Some notes about QM

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Chapter 6 Time-independent Pertunbation Theory定态微扰论

6. 1. 1 General formation

$$H^{(0)}\psi^{(0)} = E_n^{(0)}\psi_n^{(0)}$$

Orthonormal condition 正交归一性质

$$\langle\psi_n^{(0)}|\psi_m^{(0)}\rangle = \delta_{n,m}$$

其中$\langle\ \ |\ \ \rangle$称为Dirac notation, δ为克罗内克符号。

微扰论 Perturbation theory−−To obtain approximate solution based on the known exact solution.

$$H = H^{(0)} + \lambda H' \quad 其中，H' \ll H^{(0)}$$

$'$:prime（上标），| H是我们需要求解的，$H^{(0)}$是我们已知的,H'为所加微扰项。λ为任意数（往往最后令它为1,从而得到简化的结论）（在求解过程中，利用λ体现阶数）

假设：

$$\begin{aligned} E_n &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \\ \psi_n &= \psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \cdots \end{aligned}$$

将 H, E_n, ψ_n代入到 $\quad H\psi_n = E_n\psi_n$

$\Rightarrow (H^{(0)} + \lambda H')\,[\psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \cdots] = [E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots]\,[\psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \cdots]$

λ的一次项单独取出：

$$H^{(0)} \cdot (\lambda\psi_n^{(1)}) + (\lambda H')\,\psi_n^{(0)} = E_n^{(0)}\,(\lambda\psi_n^{(1)}) + \lambda E_n^{(1)}\psi_n^{(0)}$$

$$H^{(0)}\psi_n^{(1)} + H'\psi_n^{(0)} = E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)} \qquad [6.7]$$

λ的二次项单独取出：

$$H^{(0)}\,(\lambda^2\psi_n^{(2)}) + \lambda H' \cdot (\lambda\psi_n^{(1)}) = E_n^{(0)}\,(\lambda^2\psi_n^{(2)}) + \lambda E_n^{(1)} \cdot (\lambda\psi_n^{(1)}) + \lambda^2 E_n^{(2)}\psi_n^{(0)}$$

$$H^{(0)}\psi_n^{(2)} + H'\psi_n^{(1)} = E_n^{(0)}\psi_n^{(2)} + E_n^{(1)}\psi_n^{(1)} + E_n^{(2)}\psi_n^{(0)} \qquad [6.8]$$

The 1st order Theory

[Trick] Inner product $\langle\psi_n^{(0)}\,|\,[6.7]\rangle \Rightarrow$

$$\begin{aligned}
\langle\psi_n^{(0)}\,|\,H^{(0)}\,|\,\psi_n^{(1)}\rangle + \langle\psi_n^{(0)}\,|\,H'\,|\,\psi_n^{(0)}\rangle &= E_n^{(0)}\langle\psi_n^{(0)}\,|\,\psi_n^{(1)}\rangle + E_n^{(1)}\langle\psi_n^{(0)}\,|\,\psi_n^{(0)}\rangle \\
\text{(由于}H^{(0)}\text{为厄密算符可以提到前面)}\quad \text{即} & \quad \langle\psi_n^{(0)}\,|\,H^{(0)}\,|\,\psi_n^{(1)}\rangle = \langle H^{(0)}\psi_n^{(0)}\,|\,\psi_n^{(1)}\rangle = E_n^{(0)}\langle\psi_n^{(0)}\,|\,\psi_n^{(1)}\rangle \\
\Rightarrow E_n^{(0)}\langle\psi_n^{(0)}\,|\,\psi_n^{(1)}\rangle + \langle\psi_n^{(0)}\,|\,H'\,|\,\psi_n^{(0)}\rangle &= E_n^{(0)}\langle\psi_n^{(0)}\,|\,\psi_n^{(1)}\rangle + E_n^{(1)} \\
\text{一阶线性微扰解} \Rightarrow E_n^{(1)} &= \langle\psi_n^{(0)}\,|\,H'\,|\,\psi_n^{(0)}\rangle
\end{aligned}$$

Ex 6.1 1D infinite square well

量子力学的势阱能量总是与“结点数”相关。对于$x \in [0, a]$的无限深方势阱。

$$\psi_n^{(0)} = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

取微扰： $H' = V_0\,(\text{constant})$

代入$E_n^{(1)} = \langle\psi_n^{(0)}\,|\,H'\,|\,\psi_n^{(0)}\rangle \Rightarrow E_n^{(1)} = \langle\psi_n^{(0)}\,|\,V_0\,|\,\psi_n^{(0)}\rangle = V_0\langle\psi_n^{(0)}\,|\,\psi_n^{(0)}\rangle = V_0$

$E_n = E_n^{(0)} + \lambda E_n^{(1)} = E_n^{(0)} + V_0$

修改微扰为$\boldsymbol{H' = \begin{cases} V_0\,(\text{constant})\,, 0 \leqslant x \leqslant \frac{a}{2} \\ 0 \qquad\quad , \text{otherwise} \end{cases}}$

$$E_n^{(1)} = \langle\psi_n^{(0)}\,|\,H'\,|\,\psi_n^{(0)}\,\rangle \longrightarrow \int dx\,\psi_n^{(0)*}H'(x)\,\psi_n^{(0)}$$

