^t\mathrm{d}t'\widetilde{H}_I(t')+\left(\frac{1}{\mathrm{i}\hbar}\right)^2\int_0^t\mathrm{d}t'\int_{t_0}^{t'}\mathrm{d}t''\widetilde{H}_I(t')\widetilde{H}_I(t'')+\cdots\\&=\cos\left(\frac{\Omega_R t}{2}\right)+\mathrm{i}\sin\left(\frac{\Omega_R t}{2}\right)\left(\mathrm{e}^{\mathrm{i}\phi}\hat{\sigma}_++\mathrm{e}^{-\mathrm{i}\phi}\hat{\sigma}_-\right)\end{aligned} \tag{22.39}$$

3. 二能级原子的演化：

$$|\widetilde{\psi}(t)\rangle=\hat{U}(t,0)\,|e\rangle=\cos\left(\frac{\Omega_R t}{2}\right)|e\rangle+\mathrm{i}\sin\left(\frac{\Omega_R t}{2}\right)\mathrm{e}^{-\mathrm{i}\phi}\,|g\rangle \tag{22.40}$$

$$C_e(t)=\cos\left(\frac{\Omega_R t}{2}\right),\quad C_g(t)=\mathrm{i}\sin\left(\frac{\Omega_R t}{2}\right)\mathrm{e}^{-\mathrm{i}\phi} \tag{22.41}$$

22.3 密度矩阵的演化

1. 密度矩阵的演化：

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}=\frac{1}{\mathrm{i}\hbar}\left[\widetilde{H},\hat{\rho}\right] \tag{22.42}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{ee}=+\frac{\mathrm{i}}{2}(\Omega_R\mathrm{e}^{\mathrm{i}\phi}\rho_{eg}-\Omega_R\mathrm{e}^{-\mathrm{i}\phi}\rho_{eg}) \tag{22.43}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{gg}=-\frac{\mathrm{i}}{2}(\Omega_R\mathrm{e}^{\mathrm{i}\phi}\rho_{eg}-\Omega_R\mathrm{e}^{-\mathrm{i}\phi}\rho_{eg}) \tag{22.44}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{eg}=-\mathrm{i}\Delta\rho_{eg}-\mathrm{i}\frac{\Omega_R\mathrm{e}^{-\mathrm{i}\phi}}{2}(\rho_{ee}-\rho_{gg}) \tag{22.45}$$

2. Bloch 矢量：

$$\boldsymbol{\rho}=\frac{1}{2}\hat{I}+\rho_{eg}\hat{\sigma}_++\rho_{ge}\hat{\sigma}_-+\frac{1}{2}(\rho_{ee}-\rho_{gg})\hat{\sigma}_z=\frac{1}{2}(\hat{I}+R_1\hat{\sigma}_x+R_2\hat{\sigma}_y+R_3\hat{\sigma}_z) \tag{22.46}$$

$$R_1=\langle\hat{\sigma}_x\rangle=\mathrm{tr}(\hat{\sigma}_x\boldsymbol{\rho})=\rho_{eg}+\rho_{ge} \tag{22.47}$$

$$R_2=\langle\hat{\sigma}_y\rangle=\mathrm{tr}(\hat{\sigma}_y\boldsymbol{\rho})=\mathrm{i}\rho_{eg}-\rho_{ge} \tag{22.48}$$

$$R_3=\langle\hat{\sigma}_z\rangle=\mathrm{tr}(\hat{\sigma}_z\boldsymbol{\rho})=\rho_{ee}-\rho_{gg} \tag{22.49}$$

3. 光学 Bloch 方程：

$$\dot{\boldsymbol{R}}=\boldsymbol{Q}\times\boldsymbol{R} \tag{22.50}$$

$$\boldsymbol{Q}=\frac{2}{\hbar}\begin{pmatrix}\mathrm{Re}(\widetilde{H}_{ge})\\\mathrm{Im}(\widetilde{H}_{ge})\\\frac{1}{2}\hbar\Delta\end{pmatrix}=\begin{pmatrix}-\Omega\cos\phi\\\Omega\sin\phi\\\Delta\end{pmatrix} \tag{22.51}$$

共振时：

$$\boldsymbol{R}(t)=(0,-\sin\Omega t,\cos\Omega t),\quad \Delta=0,\quad \phi=0 \tag{22.52}$$

22.4 耗散密度矩阵的演化

1. 耗散的唯象表示：
   (1) 密度矩阵对角元的耗散速率：$\gamma_e = \gamma_g = \gamma$
   (2) 密度矩阵非对角元的耗散速率：$\gamma_{eg} = \frac{\gamma}{2} + \gamma_c$
2. 耗散密度矩阵的演化：

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho} = \frac{1}{\mathrm{i}\hbar}\left[\widetilde{H}, \hat{\rho}\right] - \frac{1}{2}\left\{\Gamma, \hat{\rho}\right\} \tag{22.53}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{ee} = -\gamma\rho_{ee} + \frac{\mathrm{i}}{2}(\Omega_R \mathrm{e}^{\mathrm{i}\phi}\rho_{ge} - \Omega_R \mathrm{e}^{-\mathrm{i}\phi}\rho_{eg}) \tag{22.54}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{gg} = -\gamma\rho_{gg} - \frac{\mathrm{i}}{2}(\Omega_R \mathrm{e}^{\mathrm{i}\phi}\rho_{ge} - \Omega_R \mathrm{e}^{-\mathrm{i}\phi}\rho_{eg}) \tag{22.55}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{eg} = -(\gamma_{eg} + \mathrm{i}\Delta)\rho_{eg} - \mathrm{i}\frac{\Omega_R \mathrm{e}^{\mathrm{i}\phi}}{2}(\rho_{ee} - \rho_{gg}) \tag{22.56}$$

3. 耗散的光学 Bloch 方程：

$$\dot{\boldsymbol{R}} = -\begin{pmatrix} R_1\gamma \\ R_2\gamma \\ (R_3+1)\gamma_{eg} \end{pmatrix} + \boldsymbol{Q} \times \boldsymbol{R} \tag{22.57}$$

4. 稳态下的密度矩阵元：

$$\rho_{ee} = \frac{1}{2}\frac{S}{1+S}, \quad \rho_{gg} - \rho_{ee} = \frac{1}{1+S}, \quad |\rho_{eg}|^2 = \frac{\gamma}{4\gamma_{eg}}\frac{S}{(1+S)^2} \tag{22.58}$$

5. 饱和参数：

$$S = \frac{|\Omega_R|^2/(\gamma\gamma_{eg})}{1 + \Delta^2/\gamma_{eg}^2} \sim \frac{1}{\Delta^2 + \gamma_{eg}^2} \tag{22.59}$$

$$S_0 = \frac{|\Omega_R|^2}{\gamma\gamma_{eg}} = \frac{d^2 E_0^2}{\hbar^2\gamma\gamma_{eg}} = \frac{I}{I_s}, \quad I = \frac{1}{2}\varepsilon_0 c E^2, \quad I_s = \frac{1}{2}\varepsilon_0 c \frac{\hbar^2\gamma\gamma_{eg}}{d^2} \tag{22.60}$$

