0.1 单体问题的代数解法

0.1.1 类氢原子

0.1.1.1 量级分析

$$H = \frac{\vec{p}^2}{2\mu} - \frac{Ze^2}{4\pi\epsilon_0 r}, \quad \mu = \frac{m_e M}{m_e + M}$$

使用不确定性原理临界 $\Delta x \Delta p \sim \hbar$ 可知

$$\begin{aligned} H(\Delta r) &\sim \frac{\hbar^2}{2\mu(\Delta r)^2} - \frac{Ze^2}{4\pi\epsilon_0 \Delta r} \\ \Rightarrow r &\sim \frac{4\pi\epsilon_0\hbar^2}{Ze^2\mu} \equiv \frac{1}{Z}\frac{m_e}{\mu}a_0 \\ E_0 &\sim -\frac{1}{2}\frac{\mu}{\hbar^2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2 \equiv -Z^2\frac{\mu}{m_e}\mathrm{Ry}, \quad \mathrm{Ry} = \frac{1}{2}\frac{e^2}{4\pi\epsilon_0 a_0} \end{aligned}$$

0.1.1.2 径向波函数

$$\begin{aligned} \nabla^2 &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right), \quad \psi(r,\theta,\phi) = R(r)Y(\theta,\phi) \\ &\Rightarrow \begin{cases} \frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) - \frac{2mr^2}{\hbar^2}\left[\frac{1}{4\pi\epsilon_0}\frac{1}{r} - E\right] = l(l+1) \\ \frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\} = -l(l+1) \end{cases} \end{aligned}$$

令 $\kappa \equiv \frac{\sqrt{-2m_e E}}{\hbar}$, $\rho \equiv \kappa r$, 径向波函数化为

$$\begin{aligned} \frac{\mathrm{d}^2 u}{\mathrm{d}\rho^2} &= \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]u. \quad \rho_0 \equiv \frac{m_e e^2}{2m_e\varepsilon_0\hbar^2\kappa} \\ \lim_{\rho\to\infty} u &\sim Ae^{-\rho}, \quad \lim_{\rho\to 0} u \sim C\rho^{l+1} \Rightarrow u(\rho) = \rho^{l+1}e^{-\rho}v(\rho) \\ \Rightarrow &\rho\frac{\mathrm{d}^2 v}{\mathrm{d}\rho^2} + 2(l+1-\rho)\frac{\mathrm{d}v}{\mathrm{d}\rho} + \Big[\rho_0 - 2(l+1)\Big]v = 0 \end{aligned}$$

设 $v(\rho) = \sum_{j=0}^{\infty} c_j\rho_j$, 代入得到递推关系

$$c_{j+1} = \frac{2(j+l+1) - \rho_0}{(j+1)\Big[j + 2(l+1)\Big]}c_j$$

0.1.2 简谐振子

0.1.2.1 一维谐振子

0.1.2.1.1 哈密顿量

$$\begin{aligned} H &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \quad \omega = \sqrt{\frac{k}{m}} \\ \text{无量纲化:} \quad p &= P\sqrt{\hbar m\omega}, \quad x = Q\sqrt{\frac{\hbar}{m\omega}} \\ \Rightarrow H &= \frac{1}{2}\hbar\omega(P^2 + Q^2), \quad [P,Q] = i \end{aligned}$$

0.1.2.1.2 玻色子概念 $E_n = \hbar\omega\left(n+\frac{1}{2}\right), \quad n = 0,1,2,\cdots$. 每个单位能量 $\hbar\omega$ 对应的是玻色子的激发. 产生: $a^\dagger : |0\rangle \to |1\rangle \to |2\rangle \to \cdots$, 湮灭: $a : \cdots \to |2\rangle \to |1\rangle \to |0\rangle$.