由完备性$\int dx\,|x><x| = 1$ 对应Identity operation.可以在公式间添加单位量而不引起任何变化

$$\begin{aligned}
E_n^{(1)} &= \int dx \int dx'\,\langle\psi_n^{(0)}\,|\,x\,\rangle\langle x\,|\,H'\,|\,x'\rangle\langle x'\,|\,\psi_n^{(0)}\,\rangle \\
&= \int dx \int dx'\,\langle\psi_n^{(0)}\,|\,x\,\rangle H'\langle x\,|\,x'\rangle\langle x'\,|\,\psi_n^{(0)}\,\rangle \\
&= \int dx \int dx'\,\langle\psi_n^{(0)}\,|\,x\,\rangle H'\,(\delta_{x,x'})\,\langle x'\,|\,\psi_n^{(0)}\,\rangle \\
&= \int dx\,\langle\psi_n^{(0)}\,|\,x\,\rangle H'(x)\,\langle x\,|\,\psi_n^{(0)}\,\rangle \\
&= \int dx\,\langle\psi_n^{(0)}\,|\,x\,\rangle H'(x)\,\langle x\,|\,\psi_n^{(0)}\,\rangle \\
&= \int dx\,\psi_n^{(0)*}(x)\,H'\psi_n^{(0)}
\end{aligned}$$

$$
\begin{aligned}
&= \int_0^{\frac{a}{2}} dx\,\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) V_0 \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)+0 \\
&= \frac{2V_0}{a}\int_0^{\frac{a}{2}}\sin^2\left(\frac{n\pi}{a}x\right)dx \\
E_n^{(1)} &= \frac{V_0}{2}
\end{aligned}
$$

一阶波函数修正

$$[H^{(0)}-E_n^{(0)}]\psi_n^{(1)}=-[H'-E_n^{(1)}]\psi_n^{(0)}\text{---}[6.7]\text{变式}$$

其中$\psi_n^{(1)}$是所想找到的一节波函数

因为$\sum\limits_m C_m\psi_m^{(0)}$具有表示空间中所有函数的完备性，所以可以设

$$\psi_n^{(1)}=\sum_{m\neq n}C_m^{(n)}\psi_m^{(0)}.$$

之所以有$m\neq n$，是考虑到在$[H^{(0)}-E_n^{(0)}]\psi_n^{(1)}$中，$H^{(0)}C_n^{(n)}\psi_n^{(n)}=E_n^{(0)}C_n^{(n)}\psi_n^{(n)}$，$m=n$时，左边等于0，所以$C_n^{(n)}$应为0.也就不考虑了。

$$
\begin{aligned}
[H^{(0)}-E_n^{(0)}]\sum_{m\neq n}C_m^{(n)}\psi_m^{(0)} &= -[H'-E_n^{(1)}]\psi_n^{(0)} \\
\Longrightarrow \sum_{m\neq n}C_m^{(n)}[H^{(0)}-E_n^{(0)}]\psi_m^{(0)} &= -[H'-E_n^{(1)}]\psi_n^{(0)}
\end{aligned}
$$

[Trick] $\langle\psi_l^{(0)}|\text{Inner product}\rangle$

$$
\begin{aligned}
[6.7]\Longrightarrow\left\langle\psi_l^{(0)}\left|\sum_{m\neq n}C_m^{(n)}[H^{(0)}-E_n^{(0)}]\right|\psi_m^{(0)}\right\rangle &= -\langle\psi_l^{(0)}|H'-E_n^{(1)}|\psi_n^{(0)}\rangle \\
\Longrightarrow\sum_{m\neq n}C_m^{(n)}[\langle\psi_l^{(0)}|H^{(0)}|\psi_m^{(0)}\rangle-\langle\psi_l^{(0)}|E_n^{(0)}|\psi_m^{(0)}\rangle] &= -\langle\psi_l^{(0)}|H'|\psi_n^{(0)}\rangle+\langle\psi_l^{(0)}|E_n^{(1)}|\psi_n^{(0)}\rangle \\
\sum_{m\neq n}C_m^{(n)}[E_m^{(0)}\delta_{l,m}-E_n^{(0)}\delta_{l,m}] &= -\langle\psi_l^{(0)}|H'|\psi_n^{(0)}\rangle+E_n^{(1)}\delta_{l,n}
\end{aligned}
$$

$(m\neq n)$ If $l=n$,

$$C_m^{(n)}[E_m^{(0)}\delta_{l,m}-E_n^{(0)}\delta_{l,m}]=0,\text{不能求解}C_m^{(0)},\text{且发现仅当}l=m\text{时}C\text{的系数不为0}$$

If $l=m$

$$
\begin{aligned}
C_m^{(n)}[E_m^{(0)}-E_n^{(0)}] &= -\langle\psi_l^{(0)}|H'|\psi_n^{(0)}\rangle \\
C_l^{(n)} &= \frac{-\langle\psi_l^{(0)}|H'|\psi_n^{(0)}\rangle}{E_m^{(0)}-E_n^{(0)}} \\
C_l^{(n)} &= \frac{\langle\psi_l^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}}
\end{aligned}
$$

$$\Longrightarrow\psi_n^{(1)}=\sum_{m\neq n}\frac{\langle\psi_l^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}}\psi_m^{(0)}$$

二阶波函数修正

$$H^{(0)}\psi_n^{(2)}+H'\psi_n^{(1)}=E_n^{(0)}\psi_n^{(2)}+E_n^{(1)}\psi_n^{(1)}+E_n^{(2)}\psi_n^{(0)}$$