22.5 Maxwell-Schrodinger 方程

1. 单原子的密度矩阵：

$$\hat{\rho}(z,t,t_0) = \sum_{\alpha\beta}\rho_{\alpha\beta}(z,t,t_0)\left|\alpha\right\rangle\left\langle\beta\right|, \quad \alpha,\beta \in \{e,g\} \tag{22.61}$$

2. 原子系综的密度矩阵：

$$\hat{\rho}(z,t) = \sum_{\alpha,\beta}\int_{-\infty}^{t}\mathrm{d}t_0\, r_a(z,t_0)\rho_{\alpha\beta}(z,t,t_0)\left|\alpha\right\rangle\left\langle\beta\right| \tag{22.62}$$

3. 原子系综密度矩阵的演化：

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{ee} = \lambda_e - \gamma\rho_{ee} + \frac{\mathrm{i}}{2}(\Omega_R \mathrm{e}^{\mathrm{i}\phi}\rho_{ge} - \Omega_R \mathrm{e}^{-\mathrm{i}\phi}\rho_{eg}) \tag{22.63}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{gg} = \lambda_g - \gamma\rho_{gg} - \frac{\mathrm{i}}{2}(\Omega_R \mathrm{e}^{\mathrm{i}\phi}\rho_{ge} - \Omega_R \mathrm{e}^{-\mathrm{i}\phi}\rho_{eg}) \tag{22.64}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{eg} = -(\gamma_{eg} + \mathrm{i}\Delta)\rho_{eg} - \mathrm{i}\frac{\Omega_R \mathrm{e}^{\mathrm{i}\phi}}{2}(\rho_{ee} - \rho_{gg}) \tag{22.65}$$

$$\lambda_e = r_a\rho_{ee}(z,t_0,t_0), \quad \lambda_g = r_a\rho_{gg}(z,t_0,t_0) \tag{22.66}$$

4. 光场的演化：

$$\nabla\cdot\boldsymbol{D} = 0, \quad \nabla\times\boldsymbol{E} = -\frac{\partial\boldsymbol{B}}{\partial t}, \quad \nabla\cdot\boldsymbol{B} = 0, \quad \nabla\times\boldsymbol{H} = \boldsymbol{J} - \frac{\partial\boldsymbol{D}}{\partial t} \tag{22.67}$$

$$\boldsymbol{D} = \varepsilon_0\boldsymbol{E} + \boldsymbol{P}, \quad \boldsymbol{B} = \mu_0\boldsymbol{H}, \quad \boldsymbol{J} = \sigma\boldsymbol{E} \tag{22.68}$$

$$\nabla\times(\nabla\times\boldsymbol{E}) + \mu_0\sigma\frac{\partial\boldsymbol{E}}{\partial t} + \mu_0\varepsilon_0\frac{\partial^2\boldsymbol{E}}{\partial t^2} = -\mu_0\frac{\partial^2\boldsymbol{P}}{\partial t^2} \tag{22.69}$$

5. 光场形式：

$$\boldsymbol{E}(z,t)=\frac{1}{2}\boldsymbol{e}_x\mathcal{E}(z,t)e^{-\mathrm{i}(\omega t-kz+\phi(z,t))}+c.c. \tag{22.70}$$

$$\boldsymbol{P}(z,t)=\frac{1}{2}\boldsymbol{e}_x\mathcal{P}(z,t)e^{-\mathrm{i}(\omega t-kz+\phi(z,t))}+c.c. \tag{22.71}$$

$$\mathcal{P}(z,t)=2d_{eg}\rho_{eg}e^{\mathrm{i}(\omega t-kz+\phi(z,t))} \tag{22.72}$$

6. 慢变近似：

$$\dot{\mathcal{E}}\ll\omega\mathcal{E},\quad \partial_z\mathcal{E}\ll k\mathcal{E},\quad \dot{\phi}\ll\omega,\quad \partial_z\phi\ll k,\quad \dot{\mathcal{P}}\ll\omega\mathcal{P},\quad \partial_z\mathcal{P}\ll k\mathcal{P} \tag{22.73}$$

$$\left(\frac{\partial}{\partial z}+\frac{1}{c}\frac{\partial}{\partial t}\right)\left(-\frac{\partial}{\partial z}+\frac{1}{c}\frac{\partial}{\partial t}\right)E=-\mu_0\sigma\frac{\partial E}{\partial t}-\mu_0\frac{\partial^2 P}{\partial t^2} \tag{22.74}$$

$$\left(-\frac{\partial}{\partial z}+\frac{1}{c}\frac{\partial}{\partial t}\right)E\approx-2\mathrm{i}k_0E \tag{22.75}$$

7. Maxwell-Schrodinger 方程：

$$\frac{\partial\mathcal{E}}{\partial z}+\frac{1}{c}\frac{\partial\mathcal{E}}{\partial t}=-\kappa\mathcal{E}-\frac{1}{2\varepsilon_0}k\mathrm{Im}(\mathcal{P}),\quad \kappa=\frac{\sigma}{2\varepsilon_0 c} \tag{22.76}$$

$$\frac{\partial\phi}{\partial z}+\frac{1}{c}\frac{\partial\phi}{\partial t}=k-\frac{\omega}{c}-\frac{1}{2\varepsilon_0}k\mathcal{E}^{-1}\mathrm{Re}(\mathcal{P}) \tag{22.77}$$

23 量子光场与原子相互作用

1. 调整相位的光场算符：

$$\hat{E}(\boldsymbol{r})=\sum_{\boldsymbol{k}}\boldsymbol{e}_k\mathcal{E}_k(\hat{a}_k+\hat{a}_k^\dagger) \tag{23.1}$$

2. 光场与原子相互作用系统的 Hamilton 量：

$$\hat{H}=\sum_i\hbar\omega_i\left|i\right\rangle\left\langle i\right|+\sum_k\hbar\omega_k\hat{a}_k^\dagger\hat{a}_k+\hbar\sum_k\sum_{ij}g_k^{ij}\left|i\right\rangle\left\langle j\right|(\hat{a}_k+\hat{a}_k^\dagger),\quad g_k^{ij}=-\frac{1}{\hbar}\boldsymbol{d}_{ij}\cdot\mathcal{E}_k\boldsymbol{e}_\sigma \tag{23.2}$$

3. 多模光场与二能级原子的 Hamilton 量：

$$\hat{H}=\frac{1}{2}\hbar\omega_{eg}\hat{\sigma}_z+\sum_k\hbar\omega_k\hat{a}_k^\dagger\hat{a}_k+\hbar\sum_k g_k(\hat{\sigma}_++\hat{\sigma}_-)(\hat{a}_k+\hat{a}_k^\dagger) \tag{23.3}$$

$$\hat{a}(t)=\hat{a}\mathrm{e}^{-\mathrm{i}\omega t},\quad \hat{a}^\dagger(t)=\hat{a}^\dagger\mathrm{e}^{\mathrm{i}\omega t},\quad \hat{\sigma}_-(t)=\hat{\sigma}_-\mathrm{e}^{-\mathrm{i}\omega_{eg}t},\quad \hat{\sigma}_+(t)=\hat{\sigma}_+\mathrm{e}^{\mathrm{i}\omega_{eg}t} \tag{23.4}$$

$$\hat{\sigma}_+\hat{a}\sim\mathrm{e}^{\mathrm{i}(\omega_{eg}-\omega)t},\quad \hat{\sigma}_-\hat{a}^\dagger\sim\mathrm{e}^{-\mathrm{i}(\omega_{eg}-\omega)t},\quad \hat{\sigma}_+\hat{a}^\dagger\sim\mathrm{e}^{\mathrm{i}(\omega_{eg}+\omega)t},\quad \hat{\sigma}_-\hat{a}\sim\mathrm{e}^{-\mathrm{i}(\omega_{eg}+\omega)t} \tag{23.5}$$