0.1.2.1.3 产生湮灭算符

$$
\begin{aligned}
a &= \frac{1}{\sqrt{2}}(Q+iP)\\
a^\dagger &= \frac{1}{\sqrt{2}}(Q-iP)\\
[a,a^\dagger] = 1 &\Leftrightarrow aa^\dagger = a^\dagger a + 1
\end{aligned}
$$

0.1.2.1.4 玻色子占据数表象

$$
\begin{aligned}
a|n\rangle &= \sqrt{n}|n-1\rangle\\
a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle\\
a^\dagger a|n\rangle = n|n\rangle, &\quad aa^\dagger|n\rangle = (n+1)|n\rangle
\end{aligned}
$$

0.1.2.1.5 Fock 空间的构造 定义粒子数算符 $\hat{n} = a^\dagger a$, 本征态为 $|n\rangle$, 本征值 $\lambda_n = n$.

0.1.2.1.6 矩阵表示 选定矩阵基矢为 $|0\rangle = \begin{pmatrix}1\\0\\0\\\vdots\end{pmatrix}, \quad |1\rangle = \begin{pmatrix}0\\1\\0\\\vdots\end{pmatrix}, \quad |2\rangle = \begin{pmatrix}0\\0\\1\\\vdots\end{pmatrix}, \quad \cdots$, 即可计算产生湮灭算符的矩阵表示:

$$
\begin{aligned}
a_{mn} &= \langle m|a|n\rangle = \sqrt{n}\langle m|n-1\rangle = \sqrt{n}\delta_{m,n-1}\\
a^\dagger_{mn} &= \langle m|a^\dagger|n\rangle = \sqrt{n+1}\langle m|n+1\rangle = \sqrt{n+1}\delta_{m,n+1}\\
a &= \begin{pmatrix}0 & \sqrt{1} & & & \cdots\\ & 0 & \sqrt{2} & & \cdots\\ & & 0 & \sqrt{3} & \cdots\\ & & & 0 & \ddots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}, \quad a^\dagger = \begin{pmatrix}0 & & & & \cdots\\ \sqrt{1} & 0 & & & \cdots\\ & \sqrt{2} & 0 & & \cdots\\ & & \sqrt{3} & 0 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}\\
Q &= \frac{a+a^\dagger}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & \sqrt{1} & & & \cdots\\ \sqrt{1} & 0 & \sqrt{2} & & \cdots\\ & \sqrt{2} & 0 & \sqrt{3} & \cdots\\ & & \sqrt{3} & 0 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}, \quad P = \frac{a-a^\dagger}{\sqrt{2}i} = \frac{1}{\sqrt{2}i}\begin{pmatrix}0 & +\sqrt{1} & & & \cdots\\ -\sqrt{1} & 0 & +\sqrt{2} & & \cdots\\ & -\sqrt{2} & 0 & +\sqrt{3} & \cdots\\ & & -\sqrt{3} & 0 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}
\end{aligned}
$$

0.1.2.1.7 能谱

$$
\begin{aligned}
H = \hbar\left(a^\dagger a + \frac{1}{2}\right) &\to E_n = \hbar\omega\left(n+\frac{1}{2}\right)\\
|n\rangle = \frac{1}{\sqrt{n!}}\left[a^\dagger\right]^n|0\rangle, &\quad \hat{n}|n\rangle = a^\dagger a|n\rangle = \frac{1}{\sqrt{n!}}a^\dagger a\left[a^\dagger\right]^n|0\rangle\\
a\left[a^\dagger\right]^n = aa^\dagger\left[a^\dagger\right]^{n-1} &= \left(a^\dagger a+1\right)\left[a^\dagger\right]^{n-1} = a^\dagger a\left[a^\dagger\right]^{n-1} + \left[a^\dagger\right]^{n-1}\\
a^\dagger a\left[a^\dagger\right]^{n-1} = a^\dagger aa^\dagger\left[a^\dagger\right]^{n-2} &= a^\dagger\left(a^\dagger a+1\right)\left[a^\dagger\right]^{n-2} = \left[a^\dagger\right]^2 a\left[a^\dagger\right]^{n-2} + \left[a^\dagger\right]^{n-1}\\
\Rightarrow \hat{n}|n\rangle = \frac{1}{\sqrt{n!}}a^\dagger\left\{\cancel{\left[a^\dagger\right]^n a} + n\left[a^\dagger\right]^{n-1}\right\}|0\rangle &= \frac{n}{\sqrt{n!}}\left[a^\dagger\right]^n|0\rangle = n|n\rangle
\end{aligned}
$$