[Trick] $\langle\psi_n^{(0)}|\,[6.8]\rangle$

$$\begin{aligned}
\langle\psi_n^{(0)}|H^{(0)}|\psi_n^{(2)}\rangle+\langle\psi_n^{(0)}|H'|\psi_n^{(1)}\rangle &= E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(2)}\rangle+E_n^{(1)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle+E_n^{(2)}\langle\psi_n^{(0)}|\psi_n^{(0)}\rangle\\
\text{由于}\psi_n^{(1)}=\sum_{m\neq n}\frac{\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}}\psi_m^{(0)} &,\quad \text{所以}\langle\psi_n^{(1)}|\psi_n^{(0)}\rangle=0\\
E_n^{(2)} &= \langle\psi_n^{(0)}|H'|\psi_n^{(1)}\rangle\\
&= \left\langle\psi_n^{(0)}|H'|\sum_{m\neq n}\frac{\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}}\psi_m^{(0)}\right\rangle\\
&= \sum_{m\neq n}\frac{\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}}\langle\psi_n^{(0)}|H'|\psi_m^{(0)}\rangle\\
E_n^{(2)} &= \sum_{m\neq n}\frac{\|\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle\|^2}{E_n^{(0)}-E_m^{(0)}} \qquad [6.15]
\end{aligned}$$

6.2 简并微扰论

简并微扰论就是对角化

6.2.1 二重简并

假设$H^{(0)}\psi_n^{(0)}=E^{(0)}\psi_a^{(0)}$,(假设$\psi_a^{(0)},\psi_b^{(0)}$满足正交归一性，即：$\langle\psi_a^{(0)}|\psi_b^{(0)}\rangle=0,\langle\psi_a^{(0)}|\psi_a^{(0)}\rangle=1$)

$$H^{(0)}\psi_b^{(0)}=E^{(0)}\psi_b^{(0)},$$

注意到：

$$\psi^{(0)}=\alpha\psi_a^{(0)}+\beta\psi_b^{(0)}\ \text{is an eigen state of } H^{(0)}$$

$$\|\alpha\|^2+\|\beta\|^2=1$$

Prove

$$\begin{aligned}
\langle\psi^{(0)}|H^{(0)}|\psi^{(0)}\rangle &= [\alpha^*\langle\psi_a^{(0)}|+\beta^*\langle\psi_b^{(0)}|]H'[\alpha|\psi_a^{(0)}\rangle+\beta|\psi_b^{(0)}\rangle]\\
&= \|\alpha\|^2\langle\psi_a^{(0)}|H'|\psi_a^{(0)}\rangle+\|\beta\|^2\langle\psi_b^{(0)}|H'|\psi_b^{(0)}\rangle\\
&\quad+\alpha^*\beta\langle\psi_a^{(0)}|H'|\psi_b^{(0)}\rangle+\beta^*\alpha\langle\psi_b^{(0)}|H'|\psi_a^{(0)}\rangle\\
&= (\|\alpha\|^2+\|\beta\|^2)E_0\\
&= E_0
\end{aligned}$$

We want to solve :$H\psi=E\psi$

where $H=H^{(0)}+\lambda H'\quad\lambda=1$

Assume

$$\begin{aligned}
E &= E^{(0)}+\lambda E^{(1)}+\lambda^2E^{(2)}+\cdots\\
\psi &= \psi^{(0)}+\lambda\psi^{(1)}+\lambda^2\psi^{(2)}+\cdots\\
\text{其中}\ , &\quad \psi^{(0)}=\alpha\psi_a^{(0)}+\beta\psi_b^{(0)}
\end{aligned}$$

$\psi_a^{(0)},\psi_b^{(0)}$是对角化所寻找的“good state”(用这两个作为基底表示H'为对角)

$$\Longrightarrow H^{(0)}\psi^{(0)}+\lambda(H'\psi^{(0)}+H^{(0)}\psi^{(1)})+\cdots=E_0\psi^{(0)}+\lambda(E^{(0)}\psi^{(1)}+E^{(1)}\psi^{(0)})+\cdots$$

$$H'\psi^{(0)}+H^{(0)}\psi^{(1)}=E^{(0)}\psi^{(1)}+E^{(1)}\psi^{(0)}$$

[Trick]用$\langle\psi_a^{(0)}|$与上式做内积

$$
\begin{aligned}
\langle\psi_a^{(0)}|H'|\psi^{(0)}\rangle+\langle\psi_a^{(0)}|H^{(0)}|\psi^{(1)}\rangle &= E^{(0)}\langle\psi_a^{(0)}|\psi^{(1)}\rangle+E^{(1)}\langle\psi_a^{(0)}|\psi^{(0)}\rangle\\
\langle\psi_a^{(0)}|H'|\psi^{(0)}\rangle &= E^{(1)}\langle\psi_a^{(0)}|\psi^{(0)}\rangle\\
\text{代入}\psi^{(0)}=\alpha\psi_a^{(0)}+\beta\psi_b^{(0)} &\Longrightarrow\\
\langle\psi_a^{(0)}|H'|\alpha\psi_a^{(0)}+\beta\psi_b^{(0)}\rangle &= E^{(1)}\langle\psi_a^{(0)}|\alpha\psi_a^{(0)}+\beta\psi_b^{(0)}\rangle\\
\alpha\langle\psi_a^{(0)}|H'|\psi_a^{(0)}\rangle+\beta\langle\psi_a^{(0)}|H'|\psi_b^{(0)}\rangle &= \alpha E^{(1)}
\end{aligned}
$$