4. Rabi 模型：

$$\hat{H}_R=\frac{1}{2}\hbar\omega_{eg}\hat{\sigma}_z+\hbar\omega\hat{a}^\dagger\hat{a}+\hbar g(\hat{\sigma}_++\hat{\sigma}_-)(\hat{a}+\hat{a}^\dagger) \tag{23.6}$$

5. Jaynes–Cummings 模型：

$$\hat{H}_{JC}=\frac{1}{2}\hbar\omega_{eg}\hat{\sigma}_z+\hbar\omega\hat{a}^\dagger\hat{a}+\hbar g\left(\hat{\sigma}_+\hat{a}+\hat{\sigma}_-\hat{a}^\dagger\right) \tag{23.7}$$

6. Dicke 模型：

$$\hat{H}_D=\hbar\omega_{eg}\hat{J}_z+\hbar\omega\hat{a}^\dagger\hat{a}+\frac{\hbar g}{\sqrt{N}}\left(\hat{a}+\hat{a}^\dagger\right)\left(\hat{J}_++\hat{J}_-\right),\quad \hat{J}_z=\frac{1}{2}\sum_{i=1}^N\sigma_z^i,\quad \hat{J}_\pm=\sum_{i=1}^N\sigma_\pm^i \tag{23.8}$$

7. Tavis-Cummings 模型：

$$\hat{H}_{TC}=\hbar\omega_{eg}\hat{J}_z+\hbar\omega\hat{a}^\dagger\hat{a}+\hbar g\left(\hat{a}\hat{J}_++\hat{a}^\dagger\hat{J}_-\right),\quad \hat{J}_z=\frac{1}{2}\sum_{i=1}^N\sigma_z^i,\quad \hat{J}_\pm=\sum_{i=1}^N\sigma_\pm^i \tag{23.9}$$

23.1 Jaynes-Cummings 模型

1. 单模光场与二能级原子的 Hamilton 量：

$$\hat{H}=\frac{1}{2}\hbar\omega_{eg}\hat{\sigma}_z+\hbar\omega\hat{a}^\dagger\hat{a}+\hbar g\left(\hat{\sigma}_+\hat{a}+\hat{\sigma}_-\hat{a}^\dagger\right) \tag{23.10}$$

2. 相互作用绘景下的 Hamilton 量：

$$\widetilde{H}_I=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0t}\hat{H}_I\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0t}=\hbar g\left(\hat{\sigma}_+\hat{a}\mathrm{e}^{\mathrm{i}\Delta t}+\hat{\sigma}_-\hat{a}^\dagger\mathrm{e}^{-\mathrm{i}\Delta t}\right) \tag{23.11}$$

23.1.1 概率幅方法

1. 系统的演化：

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\left|\widetilde{\psi}(t)\right\rangle=\widetilde{H}_I\left|\widetilde{\psi}(t)\right\rangle \tag{23.12}$$

$$\left|\widetilde{\psi}(t)\right\rangle=\sum_n\Big(C_{e,n}(t)\left|e,n\right\rangle+C_{g,n+1}(t)\left|g,n+1\right\rangle\Big) \tag{23.13}$$

2. 系数演化方程：

$$\dot{C}_{e,n}(t)=-\mathrm{i}g\sqrt{n+1}\mathrm{e}^{\mathrm{i}\Delta t}C_{g,n+1}(t) \tag{23.14}$$

$$\dot{C}_{g,n+1}(t)=-\mathrm{i}g\sqrt{n+1}e^{-\mathrm{i}\Delta t}C_{e,n}(t) \tag{23.15}$$

3. 系数的形式解:

$$\begin{pmatrix} C_{e,n}(t) \\ C_{g,n+1}(t) \end{pmatrix} = \begin{pmatrix} \cos\frac{\Omega_n t}{2} - \mathrm{i}\frac{\Delta}{\Omega_n}\sin\frac{\Omega_n t}{2} & -\frac{2\mathrm{i}g\sqrt{n+1}}{\Omega_n}\sin\frac{\Omega_n t}{2}e^{\mathrm{i}\frac{\Delta t}{2}} \\ -\frac{2\mathrm{i}g\sqrt{n+1}}{\Omega_n}\sin\frac{\Omega_n t}{2}e^{-\mathrm{i}\frac{\Delta t}{2}} & \cos\frac{\Omega_n t}{2} + \mathrm{i}\frac{\Delta}{\Omega_n}\sin\frac{\Omega_n t}{2} \end{pmatrix} \begin{pmatrix} C_{e,n}(0) \\ C_{g,n+1}(0) \end{pmatrix} \tag{23.16}$$

$$\Omega_n^2 = \Delta^2 + 4g^2(n+1) \tag{23.17}$$

4. 原子初始处于激发态 $|e\rangle$:

$$C_{e,n}(0) = C_n(0), \quad C_{g,n+1}(0) = 0 \tag{23.18}$$

$$C_{e,n}(t) = C_n(0)\left(\cos\frac{\Omega_n t}{2} - \mathrm{i}\frac{\Delta}{\Omega_n}\sin\frac{\Omega_n t}{2}\right)e^{\mathrm{i}\Delta t/2} \tag{23.19}$$

$$C_{g,n+1}(t) = -C_n(0)\frac{2\mathrm{i}g\sqrt{n+1}}{\Omega_n}\sin\frac{\Omega_n t}{2}e^{-\mathrm{i}\Delta t/2} \tag{23.20}$$

5. 光场具有 n 个光子概率的演化:

$$\begin{aligned} P(n) &= \langle n|\,\hat{\rho}_F(t)\,|n\rangle = |C_{e,n}(t)|^2 + |C_{g,n}(t)|^2 \\ &= |C_n(0)|^2\left[\cos^2\frac{\Omega_n t}{2} + \left(\frac{\Delta}{\Omega_n}\right)^2\sin^2\frac{\Omega_n t}{2}\right] + |C_{n-1}(0)|^2\frac{4g^2 n}{\Omega_{n-1}^2}\sin^2\frac{\Omega_{n-1}t}{2} \end{aligned} \tag{23.21}$$

6. 原子能级布居反转的演化:

$$W(t) = \sum_n\left(|C_{e,n}(t)|^2 - |C_{g,n}(t)|^2\right) = \sum_n |C_n(0)|^2\left(\frac{\Delta^2}{\Omega_n^2} + \frac{4g^2(n+1)}{\Omega_n^2}\cos\Omega_n t\right) \tag{23.22}$$