0.1.2.1.8 波函数 根据 $a|0\rangle = 0$, 且应用 $P = -i\dfrac{\partial}{\partial Q}$, 基态 $|0\rangle$ 满足 $\left(Q + \dfrac{\partial}{\partial Q}\right)\psi_0(Q) = 0$. 所以 $\psi_0(Q) = \dfrac{1}{\pi^{\frac{1}{4}}}e^{-\frac{1}{2}Q^2}$. 通过 $a^\dagger$ 产生激发态, 如第一激发态 $|1\rangle = a^\dagger|0\rangle$:

$$\begin{aligned}
\psi_1(Q) &= \frac{1}{\sqrt{2}}\left(Q - \frac{\partial}{\partial Q}\right)\psi_0(Q) = \frac{1}{\pi^{\frac{1}{4}}}\sqrt{2}Qe^{-\frac{1}{2}Q^2} \\
\psi_n(Q) &= \frac{1}{\pi^{\frac{1}{4}}\sqrt{2^n n!}}H_n(Q)e^{-\frac{1}{2}Q^2} \\
\bar{\psi}_n(P) &= \frac{1}{\pi^{\frac{1}{4}}\sqrt{2^n n!}}H_n(P)e^{-\frac{1}{2}P^2}
\end{aligned}$$

0.1.2.1.9 不确定性关系

$$\Delta Q\delta P \geq \frac{1}{2}\Big|[Q, P]\Big|^2 = \frac{1}{2}$$

使用 Fock 态 $|n\rangle$ 检验. ΔQ 和 ΔP 即标准差, 有

$$\begin{aligned}
Q &= \frac{a + a^\dagger}{\sqrt{2}}, \quad P = \frac{a - a^\dagger}{\sqrt{2}i} \\
\langle n|Q|n\rangle &= 0, \quad \langle n|Q^2|n\rangle = \frac{1}{2}\langle n|(a + a^\dagger)^2|n\rangle = n + \frac{1}{2} \\
\to \Delta Q &= \sqrt{\langle n|q^2|n\rangle - (\langle n|Q|n\rangle)^2} = \sqrt{n + \frac{1}{2}} \\
\langle n|P|n\rangle &= 0, \quad \langle n|P^2|n\rangle = -\frac{1}{2}\langle n|(a - a^\dagger)^2|n\rangle = -n - \frac{1}{2} \\
\to \Delta P &= \sqrt{\langle n|P^2|n\rangle - (\langle n|P|n\rangle)^2} = \sqrt{n + \frac{1}{2}} \\
\Rightarrow \Delta Q\Delta P &= \sqrt{n + \frac{1}{2}}\sqrt{n + \frac{1}{2}} = n + \frac{1}{2} \geq \frac{1}{2}
\end{aligned}$$

0.1.2.2 相干态

0.1.2.2.1 定义 相干态是湮灭算符 a 的本征态, 也是使得不确定性最小的态.