同理，我们用$\langle\psi_b^{(0)}|$与上式做内积，将得到

$$\alpha\langle\psi_b^{(0)}|H'|\psi_a^{(0)}\rangle+\beta\langle\psi_b^{(0)}|H'|\psi_b^{(0)}\rangle=\beta E^{(1)}$$

我们把$\langle\psi_a^{(0)}|H'|\psi_a^{(0)}\rangle$,$\langle\psi_a^{(0)}|H'|\psi_b^{(0)}\rangle$,$\langle\psi_b^{(0)}|H'|\psi_a^{(0)}\rangle$,$\langle\psi_b^{(0)}|H'|\psi_b^{(0)}\rangle$看作四个矩阵元，为了方便期间，记$w_{ij}=\langle\psi_i^{(0)}|H'|\psi_j^{(0)}\rangle$

$$
\begin{aligned}
\begin{bmatrix} w_{aa} & w_{ab}\\ w_{ba} & w_{bb}\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix} &= \begin{bmatrix} E' & 0\\ 0 & E'\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix}\\
\begin{bmatrix} w_{aa}-E' & w_{ab}\\ w_{ba} & w_{bb}-E'\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix} &= 0
\end{aligned}
$$

为得到非平庸阶，要求：

$$
\begin{aligned}
\det\begin{vmatrix} w_{aa}-E' & w_{ab}\\ w_{ba} & w_{bb}-E'\end{vmatrix} &= 0\\
(w_{aa}-E')(w_{bb}-E')-w_{ba}\cdot w_{ab} &= 0\\
(E')^2-(w_{aa}+w_{bb})E'+w_{aa}\cdot w_{bb}-w_{ba}\cdot w_{ab} &= 0\\
\left(E'-\frac{w_{aa}+w_{bb}}{2}\right)^2 &= w_{ba}\cdot w_{ab}-w_{aa}\cdot w_{bb}+\left(\frac{w_{aa}+w_{bb}}{2}\right)^2\\
\left(E'-\frac{w_{aa}+w_{bb}}{2}\right)^2 &= w_{ba}\cdot w_{ab}+\left(\frac{w_{aa}-w_{bb}}{2}\right)^2\\
E_{\pm}'-\frac{w_{aa}+w_{bb}}{2} &= \pm\sqrt{\left(\frac{w_{aa}-w_{bb}}{2}\right)^2+w_{ba}\cdot w_{ab}}\\
E_{\pm}' &= \frac{w_{aa}+w_{bb}}{2}\pm\sqrt{\left(\frac{w_{aa}-w_{bb}}{2}\right)^2+w_{ba}\cdot w_{ab}}\\
\text{不妨, 设}\Delta E &= \sqrt{\left(\frac{w_{aa}-w_{bb}}{2}\right)^2+w_{ba}\cdot w_{ab}}\\
E_{\pm}' &= \frac{w_{aa}+w_{bb}}{2}\pm\Delta E
\end{aligned}
$$

$W=\begin{bmatrix} w_{aa} & w_{ab}\\ w_{ba} & w_{bb}\end{bmatrix}$ is the matrix of the perturbation H' in the Hilbert space spanned by $|\psi_a^{(0)}\rangle$ and $|\psi_b^{(0)}\rangle$.

To find the 1st order correction to the energy, $E^{(1)}$ is eigenvalue fo W.

例. Pro 6.6 Eigenstate of W

for $E_+^{(1)}$:

$$\psi_+^{(0)}=\alpha_+\psi_a^{(0)}+\beta_+\psi_b^{(0)}$$

for $E_-^{(1)}$:

$$\psi_-^{(0)}=\alpha_-\psi_a^{(0)}+\beta_-\psi_b^{(0)}$$

例. Pro 4.30

$$\psi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\left(\frac{\theta}{2}\right)\cdot e^{i\phi} \end{pmatrix} \qquad \psi_- = \begin{pmatrix} \sin\left(\frac{\theta}{2}\right)\cdot e^{-i\phi} \\ -\cos\frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} \sin\left(\frac{\theta}{2}\right) \\ -\cos\frac{\theta}{2}\cdot e^{i\phi} \end{pmatrix}$$

选择这种表示形式时的基底为$\psi_a^{(0)}$, $\psi_b^{(0)}$,即：

$$\psi_+ \;=\; \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\left(\frac{\theta}{2}\right)\cdot e^{i\phi} \end{pmatrix} = \cos\frac{\theta}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sin\frac{\theta}{2}\cdot e^{i\phi}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \cos\frac{\theta}{2}\psi_a^{(0)} + \sin\frac{\theta}{2}\cdot e^{i\phi}\psi_b^{(0)}$$

$$\cos\theta = \frac{\frac{w_{aa}-w_{bb}}{2}}{\sqrt{\left(\frac{w_{aa}-w_{bb}}{2}\right)^2 + w_{ab}w_{ba}}}$$

$$\cos\frac{\theta}{2} = \sqrt{\frac{1}{2}(1+\cos\theta)}\,,\quad \sin\frac{\theta}{2} = \sqrt{\frac{1}{2}(1-\cos\theta)}\,,\quad w_{ab} = |w_{ab}|e^{i\phi}$$