7. 初始光场为相干态:

$$|C_n(0)|^2 = |\langle\alpha|n\rangle|^2 = \frac{\langle n\rangle^n}{n!}e^{-\langle n\rangle} \tag{23.23}$$

(1) Rabi 振荡周期:

$$t_R \sim \frac{1}{\Omega_{\langle n\rangle}} = \frac{1}{\sqrt{\Delta^2 + 4g^2\langle n\rangle}} \tag{23.24}$$

(2) 崩塌时间:

$$t_c \sim \frac{1}{\Omega_{\langle n\rangle+\sqrt{\langle n\rangle}} - \Omega_{\langle n\rangle-\sqrt{\langle n\rangle}}} \approx \frac{1}{2g}\sqrt{1 + \frac{\Delta^2}{4g^2\langle n\rangle}} \tag{23.25}$$

(3) 复原周期:

$$t_r = \frac{2\pi m}{\Omega_{\langle n\rangle} - \Omega_{\langle n\rangle-1}} \approx \frac{2\pi m\sqrt{\langle n\rangle}}{g}\sqrt{1 + \frac{\Delta^2}{4g^2\langle n\rangle}} \tag{23.26}$$

8. 初始光场为真空态:

$$|C_n(0)|^2 = \delta_{n0} \tag{23.27}$$

$$W(t) = \frac{1}{\Delta^2 + 4g^2}\left[\Delta^2 + 4g^2\cos\left(\sqrt{\Delta^2 + 4g^2}t\right)\right] \xrightarrow{\Delta=0} \cos 2gt \tag{23.28}$$

23.1.2 Heisenberg 绘景方法

1. Heidenberg 运动方程:

$$\dot{\hat{a}} = -\mathrm{i}\omega\hat{a} - \mathrm{i}g\hat{\sigma}_- \tag{23.29}$$

$$\dot{\hat{\sigma}}_- = \mathrm{i}\omega_{eg}\hat{\sigma}_- + \mathrm{i}g\hat{\sigma}_z\hat{a} \tag{23.30}$$

$$\dot{\hat{\sigma}}_z = 2\mathrm{i}g\left(\hat{a}^\dagger\hat{\sigma}_- - \hat{\sigma}_-\hat{a}\right) \tag{23.31}$$

2. 运动常数算符:

$$\hat{N} = \hat{a}^\dagger\hat{a} + \hat{\sigma}_+\hat{\sigma}_- \tag{23.32}$$

$$\hat{C} = \frac{1}{2}\Delta\hat{\sigma}_z + g\left(\hat{\sigma}_+\hat{a} + \hat{a}^\dagger\hat{\sigma}_-\right) \tag{23.33}$$

$$[\hat{N}, \hat{H}] = [\hat{C}, \hat{H}] = 0 \tag{23.34}$$

$$\hat{C}^2 = \frac{\Delta^2}{4} + g^2\hat{N}, \quad g\hat{\sigma}_z\hat{a} = 2\hat{C}\hat{\sigma}_- + \Delta\hat{\sigma}_- - g\hat{a} \tag{23.35}$$

3. 算符的形式解:

$$\begin{pmatrix}\hat{\sigma}_-(t)\\ \hat{a}(t)\end{pmatrix} = e^{-\mathrm{i}\omega t}e^{\mathrm{i}\hat{C}t}\begin{pmatrix}\cos\hat{\kappa}t + \mathrm{i}\hat{C}\dfrac{\sin\hat{\kappa}t}{\hat{\kappa}} & -\mathrm{i}g\dfrac{\sin\hat{\kappa}t}{\hat{\kappa}}\\ -\mathrm{i}g\dfrac{\sin\hat{\kappa}t}{\hat{\kappa}} & \cos\hat{\kappa}t - \mathrm{i}\hat{C}\dfrac{\sin\hat{\kappa}t}{\hat{\kappa}}\end{pmatrix}\begin{pmatrix}\hat{\sigma}_-(0)\\ \hat{a}(0)\end{pmatrix} \tag{23.36}$$

$$\hat{\kappa}^2 = \frac{\Delta^2}{4} + g^2(\hat{N}+1) \tag{23.37}$$

4. 原子能级布居反转的演化:

$$W(t) = \langle\psi(0)|\hat{\sigma}_z(t)|\psi(0)\rangle = 2\langle\psi(0)|\hat{\sigma}_+(t)\hat{\sigma}_-(t)|\psi(0)\rangle - \hat{I} \tag{23.38}$$

5. 偶极-偶极相关函数:

$$\langle\psi(0)|\hat{\sigma}_+(t)\hat{\sigma}_-(t+\tau)|\psi(0)\rangle = \mathrm{tr}\left[\hat{\sigma}_+(t)\hat{\sigma}_-(t+\tau)\hat{\rho}(0)\right] \tag{23.39}$$

$$\begin{aligned}\langle e,\alpha|\hat{\sigma}_+(t)\hat{\sigma}_-(t+\tau)|e,\alpha\rangle = {}& e^{-i\omega\tau-|\alpha|^2}\sum_{n=0}^{+\infty}\frac{|\alpha|^{2n}}{n!}\frac{1}{4\Omega_n^2}\left(\cos\frac{\Omega_{n-1}\tau}{2} - \frac{i\Delta}{2\Omega_{n-1}}\sin\frac{\Omega_{n-1}\tau}{2}\right)\\ &\times\left((\Omega_n+\Delta)^2e^{-i\frac{\Omega_n\tau}{2}} + (\Omega_n-\Delta)^2e^{i\frac{\Omega_n\tau}{2}} + 8g^2(n+1)\cos\frac{\Omega_n(\tau+2t)}{2}\right)\end{aligned} \tag{23.40}$$

23.1.3 相互作用绘景方法

1. 相互作用绘景中的 Hamilton 量:

$$\widetilde{H}_I = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0 t}\hat{H}_I\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0 t} = \hbar g\left(\hat{\sigma}_+\hat{a} + \hat{\sigma}_-\hat{a}^\dagger\right), \quad \Delta = 0 \tag{23.41}$$

$$\left(\hat{\sigma}_+\hat{a} + \hat{\sigma}_-\hat{a}^\dagger\right)^{2l} = (\hat{a}\hat{a}^\dagger)^l|e\rangle\langle e| + (\hat{a}^\dagger\hat{a})^l|g\rangle\langle g| \tag{23.42}$$

$$\left(\hat{\sigma}_+\hat{a} + \hat{\sigma}_-\hat{a}^\dagger\right)^{2l+1} = (\hat{a}\hat{a}^\dagger)^l\hat{a}|e\rangle\langle g| + \hat{a}^\dagger(\hat{a}^\dagger\hat{a})^l|g\rangle\langle e| \tag{23.43}$$