$$\begin{aligned}
&a|\alpha\rangle = \alpha|\alpha\rangle, \quad \alpha \in \mathbb{C}, \quad \langle\alpha_1|\alpha_2\rangle \neq \delta(\alpha_1 - \alpha_2) \\
&\langle\alpha|Q|\alpha\rangle = \langle\alpha|\frac{a + a^\dagger}{\sqrt{2}}|\alpha\rangle = \frac{\alpha^* + \alpha}{\sqrt{2}} = \sqrt{2}\mathrm{Re}(\alpha) \\
&\langle\alpha|Q^2|\alpha\rangle = \langle\alpha|\frac{[a^\dagger]^2 + aa^\dagger + a^\dagger a + a^2}{2}|\alpha\rangle = \frac{\alpha^2 + 2\alpha^*\alpha + [\alpha^*]^2 + 1}{2} = \frac{(\alpha^* + \alpha)}{2} + \frac{1}{2} = 2[\mathrm{Re}\alpha]^2 + \frac{1}{2} \\
&\Rightarrow \Delta Q = \sqrt{\langle\alpha|x^2|\alpha\rangle - (\langle\alpha|x|\alpha\rangle)^2} = \frac{1}{\sqrt{2}} \\
&\langle\alpha|P|\alpha\rangle = \langle\alpha|\frac{a - a^\dagger}{\sqrt{2}i}|\alpha\rangle = \frac{\alpha^* - \alpha}{\sqrt{2}i} = \sqrt{2}\mathrm{Im}(\alpha) \\
&\langle\alpha|P^2|\alpha\rangle = \langle\alpha|\frac{[a^\dagger]^2 - aa^\dagger - a^\dagger a + a^2}{2}|\alpha\rangle = \frac{\alpha^2 - 2\alpha^*\alpha + [\alpha^*]^2 + 1}{2} = \frac{(\alpha^* - \alpha)}{2} + \frac{1}{2} = 2[\mathrm{Im}\alpha]^2 + \frac{1}{2} \\
&\Rightarrow \Delta P = \sqrt{\langle\alpha|P^2|\alpha\rangle - (\langle\alpha|P|\alpha\rangle)^2} = \frac{1}{\sqrt{2}} \\
&\Delta Q\Delta P = \frac{1}{2}
\end{aligned}$$

0.1.2.2.2 Fock 态表象 以 Fock 态为基矢展开相干态 $|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\dfrac{\alpha^n}{\sqrt{n!}}|n\rangle$. 它的含义是, 遍历所有可能的 $|n\rangle$, 并使用对应的 n 个湮灭算符将其降阶至基态 $|0\rangle$.

1. $|0\rangle$ 也是相干态, 相当于 $\alpha = 0$.

2. 相干态 $|\alpha = n\rangle$ 和粒子数表象的 $|n\rangle$ 不同.

3. 在相干态 $|\alpha\rangle$ 中测得 n 个玻色子的概率为 $p_\alpha(n) = |\langle n|\alpha\rangle|^2 = \dfrac{|\alpha|^{2n}}{n!}e^{-|\alpha|^2} \equiv \dfrac{\lambda^2}{n!}e^{-\lambda}$, 也就是说这是一个 Poisson 分布. 这也是 $\langle n\rangle_\alpha = \langle\alpha|\hat{n}|\alpha\rangle = |\alpha|^2$ 的例证.

0.1.2.2.3 时间演化

$$
\begin{aligned}
U(t) &= e^{-iHt/\hbar} = e^{-i\omega\left(\hat{n}+\frac{1}{2}\right)t} = e^{-\frac{i\omega t}{2}}e^{-i\omega t\hat{n}} \\
U(t)|\alpha\rangle &= e^{-\frac{i\omega t}{2}}e^{-i\omega t\hat{n}}e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle = e^{-\frac{i\omega t}{2}}e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-i\omega tn}|n\rangle \\
&= e^{-\frac{i\omega t}{2}}e^{-\frac{1}{2}|\alpha e^{-i\omega t}|^2}\sum_{n=0}^{\infty}\frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}}|n\rangle = |\alpha e^{-i\omega t}\rangle \\
&\Rightarrow \alpha(t) = \alpha(0)e^{-i\omega t}
\end{aligned}
$$

0.1.2.2.4 U(1)对称性

0.1.2.2.5 坐标表象

0.1.2.2.6 BCH 公式

0.1.2.2.7 位移公式

0.1.2.2.8 超完备性

$$
\langle\beta|\alpha\rangle = e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)+\alpha\beta^*} \to P(|\alpha\rangle->|\beta\rangle) = |\langle\beta|\alpha\rangle|^2 = e^{-|\alpha-\beta|^2}
$$

1. 非正交性: $\langle\beta|\alpha\rangle \neq \delta_{\alpha\beta}$.