利用Pauli matrix in σ_z表象(在哪个表象内哪个就是对角化的)， 利用“自旋模型”表示因为微扰H'所造成的能级分裂之后的两能级。(任意的2×2矩阵都可以用Pauli 矩阵表示)

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$W = \frac{w_{aa}+w_{bb}}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{w_{aa}-w_{bb}}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \frac{w_{ab}+w_{ba}}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \frac{w_{ab}-w_{ba}}{2}i\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\begin{aligned} W &= \frac{w_{aa}+w_{bb}}{2}\sigma_0 + \Delta E\begin{bmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{bmatrix} \\ &= \frac{w_{aa}+w_{bb}}{2}\sigma_0 + \Delta E\,(\sin\theta\cos\phi\sigma_x + \sin\theta\sin\phi\sigma_y + \cos\theta\sigma_z) \end{aligned}$$

check the orthonormal properties

$$\langle\psi_+^{(0)}|\psi_-^{(0)}\rangle = \left(\cos\frac{\theta}{2} \quad ,\sin\frac{\theta}{2}e^{-i\phi}\right)\begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} = 0$$

$\langle\psi_+^{(0)}|H'|\psi_+^{(0)}\rangle$ in the basis $\{\psi_a^{(0)}, \psi_b^{(0)}\}$

$$\begin{aligned} \langle\psi_+^{(0)}|H'|\psi_+^{(0)}\rangle &= \left(\cos\frac{\theta}{2}, \sin\left(\frac{\theta}{2}\right)\cdot e^{-i\phi}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\frac{w_{aa}+w_{bb}}{2}\begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix} \\ &\quad + \left(\cos\frac{\theta}{2} \quad \sin\left(\frac{\theta}{2}\right)\cdot e^{-i\phi}\right)\begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}\Delta E\begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\left(\frac{\theta}{2}\right)\cdot e^{i\phi} \end{pmatrix} \\ &= \frac{w_{aa}+w_{bb}}{2} + (+1)\,\Delta E \end{aligned}$$

同理可计算出：

$$
\begin{aligned}
\langle\psi_-^{(0)}|H'|\psi_-^{(0)}\rangle &= \left(\sin\left(\frac{\theta}{2}\right)\cdot e^{i\phi}, -\cos\left(\frac{\theta}{2}\right)\right)\begin{pmatrix}1&0\\0&1\end{pmatrix}\frac{w_{aa}+w_{bb}}{2}\begin{pmatrix}\sin\left(\frac{\theta}{2}\right)\cdot e^{-i\phi}\\ -\cos\frac{\theta}{2}\end{pmatrix}\\
&\quad+\left(\sin\left(\frac{\theta}{2}\right)\cdot e^{i\phi}, -\cos\left(\frac{\theta}{2}\right)\right)\begin{pmatrix}\cos\theta & \sin\theta e^{-i\phi}\\ \sin\theta e^{i\phi} & -\cos\theta\end{pmatrix}\Delta E\begin{pmatrix}\sin\left(\frac{\theta}{2}\right)\cdot e^{-i\phi}\\ -\cos\frac{\theta}{2}\end{pmatrix}\\
&= \frac{w_{aa}+w_{bb}}{2}+(-1)\Delta E\\
\langle\psi_-^{(0)}|H'|\psi_+^{(0)}\rangle &= \left(\sin\left(\frac{\theta}{2}\right)\cdot e^{i\phi}, -\cos\left(\frac{\theta}{2}\right)\right)\begin{pmatrix}1&0\\0&1\end{pmatrix}\frac{w_{aa}+w_{bb}}{2}\begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix}\\
&\quad+\left(\sin\left(\frac{\theta}{2}\right)\cdot e^{i\phi}, -\cos\left(\frac{\theta}{2}\right)\right)\begin{pmatrix}\cos\theta & \sin\theta e^{-i\phi}\\ \sin\theta e^{i\phi} & -\cos\theta\end{pmatrix}\Delta E\begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix}\\
&= 0\\
\langle\psi_+^{(0)}|H'|\psi_-^{(0)}\rangle &= 0
\end{aligned}
$$

```
In[10]:= Simplify[(Sin[θ/2] E^(I ϕ)  -Cos[θ/2]).
         化简
          (    Cos[θ]        Sin[θ] E^(-I ϕ) ).( Sin[θ/2] E^(-I ϕ) )]
          ( Sin[θ] E^(I ϕ)      -Cos[θ]      )  (    -Cos[θ/2]      )
Out[10]= {{-1}}

In[15]:= Simplify[(Sin[θ/2] E^(I ϕ)  -Cos[θ/2]).
         化简
          (    Cos[θ]        Sin[θ] E^(-I ϕ) ).(     Cos[θ/2]      )]
          ( Sin[θ] E^(I ϕ)      -Cos[θ]      )  ( Sin[θ/2] E^(I ϕ)  )
Out[15]= {{0}}

In[16]:= Simplify[(Sin[θ/2] E^(I ϕ)  -Cos[θ/2]).( Cos[θ/2] E^(-I ϕ) )]
         化简                                    (     Sin[θ/2]      )
Out[16]= {{0}}
```