2. 系统的演化:

$$|\widetilde{\psi}(t)\rangle = \hat{U}(t,0)\,|\widetilde{\psi}(0)\rangle \tag{23.44}$$

$$\begin{aligned}\hat{U}(t,0) &= \hat{P}\exp\left(\frac{1}{\mathrm{i}\hbar}\int_0^t \mathrm{d}t'\widetilde{H}_I\right) = \exp\left(-\frac{\mathrm{i}}{\hbar}\widetilde{H}_I t\right)\\ &= \cos\left(gt\sqrt{\hat{a}^\dagger\hat{a}+1}\right)|e\rangle\langle e| + \cos\left(gt\sqrt{\hat{a}^\dagger\hat{a}}\right)|g\rangle\langle g|\\ &\quad - \mathrm{i}\frac{\sin\left(gt\sqrt{\hat{a}^\dagger\hat{a}+1}\right)}{\sqrt{\hat{a}^\dagger\hat{a}+1}}\hat{a}|e\rangle\langle g| - \mathrm{i}\hat{a}^\dagger\frac{\sin\left(gt\sqrt{\hat{a}^\dagger\hat{a}+1}\right)}{\sqrt{\hat{a}^\dagger\hat{a}+1}}|g\rangle\langle e|\end{aligned} \tag{23.45}$$

3. 系统的演化:

$$|\widetilde{\psi}(t)\rangle = \hat{U}(t,0)\sum_{n=0}^{+\infty}C_n(0)|e,n\rangle = \sum_{n=0}^{+\infty}C_n(0)\Big[\cos\left(gt\sqrt{n+1}\right)|e,n\rangle - i\sin\left(gt\sqrt{n+1}\right)|g,n+1\rangle\Big] \tag{23.46}$$

$$C_{e,n}(t) = C_n(0)\cos\left(gt\sqrt{n+1}\right), \quad C_{g,n+1}(t) = -\mathrm{i}C_n(0)\sin\left(gt\sqrt{n+1}\right) \tag{23.47}$$

23.2 二能级原子自发辐射的 Weisskopf-Wigner 理论

1. 多模光场与二能级原子的 Hamilton 量:

$$\hat{H}=\frac{1}{2}\hbar\omega_{eg}\hat{\sigma}_z+\sum_k\hbar\omega_k\hat{a}_k^\dagger\hat{a}_k+\hbar\sum_k g_k(\hat{\sigma}_+\hat{a}_k+\hat{\sigma}_-\hat{a}_k^\dagger) \tag{23.48}$$

2. 相互作用绘景中的 Hamilton 量:

$$\widetilde{H}_I=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_0t}\hat{H}_I\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0t}=\hbar\sum_k\left(g_k^*\hat{\sigma}_+\hat{a}_k\mathrm{e}^{\mathrm{i}(\omega_{eg}-\omega_k)t}+h.c.\right) \tag{23.49}$$

3. 系统的演化:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\widetilde{\psi}(t)\rangle=\widetilde{H}_I|\widetilde{\psi}(t)\rangle \tag{23.50}$$

$$|\widetilde{\psi}(t)\rangle=C_e(t)|e,0\rangle+\sum_k C_{g,k}(t)|g,1_k\rangle \tag{23.51}$$

$$C_e(0)=1,\quad C_{g,k}(0)=0 \tag{23.52}$$

4. 系数演化方程:

$$\dot{C}_e(t)=-\mathrm{i}\sum_k g_k^*e^{i(\omega_{eg}-\omega_k)t}C_{g,k}(t) \tag{23.53}$$

$$\dot{C}_{g,k}(t)=-\mathrm{i}g_ke^{-i(\omega_{eg}-\omega_k)t}C_e(t) \tag{23.54}$$

5. 系数的形式解:

$$\begin{aligned}\dot{C}_e(t)&=-\sum_k|g_k|^2\int_0^t\mathrm{d}t'\,\mathrm{e}^{\mathrm{i}(\omega_{eg}-\omega_k)(t-t')}C_e(t'),\quad |g_k|^2=\frac{\omega_k}{2\hbar\varepsilon_0V}|\boldsymbol{d}_{eg}|^2\cos^2\theta\\&\to-\frac{4|\boldsymbol{d}_{eg}|^2}{(2\pi)^26\hbar\varepsilon_0c^3}\int_0^{+\infty}\mathrm{d}\omega_k\,\omega_k^3\int_0^t\mathrm{d}t'\,\mathrm{e}^{\mathrm{i}(\omega_{eg}-\omega_k)(t-t')}C_e(t')\xrightarrow{\omega_k=\omega_{eg}}-\frac{\varGamma}{2}C_e(t)\end{aligned} \tag{23.55}$$

$$C_e(t)=\mathrm{e}^{-\varGamma t/2},\quad \varGamma=\frac{1}{4\pi\varepsilon_0}\frac{4\omega^3|\boldsymbol{d}_{eg}|^2}{3\hbar c^3} \tag{23.56}$$

$$C_{g,k}(t)=-\mathrm{i}g_k\int_0^t\mathrm{d}t'\,\mathrm{e}^{-\mathrm{i}(\omega_{eg}-\omega_k)t'}C_e(t')=g_k\left[\frac{1-\mathrm{e}^{-\mathrm{i}(\omega_{eg}-\omega_k)t-\varGamma t/2}}{(\omega_k-\omega_{eg})+\mathrm{i}\varGamma/2}\right] \tag{23.57}$$

6. 原子激发态的布居演化:

$$\rho_{ee}(t)=|C_e(t)|^2=\mathrm{e}^{-\varGamma t} \tag{23.58}$$

7. 系统的演化:

$$|\psi(t)\rangle=\mathrm{e}^{-\varGamma t/2}|e,0\rangle+\sum_k g_k\left[\frac{1-\mathrm{e}^{\mathrm{i}(\omega_{eg}-\omega_k)t-\varGamma t/2}}{(\omega_k-\omega_{eg})+\mathrm{i}\varGamma/2}\right]|g,1_k\rangle\xrightarrow{t\to+\infty}|g,\gamma_0\rangle \tag{23.59}$$

8. 远场光强:

$$\langle0|\hat{E}^+(\boldsymbol{r},t)|\gamma_0\rangle=\sqrt{\frac{\hbar}{2\varepsilon_0V}}\sum_{kk'}\langle0|\sqrt{\omega_{k'}}\hat{a}_{k'}\mathrm{e}^{-\mathrm{i}\omega_{k'}t+\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}}g_k\frac{1}{(\omega_k-\omega_{eg})+\mathrm{i}\varGamma/2}|1_k\rangle \tag{23.60}$$

$$=\sqrt{\frac{\hbar}{2\varepsilon_0V}}\sum_k\sqrt{\omega_k}\hat{a}_k\mathrm{e}^{-\mathrm{i}\omega_kt+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}g_k\frac{1}{(\omega_k-\omega_{eg})+\mathrm{i}\varGamma/2} \tag{23.61}$$

$$\approx-\frac{\mathrm{i}c}{8\pi^2\varepsilon_0r}\left(\boldsymbol{d}\times\frac{\boldsymbol{r}}{r}\right)\times\frac{\boldsymbol{r}}{r}\int_0^{+\infty}\mathrm{d}k\,k^2\frac{\mathrm{e}^{\mathrm{i}kr}-\mathrm{e}^{-\mathrm{i}kr}}{(\omega_k-\omega_{eg})+\mathrm{i}\varGamma/2}\mathrm{e}^{-\mathrm{i}\omega_kt} \tag{23.62}$$

$$=\frac{\omega_{eg}^2}{4\pi^2\varepsilon_0c^2r}\left(\boldsymbol{d}\times\frac{\boldsymbol{r}}{r}\right)\times\frac{\boldsymbol{r}}{r}\varTheta\left(t-\frac{r}{c}\right)\mathrm{e}^{-\mathrm{i}(\omega_{eg}-\mathrm{i}\varGamma/2)(t-r/c)} \tag{23.63}$$

$$|\boldsymbol{E}(\boldsymbol{r},t)|^2=\langle\gamma_0|\hat{E}^-(\boldsymbol{r},t)\hat{E}^+(\boldsymbol{r},t)|\gamma_0\rangle=\left|\langle0|\hat{E}^+(\boldsymbol{r},t)|\gamma_0\rangle\right|^2=\frac{|\mathcal{E}_0|^2}{r^2}\varTheta\left(t-\frac{r}{c}\right)\mathrm{e}^{-\varGamma(t-r/c)} \tag{23.64}$$