2. 完备性关系:

$$
\begin{aligned}
\frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}\alpha|\alpha\rangle\langle\alpha| &= \frac{1}{\pi}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{\sqrt{m!n!}}\int_{\mathbb{C}}\mathrm{d}\alpha e^{-|\alpha|^2}\alpha^m[\alpha^*]^n|m\rangle\langle n| \\
\alpha = re^{i\varphi}:\quad &= \frac{1}{\pi}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{\sqrt{m!n!}}\int_0^{\infty}r\mathrm{d}re^{-r^2}r^{m+n}\int_0^{2\pi}\mathrm{d}\varphi e^{i(m-n)\varphi}|m\rangle\langle n| \\
&= \frac{1}{\pi}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{\sqrt{m!n!}}2\pi\delta_{mn}\int_0^{\infty}r\mathrm{d}re^{-r^2}r^{m+n}|m\rangle\langle n| \\
s = r^2:\quad &= \frac{1}{\pi}\sum_{n=0}^{\infty}\frac{1}{n!}\pi\int_0^{\infty}\mathrm{d}se^{-s}s^n|n\rangle\langle n| \\
&= \frac{1}{\pi}\sum_{n=0}^{\infty}\frac{1}{\cancel{n!}}\pi\cancel{\Gamma(n+1)}|n\rangle\langle n| \\
&= \sum_{n=0}^{\infty}|n\rangle\langle n| = \mathbb{I}
\end{aligned}
$$

3. 超完备性(任何相干态都可以用其它相干态展开):

$$
|\alpha\rangle = \frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}\beta|\beta\rangle\langle\beta|\alpha\rangle = \frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}\beta|\beta\rangle e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)+\alpha\beta^*}
$$

0.1.2.3 三维谐振子

0.1.2.3.1 哈密顿量

$$
\begin{aligned}
H &= \frac{\hbar\omega}{2}\left(\vec{P}^2 + \vec{Q}^2\right), \quad [Q_i, P_j] = i\delta_{ij}, \quad [Q_i, Q_j] = [P_i, P_j] = 0 \\
\vec{a} &= \frac{1}{\sqrt{2}}(\vec{Q} + i\vec{P}), \quad \vec{a}^\dagger = \frac{1}{\sqrt{2}}(\vec{Q} - i\vec{P}), \quad [a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0 \\
H &= \hbar\omega\left(\vec{a}^\dagger \cdot \vec{a} + \frac{3}{2}\right) = \hbar\omega\left(a_1^\dagger a_1 + a_2^\dagger a_2 + a_3^\dagger a_3 + \frac{3}{2}\right)
\end{aligned}
$$

0.1.2.3.2 能级和简并

$$
\begin{aligned}
E &= \hbar\omega\left(n_1 + n_2 + n_3 + \frac{3}{2}\right) = \hbar\omega\left(N + \frac{3}{2}\right) \\
D &= \sum_{n_1, n_2, n_3} \delta_{N, n_1+n_2, n_3} = \frac{1}{2}(N+1)(N+2)
\end{aligned}
$$

0.1.2.3.3 角动量算符

$$
\vec{L} = \vec{x} \times \vec{p} \iff L_i = \epsilon_{ijk} x_j p_k \iff L_i = -i\epsilon_{ijk} a_j^\dagger a_k
$$

0.1.2.3.4 Fock 态表象

0.1.2.3.5 角动量表象