图. 一些计算

经过微扰之后我们发现$\langle\psi_+^{(0)}|H'|\psi_+^{(0)}\rangle\neq\langle\psi_-^{(0)}|H'|\psi_-^{(0)}\rangle$，这是由于微扰破坏了简并度（微扰破坏了其对称性）

6.2.2 多重简并

use $\{\psi_1,\psi_2,\ldots,\psi_n\}$ to express H' and digonalize

例. 3D cubical well

$$V(x,y,z)=\begin{cases}0, & x,y,z\in[0,a]\\ \infty, & \text{elsewhere}\end{cases}$$

未经微扰波函数与能量：

$$
\begin{aligned}
\psi_{n_x,n_y,n_z} &= \left(\frac{2}{a}\right)^{\frac{3}{2}}\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{a}y\right)\sin\left(\frac{n_z\pi}{a}z\right)\\
E_{n_x,n_y,n_z} &= \frac{\pi^2\hbar^2}{2ma^2}(n_x^2+n_y^2+n_z^2)
\end{aligned}
$$

基态$(n_x = n_y = n_z = 1)$：

$$\begin{aligned}\psi_{111} &= \left(\frac{2}{a}\right)^{\frac{3}{2}} \sin\left(\frac{\pi}{a}x\right) \sin\left(\frac{\pi}{a}y\right) \sin\left(\frac{\pi}{a}z\right)\\ E_{111} &= \frac{\pi^2\hbar^2}{2ma^2}(1+1+1)\end{aligned}$$

第一激发态$(\psi_{112}, \psi_{121}, \psi_{211}$三重简并)：

$$\begin{aligned}E_1 &= \frac{\pi^2\hbar^2}{2ma^2}(1+1+4)\\ &= \frac{3\pi^2\hbar^2}{ma^2}\end{aligned}$$

设存在微扰

$$H' = \begin{cases} V_0 & x, y \in \left[0, \frac{a}{2}\right] \\ 0 & \text{else where}\end{cases}$$

基态能量修正：$E^{(1)} = \langle \psi_{111} | H' | \psi_{111} \rangle = \left(\frac{2}{a}\right)^{\frac{3}{2}} V_0 \int_0^{a/2} dx \sin^2\left(\frac{\pi}{a}x\right) \int_0^{a/2} dy \sin^2\left(\frac{\pi}{a}y\right) \int_0^{a/2} dz \sin^2\left(\frac{\pi}{a}z\right)$

$$E^{(1)} = \frac{V_0}{4}$$

第一激发态能量修正:

$$\langle \psi_{简并1\times3} | H' | \psi_{简并1\times3} \rangle \longrightarrow \begin{bmatrix} w_{aa} & w_{ab} & w_{ac} \\ w_{ba} & w_{bb} & w_{bc} \\ w_{ca} & w_{cb} & w_{cc} \end{bmatrix} \quad \text{basis: } \{\psi_a, \psi_b, \psi_c\}$$

[tips] w_{ij}的物理含义为：从j状态转变为i状态的概率

即：$|H'\psi_a>$为H'作用于ψ_a，由于ψ_a并非关于H'的本征态，所以$|H'\psi_a>$为ψ_a, ψ_b, ψ_c的线性组合，而非仅为ψ_a的倍数。为了得到在三个态上的概率（线性组合的系数），只需做相应投影（利用ψ_a, ψ_b, ψ_c彼此正交），故有$\langle \psi_a | H' | \psi_a \rangle = w_{aa}$。一般的，有$w_{ij} = \langle \psi_i | H' | \psi_j \rangle$。

$$\begin{aligned}w_{aa} &= \langle \psi_a | H' | \psi_a \rangle = \langle \psi_{112} | H' | \psi_{112} \rangle\\ &= \left(\frac{2}{a}\right)^{\frac{3}{2}} V_0 \int_0^{\frac{a}{2}} dx \sin^2\left(\frac{\pi}{a}x\right) \int_0^{\frac{a}{2}} dy \sin^2\left(\frac{\pi}{a}y\right) \int_0^{a} dz \sin^2\left(\frac{2\pi}{a}z\right) = \frac{V_0}{4}\end{aligned}$$

$$\begin{aligned}w_{ab} &= \langle \psi_a | H' | \psi_b \rangle = \langle \psi_{112} | H' | \psi_{121} \rangle\\ &= \left(\frac{2}{a}\right)^{\frac{3}{2}} V_0 \int_0^{\frac{a}{2}} dx \sin^2\left(\frac{\pi}{a}x\right) \int_0^{\frac{a}{2}} dy \sin\left(\frac{2\pi}{a}y\right) \sin\left(\frac{\pi}{a}u\right) \int_0^{a} dz \sin\left(\frac{2\pi}{a}z\right) \sin\left(\frac{\pi}{a}z\right) = 0\end{aligned}$$

$$w_{ab} = 0, \text{说明} H' \text{ does not couple } \psi_a \text{ and } \psi_b, (\psi_a, \psi_b\text{无耦合})$$

$$\begin{aligned}w_{\text{bc}} &= \langle \psi_b | H' | \psi_c \rangle = \langle \psi_{121} | H' | \psi_{211} \rangle\\ &= \left(\frac{2}{a}\right)^{\frac{3}{2}} V_0 \int_0^{\frac{a}{2}} dx \sin\left(\frac{2\pi}{a}x\right) \sin\left(\frac{\pi}{a}x\right) \int_0^{\frac{a}{2}} dy \sin\left(\frac{2\pi}{a}y\right) \sin\left(\frac{\pi}{a}y\right) \int_0^{a} dz \sin^2\left(\frac{\pi}{a}z\right) = \frac{16}{9\pi^2} V_0\\ w_{\text{bc}} &\neq 0\text{，说明} H' \text{ couple} |\psi_b> \text{and} |\psi_c>, \text{令}\kappa =\end{aligned}$$