23.3 双光子级联

1. 多模光场与三能级原子的 Hamilton 量：

$$\hat{H}_I = \hbar \sum_k \left(g_{h,k}^* \hat{\sigma}_+^{(h)} \hat{a}_k + h.c. \right) + \hbar \sum_q \left(g_{e,q}^* \hat{\sigma}_+^{(e)} \hat{a}_q + h.c. \right) \tag{23.65}$$

2. 相互作用绘景中的 Hamilton 量：

$$\widetilde{H}_I = \hbar \sum_k \left(g_{h,k}^* \hat{\sigma}_+^{(h)} \hat{a}_k \mathrm{e}^{\mathrm{i}(\omega_{he}-\omega_k)t} + h.c. \right) + \hbar \sum_q \left(g_{e,q}^* \hat{\sigma}_+^{(e)} \hat{a}_q \mathrm{e}^{\mathrm{i}(\omega_{eg}-\omega_q)t} + h.c. \right) \tag{23.66}$$

3. 系统的演化：

$$\mathrm{i}\hbar \frac{\partial}{\partial t} |\widetilde{\psi}(t)\rangle = \widetilde{H}_I |\widetilde{\psi}(t)\rangle \tag{23.67}$$

$$|\widetilde{\psi}(t)\rangle = C_h(t) |h,0,0\rangle + \sum_k C_{e,k}(t) |e,1_k,0\rangle + \sum_{kq} C_{g,k,q} |g,1_k,1_q\rangle \tag{23.68}$$

$$C_h(0) = 1, \quad C_{e,k}(0) = C_{g,k,q}(0) = 0 \tag{23.69}$$

4. 系数演化方程：

$$\dot{C}_h(t) = -\mathrm{i} \sum_k g_{h,k}^* C_{e,k}(t) \mathrm{e}^{\mathrm{i}(\omega_{he}-\omega_k)t} \tag{23.70}$$

$$\dot{C}_{e,k}(t) = -\mathrm{i} g_{h,k} C_h(t) \mathrm{e}^{-\mathrm{i}(\omega_{he}-\omega_k)t} - \mathrm{i} \sum_q g_{e,q}^* C_{g,k,q} \mathrm{e}^{\mathrm{i}(\omega_{eg}-\omega_q)t} \tag{23.71}$$

$$\dot{C}_{g,k,q}(t) = -\mathrm{i} g_{e,q} C_{e,k}(t) \mathrm{e}^{-\mathrm{i}(\omega_{eg}-\omega_q)t} \tag{23.72}$$

Weisskopf-Wigner 理论给出：

$$\dot{C}_h(t) = -\mathrm{i} \sum_k g_{h,k}^* C_{e,k}(t) \mathrm{e}^{\mathrm{i}(\omega_{he}-\omega_k)t} = -\frac{\Gamma_h}{2} C_h(t) \tag{23.73}$$

$$-\mathrm{i} \sum_q g_{e,k}^* C_{g,k,q}(t) \mathrm{e}^{\mathrm{i}(\omega_{eg}-\omega_q)t} = -\frac{\Gamma_e}{2} C_{e,k}(t) \tag{23.74}$$

简化为：

$$\dot{C}_h(t) = -\frac{\Gamma_h}{2} C_h(t) \tag{23.75}$$

$$\dot{C}_{e,k}(t) = -\mathrm{i} g_{h,k} \mathrm{e}^{-\mathrm{i}(\omega_{he}-\omega_k)t - \Gamma_h t/2} - \frac{\Gamma_e}{2} C_{e,k}(t) \tag{23.76}$$

$$\dot{C}_{g,k,q}(t) = -\mathrm{i} g_{e,q} C_{e,k}(t) \mathrm{e}^{-\mathrm{i}(\omega_{eg}-\omega_q)t} \tag{23.77}$$

5. 系数的解：

$$C_{e,k}(t) = -\mathrm{i} g_{h,k} \frac{\mathrm{e}^{\mathrm{i}(\omega_k-\omega_{he})t - \Gamma_h t/2} - \mathrm{e}^{-\Gamma_e t/2}}{\mathrm{i}(\omega_k - \omega_{he}) - (\Gamma_h - \Gamma_e)/2} \xrightarrow{t\to+\infty} 0 \tag{23.78}$$

$$C_{g,k,q}(+\infty) = \frac{-g_{h,k} g_{e,q}}{[\mathrm{i}(\omega_k + \omega_q - \omega_{hg}) - \Gamma_h/2]\,[\mathrm{i}(\omega_q - \omega_{eg}) - \Gamma_e/2]} \tag{23.79}$$

6. 辐射光场态：

$$|\gamma,\phi\rangle = \sum_{kq} \frac{-g_{h,k} g_{e,q}}{[\mathrm{i}(\omega_k + \omega_q - \omega_{hg}) - \Gamma_h/2]\,[\mathrm{i}(\omega_q - \omega_{eg}) - \Gamma_e/2]} |1_k, 1_q\rangle \tag{23.80}$$

A 变分法

1. 试探波函数:

$$|\psi(\lambda)\rangle = \sum_n c_n |n\rangle \tag{A.1}$$

2. 变分原理:

$$\langle H\rangle = \sum_n E_n |c_n|^2 \geqslant E_{gs} \sum_n |c_n|^2 = E_{gs} \tag{A.2}$$

$$\frac{\partial}{\partial\lambda}\langle H\rangle = 0 \tag{A.3}$$

3. 氦原子基态:

$$\hat{H} = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}\right) \tag{A.4}$$

$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{Z^3}{\pi a^3}\mathrm{e}^{-Z(r_! + r_2)/a} \tag{A.5}$$

$$\langle H\rangle = (2Z^2 - 4Z(Z-2) - \frac{5}{4}Z)E_1 = (-2Z^2 + \frac{27}{4}Z)E_1 \tag{A.6}$$

$$\frac{\partial}{\partial Z}\langle H\rangle = 0 \Rightarrow Z = \frac{27}{16} \Rightarrow \langle H\rangle_{min} = \frac{1}{2}\left(\frac{3}{2}\right)^6 E_1 = -77.5\ \mathrm{eV} \tag{A.7}$$