$\cdots \quad \cdots$

$$W = \frac{V_0}{4}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \kappa \\ 0 & \kappa & 1 \end{bmatrix}，对角化W \Rightarrow \begin{cases} E_1 = \frac{V_0}{4} \\ E_2 = \frac{V_0}{4}(1+\kappa) \\ E_3 = \frac{V_0}{4}(1-\kappa) \end{cases}$$

Dr. Lu:

1.calculate

$$\begin{bmatrix} w_{aa} & w_{ab} \\ w_{ba} & w_{ba} \end{bmatrix} = \frac{w_{aa}+w_{bb}}{2}\sigma_0 + \Delta E(\cos\theta\sigma_z + \sin\theta\cos\phi\sigma_x + \sin\theta\sin\phi\sigma_y)$$

2.Projection along the z axis

$$\cos\theta \equiv \frac{\frac{w_{aa}-w_{bb}}{2}}{\sqrt{\left(\frac{w_{aa}-w_{bb}}{2}\right)^2 + w_{ab}w_{ba}}}$$

$$\Delta E = \sqrt{\left(\frac{w_{aa}-w_{bb}}{2}\right)^2 + w_{ab}w_{ba}} \quad (''\text{length magnitude of the spin}'')$$

Projection along on the $x-y$ plane

$$\sin\theta \equiv \frac{w_{\mathrm{ab}}w_{ba}}{\sqrt{\left(\frac{w_{aa}-w_{bb}}{2}\right)^2 + w_{ab}w_{ba}}}$$

3.calculate $\psi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}, \psi_- = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix}$

4. calculate $E_\pm = \frac{w_{aa}+w_{bb}}{2} \pm \Delta E$

用Pauli matrix 表示，将二能级系统类似为自旋系统，在微扰问题中，类似于表示球坐标下的$(\Delta E, \theta, \phi)$

已知$W = \begin{bmatrix} w_{aa} & w_{ab} \\ w_{ab} & w_{bb} \end{bmatrix}$，为$H'$再以$|\psi_a^{(0)}>$,与$|\psi_b^{(0)}>$为基 下的展开。

即此时$|\psi_a^{(0)}> = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, |\psi_b^{(0)}> \begin{bmatrix} 0 \\ 1 \end{bmatrix}$,

对比$H = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$寻找特征值：$H\psi = E\psi$

$$\begin{aligned}
\Rightarrow \det\begin{vmatrix} a-E_\pm & b \\ c & d-E_\pm \end{vmatrix} &= 0 \\
(a-E_\pm)(d-E_\pm) - bc &= 0 \\
E_\pm &= \frac{a+d \pm \sqrt{(a+d)^2 - 4(ad-bc)}}{2} \\
E_\pm &= \frac{a+d}{2} \pm \sqrt{\left(\frac{a-d}{2}\right)^2 + \mathrm{bc}}
\end{aligned}$$

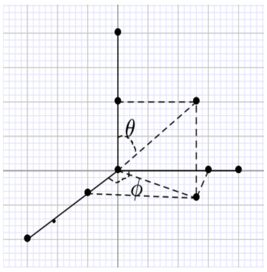
现将H'用Pauli 矩阵表达

$$H=d_0(\text{未扰动})+d\cdot\boldsymbol{\sigma}\ (\text{扰动}) \tag{1}$$

$$\sigma_x=\begin{bmatrix}0&1\\1&0\end{bmatrix},\ \sigma_y=\begin{bmatrix}0&-i\\i&0\end{bmatrix},\ \sigma_z=\begin{bmatrix}1&0\\0&-1\end{bmatrix},$$

$$\boldsymbol{d}=dx\,\hat{\boldsymbol{x}}+dy\,\hat{\boldsymbol{y}}+dz\,\hat{\boldsymbol{z}}$$

$$d\cdot\boldsymbol{\sigma}=\begin{bmatrix}\mathrm{dz}&\mathrm{dx}-i\,\mathrm{dy}\\\mathrm{dx}+i\,\mathrm{dy}&-\mathrm{dz}\end{bmatrix}=d\begin{bmatrix}\frac{\mathrm{dz}}{d}&\frac{\mathrm{dx}-i\mathrm{dy}}{d}\\\frac{\mathrm{dx}+i\mathrm{dy}}{d}&\frac{-\mathrm{dz}}{d}\end{bmatrix}$$



由图可知$\frac{\mathrm{dz}}{d}=\cos\theta,\frac{\mathrm{dx}}{d}=\frac{\mathrm{dx}}{d\sin\theta}\cdot\frac{\mathrm{dz}}{d}=\cos\phi\sin\theta,\frac{\mathrm{dy}}{d}=\sin\phi\sin\theta$

$$\begin{aligned}d\cdot\sigma&=d\begin{bmatrix}\cos\theta&\sin\theta(\cos\phi-i\sin\phi)\\\sin\theta(\cos\phi+i\sin\phi)&-\cos\theta\end{bmatrix}\\&=d\begin{bmatrix}\cos\theta&\sin\theta\cdot e^{i\phi}\\\sin\theta&-\cos\theta\end{bmatrix}\end{aligned}$$