4. 氢分子离子:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r} + \frac{1}{r'} - \frac{1}{R}\right) \tag{A.8}$$

$$\psi(r) = A(\psi_0(r) + \psi_0(r')), \quad A = \frac{1}{2(1+I)}, \quad \psi_0(r) = \frac{1}{\sqrt{\pi a^3}}\mathrm{e}^{-\frac{r}{a}} \tag{A.9}$$

$$\langle H\rangle = \left(1 + 2\frac{D+X}{1+I} - \frac{2}{x}\right)E_1 \tag{A.10}$$

$$I = \left(1 + x + \frac{1}{3}x^3\right)\mathrm{e}^{-x}, \quad D = \frac{1}{x} - \left(1 + \frac{1}{x}\right)\mathrm{e}^{-2x}, \quad X = \left(1 + \frac{1}{x}\right)\mathrm{e}^{-x}, \quad x = \frac{R}{a} \tag{A.11}$$

5. 氢分子:

$$\hat{H} = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r_1'} + \frac{1}{r_1'} + \frac{1}{r_2} + \frac{1}{r_2'} - \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} - \frac{1}{R}\right) \tag{A.12}$$

$$\psi_\pm(\boldsymbol{r}_1, \boldsymbol{r}_2) = A_\pm\left(\psi_0(r_1)\psi_0(r_2') \pm \psi_0(r_1')\psi_0(r_2)\right), \quad \psi_0(r) = \frac{1}{\sqrt{\pi a^3}}\mathrm{e}^{-\frac{r}{a}} \tag{A.13}$$

$$\langle H\rangle_\pm = 2\left(1 - \frac{1}{x} + \frac{2D - D_2 \pm (2IX - X_2)}{1 \pm I^2}\right)E_1 \tag{A.14}$$

B WKB 近似

1. 势场缓变：

$$\left|\frac{\lambda(x)}{4\pi(E-V(x))}\frac{\mathrm{d}V(x)}{\mathrm{d}x}\right| \ll 1 \Longleftrightarrow \left|\frac{1}{k^2(x)}\frac{\mathrm{d}k(x)}{\mathrm{d}x}\right| \ll 1 \tag{B.1}$$

2. 波函数：

$$\psi(x) = \begin{cases} A(x)\mathrm{e}^{\pm \mathrm{i}k(x)x} & E > V(x) \\ A(x)\mathrm{e}^{\mp|k(x)|x} & E < V(x) \end{cases}, \quad k^2(x) = \frac{2m(E-V(x))}{\hbar^2} \tag{B.2}$$

转折点：$E \approx V(x) \Rightarrow \lambda(x) \to \infty$，WKB 近似不适用

3. 经典区域：

(1) Schrodinger 方程：

$$\psi'' = -\frac{p^2}{\hbar^2}\psi, \quad p(x) = \sqrt{2m(E-V(x))} > 0 \tag{B.3}$$

$$\psi(x) = A(x)\mathrm{e}^{\mathrm{i}\phi(x)} \tag{B.4}$$

$$A'' + 2\mathrm{i}A'\phi' + \mathrm{i}A\phi'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A \tag{B.5}$$

(2) 虚部：

$$2A'\phi' + A\phi'' = 0 \Rightarrow (A^2\phi')' = 0 \Rightarrow A = \frac{C}{\sqrt{|\phi'|}} \tag{B.6}$$

(3) 实部：忽略缓变的 A''

$$A'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A \Rightarrow (\phi')^2 - \frac{p^2}{\hbar^2} = 0 \Rightarrow \phi(x) = \pm\frac{1}{\hbar}\int p(x)\mathrm{d}x \tag{B.7}$$

(4) 波函数：

$$\psi(x) = \frac{C}{\sqrt{p(x)}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int p(x)\mathrm{d}x} + \frac{D}{\sqrt{p(x)}}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int p(x)\mathrm{d}x} \tag{B.8}$$

4. 隧道效应：

(1) 当 $x < 0$ 时：

$$\psi(x) = A\mathrm{e}^{\mathrm{i}kx} + B\mathrm{e}^{-\mathrm{i}kx} \tag{B.9}$$

(2) 当 $x > a$ 时：

$$\psi(x) = F\mathrm{e}^{\mathrm{i}kx} \tag{B.10}$$

(3) 当 $0 < x < a$ 时：

$$\psi(x) = \frac{C}{\sqrt{|p(x)|}}\mathrm{e}^{\frac{1}{\hbar}\int_0^x |p(x')|\mathrm{d}x'} + \frac{D}{\sqrt{|p(x)|}}\mathrm{e}^{-\frac{1}{\hbar}\int_0^x |p(x')|\mathrm{d}x'} \tag{B.11}$$

5. 连接公式：

(1) 经典区域和非经典区域的波函数：

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{p(x)}}\left[B\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int_x^0 p(x')\mathrm{d}x'} + C\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_x^0 p(x')\mathrm{d}x'}\right] & x < 0 \\ \frac{1}{\sqrt{|p(x)|}}D\mathrm{e}^{-\frac{1}{\hbar}\int_0^x |p(x')|\mathrm{d}x'} & x > 0 \end{cases} \tag{B.12}$$

(2) 原点邻域的线性势：

$$V(x) = E + V'(0)x \tag{B.13}$$

(3) 原点邻域的 Schrodinger 方程：

$$-\frac{\hbar^2}{2m}\psi_p(x) + (E + V'(0)x)\psi_p(x) = E\psi_p(x) \tag{B.14}$$

$$\frac{\mathrm{d}^2\psi_p}{\mathrm{d}x^2} = \alpha^3 x\psi_p, \quad \alpha = \left[\frac{2m}{\hbar^2}V'(0)\right]^{\frac{1}{3}} \Rightarrow \frac{\mathrm{d}^2\psi_p}{\mathrm{d}z^2} = z\psi_p, \quad z = \alpha x \tag{B.15}$$

(4) 原点邻域的修补波函数：

$$\psi_p(x) = a\mathrm{Ai}(\alpha x) + b\mathrm{Bi}(\alpha x) \tag{B.16}$$

$$p(x) = \sqrt{-2mV'(0)x} = \hbar\alpha^{\frac{3}{2}}\sqrt{-x} \tag{B.17}$$

(5) 第二交叠区：

$$\int_0^x |p(x')|\mathrm{d}x' = \hbar\alpha^{\frac{3}{2}}\int_0^x \sqrt{x'}\mathrm{d}x' = \frac{2}{3}\hbar(\alpha x)^{\frac{3}{2}} \tag{B.18}$$

$$\psi(x) = \frac{D}{\sqrt{\hbar}\alpha^{\frac{3}{4}}x^{\frac{1}{4}}}\mathrm{e}^{-\frac{2}{3}(\alpha x)^{3/2}} \tag{B.19}$$

$$\psi_p(x) \approx \frac{a}{2\sqrt{\pi}(\alpha x)^{\frac{1}{4}}}\mathrm{e}^{-\frac{2}{3}(\alpha x)^{3/2}} + \frac{b}{\sqrt{\pi}(\alpha x)^{\frac{1}{4}}}\mathrm{e}^{\frac{2}{3}(\alpha x)^{3/2}} \tag{B.20}$$

$$\psi(x) \sim \psi_p(x) \Rightarrow a = \sqrt{\frac{4\pi}{\alpha\hbar}}D, \quad b = 0 \tag{B.21}$$

(6) 第一交叠区：

$$\int_x^0 p(x')\mathrm{d}x' = \hbar\alpha^{\frac{3}{2}}\int_x^0 \sqrt{-x'}\mathrm{d}x' = \frac{2}{3}\hbar(-\alpha x)^{\frac{3}{2}} \tag{B.22}$$

$$\psi(x) = \frac{1}{\sqrt{\hbar}\alpha^{\frac{3}{4}}(-x)^{\frac{1}{4}}}\left[B\mathrm{e}^{\mathrm{i}\frac{2}{3}(-\alpha x)^{3/2}} + C\mathrm{e}^{-\mathrm{i}\frac{2}{3}(-\alpha x)^{3/2}}\right] \tag{B.23}$$

$$\psi_p(x) \approx \frac{a}{\sqrt{\pi}(-\alpha x)^{\frac{1}{4}}}\sin\left[\frac{2}{3}(-\alpha x)^{\frac{3}{2}} + \frac{\pi}{4}\right] = \frac{a}{\sqrt{\pi}(-\alpha x)^{\frac{1}{4}}}\frac{1}{2\mathrm{i}}\left[\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}\mathrm{e}^{\mathrm{i}\frac{2}{3}(-\alpha x)^{3/2}} - \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}\mathrm{e}^{-\mathrm{i}\frac{2}{3}(-\alpha x)^{3/2}}\right] \tag{B.24}$$

$$\psi(x) \sim \psi_p(x) \Rightarrow \frac{a}{2\mathrm{i}\sqrt{\pi}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}} = \frac{B}{\sqrt{\hbar\alpha}}, \quad \frac{-a}{2\mathrm{i}\sqrt{\pi}}\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} = \frac{C}{\sqrt{\hbar\alpha}} \tag{B.25}$$

(7) 连接公式：

$$B = -\mathrm{i}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}D, \quad C = \mathrm{i}\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}D \tag{B.26}$$

(8) 波函数：转折点为 x_0

$$\psi(x) = \begin{cases} \dfrac{2D}{\sqrt{p(x)}}\sin\left[\dfrac{1}{\hbar}\displaystyle\int_0^{x_0} p(x')\mathrm{d}x' + \dfrac{\pi}{4}\right] & x < x_0 \\ \dfrac{D}{\sqrt{|p(x)|}}\mathrm{e}^{-\frac{1}{\hbar}\int_{x_0}^x |p(x')|\mathrm{d}x'} & x > x_0 \end{cases} \tag{B.27}$$

C 量子相位算符

1. 相位算符：非幺正、非 Hermite

$$e^{i\hat{\phi}} = \frac{1}{\sqrt{\hat{a}\hat{a}^\dagger}}\hat{a}, \quad e^{-i\hat{\phi}} = \hat{a}^\dagger\frac{1}{\sqrt{\hat{a}\hat{a}^\dagger}} \tag{C.1}$$

$$e^{i\hat{\phi}} = \sum_{n=0}^{+\infty}|n\rangle\langle n+1|, \quad e^{-i\hat{\phi}} = \sum_{n=0}^{+\infty}|n+1\rangle\langle n| \tag{C.2}$$

$$e^{i\hat{\phi}}e^{-i\hat{\phi}} = \hat{I}, \quad e^{-i\hat{\phi}}e^{i\hat{\phi}} = \hat{I} - |0\rangle\langle 0|, \quad [e^{i\hat{\phi}}, e^{-i\hat{\phi}}] = 0 \tag{C.3}$$

$$[\hat{n}, e^{i\hat{\phi}}] = -e^{i\hat{\phi}}, \quad [\hat{n}, e^{-i\hat{\phi}}] = e^{-i\hat{\phi}} \tag{C.4}$$

2. 相位算符的本征态：

$$|\phi\rangle = \frac{1}{\sqrt{2\pi}}\sum_{n=0}^{+\infty}e^{in\phi}|n\rangle, \quad e^{i\hat{\phi}}|\phi\rangle = e^{i\phi}|\phi\rangle \tag{C.5}$$

3. 正规化的相位算符：幺正、Hermite

$$e^{i\hat{\phi}_\theta} = \sum_k e^{i\theta_k}|\theta_k\rangle\langle\theta_k|, \quad \theta_k = \theta_0 + \frac{2k\pi}{M+1}, \quad k = 0, 1, \ldots, M \tag{C.6}$$

$$|\theta_k\rangle = \frac{1}{\sqrt{M+1}}\sum_{n=0}^{M}e^{in\theta_k}|n\rangle, \quad |n\rangle = \frac{1}{\sqrt{M+1}}\sum_{k=0}^{M}e^{-in\theta_k}|\theta_k\rangle \tag{C.7}$$

4. 正规化相位算符的本征态：

$$e^{i\hat{\phi}}|\theta_k\rangle = e^{i\theta}|\theta_k\rangle, \quad \hat{\phi}_\theta = \sum_k \theta_k|\theta_k\rangle\langle\theta_k| \tag{C.8}$$

5. 相位分布函数：

$$W(\theta_k) = |\langle\theta_k|\psi\rangle|^2 = \frac{1}{M+1}\left|\sum_{n=0}^{M}c_n e^{-in\theta_k}\right|^2 = \frac{1}{2\pi}\left|\sum_{n=0}^{M}c_n e^{-in\theta_k}\right|^2\frac{2\pi}{M+1} \tag{C.9}$$

$$M\to\infty \Rightarrow \int_0^{2\pi}W(\theta)d\theta = \frac{1}{2\pi}\int_0^{2\pi}\left|\sum_{n=0}^{M}c_n e^{-in\theta}\right|^2 d\theta = 1 \tag{C.10}$$

6. 力学量的平均值：

$$\langle\psi|\hat{O}(\hat{\phi}_\theta)|\psi\rangle = \int_0^{2\pi}O(\theta)W(\theta)d\theta \tag{C.11}$$

D 局域实在论与量子力学的矛盾

1. Bell 不等式：

$$|P(\boldsymbol{a},\boldsymbol{b})-P(\boldsymbol{a},\boldsymbol{c})|\leqslant 1+P(\boldsymbol{b},\boldsymbol{c}) \tag{D.1}$$

2. CHSH 不等式：

$$|P(\boldsymbol{a},\boldsymbol{b})+P(\boldsymbol{a}',\boldsymbol{b})-P(\boldsymbol{a},\boldsymbol{b}')+P(\boldsymbol{a}',\boldsymbol{b}')|\leqslant 2 \tag{D.2}$$

3. GHZ 定理：

$$m_{1x}m_{2y}m_{3y}=m_{1y}m_{2x}m_{3y}=m_{1y}m_{2y}m_{3x}=1,\ m_{i\alpha}^2=1 \tag{D.3}$$

$$\Rightarrow (m_{1x}m_{2y}m_{3y})(m_{1y}m_{2x}m_{3y})(m_{1y}m_{2y}m_{3x})=m_{1x}m_{2x}m_{3x}=1 \tag{D.4}$$

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