此时H'可写成：

$$H'=\begin{bmatrix}d_0+d\cos\theta&\sin\theta\cdot e^{-i\phi}\\\sin\theta\cdot e^{i\phi}&-\cos\theta\end{bmatrix} \tag{2}$$

由(1)式可知

$$H'=\begin{bmatrix}d_0+\mathrm{dz}&\mathrm{dx}-i\,\mathrm{dy}\\\mathrm{dx}+i\,\mathrm{dy}&d_0-\mathrm{dz}\end{bmatrix}$$

特征值：

$$(d_0-\lambda)^2-(\mathrm{dz})^2-(\mathrm{dx})^2-(\mathrm{dy})^2=0$$

$$\lambda=d_0\pm d\quad 即E_\pm=d_0+d$$

先讲$E_\pm$回代到2,可得

$$\begin{aligned}H'-\begin{bmatrix}E_+&\\&E_+\end{bmatrix}&=\begin{bmatrix}d\cos\theta-d&d\sin\theta\cdot e^{i\phi}\\d\sin\theta\cdot e^{i\phi}&-d\cos\theta-d\end{bmatrix}\\&=d\begin{bmatrix}\cos\theta-1&\sin\theta e^{-i\phi}\\\sin\theta e^{i\phi}&-\cos\theta-1\end{bmatrix}\end{aligned}$$

$$即\begin{bmatrix}\cos\theta-1&\sin\theta e^{i\phi}\\\sin\theta\cdot e^{i\phi}&-\cos\theta-1\end{bmatrix}\begin{bmatrix}x\\y\end{bmatrix}=0$$

$$\begin{aligned}
(\cos\theta-1)x+\sin\theta\cdot e^{-i\phi}y &= 0\\
(1-\cos\theta)x &= \sin\theta e^{-i\phi}y\\
\frac{x}{y} &= \frac{2\sin\frac{\theta}{2}\cos\frac{\theta}{2}\cdot e^{-i\phi}}{2\sin^2\left(\frac{\theta}{2}\right)}=\frac{\cos\frac{\theta}{2}}{\sin\frac{\theta}{2}\cdot e^{i\phi}}\\
\Longrightarrow\psi_+ &= \begin{bmatrix} x\\ y\end{bmatrix}=\begin{bmatrix}\cos\dfrac{\theta}{2}\\ \sin\dfrac{\theta}{2}e^{i\phi}\end{bmatrix}\\
\text{同理，}\psi_- &= \begin{bmatrix} x\\ y\end{bmatrix}=\begin{bmatrix}\sin\dfrac{\theta}{2}\\ -\cos\dfrac{\theta}{2}e^{i\phi}\end{bmatrix}
\end{aligned}$$

现在比较$H_1=\begin{bmatrix} a & b\\ c & d\end{bmatrix}$与$H_2=d_0+\boldsymbol{d}\cdot\boldsymbol{\sigma}$

$$\begin{aligned}
E_1{}' &= \frac{a+d}{2}\pm\sqrt{\left(\frac{a-d}{2}\right)^2+\mathrm{bc}}\\
E_2{}' &= d_0\pm d\\
\text{即，}d_0=\frac{a+d}{2} & \qquad d=\sqrt{\left(\frac{a-d}{2}\right)^2+\mathrm{bc}},\\
& \qquad d\text{为扰动后的}H'\text{的本征值}\\
\text{而}\cos\theta &= \frac{\mathrm{dz}}{d}\\
\because H_2-d_0 &= \begin{bmatrix}\mathrm{dz} & \mathrm{dx}-i\,\mathrm{dy}\\ \mathrm{dx}+i\,\mathrm{dy} & -\mathrm{dz}\end{bmatrix}\\
H_1-d_0 &= \begin{bmatrix} a-\dfrac{a+d}{2} & b\\ c & d-\dfrac{a+d}{2}\end{bmatrix}\\
&= \begin{bmatrix}\dfrac{a-d}{2} & b\\ c & \dfrac{d-a}{2}\end{bmatrix}
\end{aligned}$$

$$\begin{aligned}
\text{通过对应关系}\Rightarrow\mathrm{dz} &= \frac{a-d}{2}\\
\cos\theta &= \frac{\mathrm{dz}}{d}=\frac{\frac{a-d}{2}}{\sqrt{\left(\frac{a-d}{2}\right)^2+\mathrm{bc}}}
\end{aligned}$$

$$\begin{aligned}
\text{即在}W\text{中},\cos\theta &= \frac{\frac{w_{aa}-w_{bb}}{2}}{\sqrt{\left(\frac{w_{aa}-w_{bb}}{2}\right)^2+w_{ab}w_{ba}}}\\
W &= d_0+\boldsymbol{d}\cdot\boldsymbol{\sigma}\\
&= \frac{w_{aa}+w_{bb}}{2}+d\begin{bmatrix}\cos\theta & \sin\theta e^{i\phi}\\ \sin\theta\cdot e^{i\phi} & -\cos\theta\end{bmatrix},d\text{即为}\Delta E\\
&= \frac{w_{aa}+w_{bb}}{2}+d\cos\theta\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}+\mathrm{d}\sin\theta\cos\phi\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}+d\sin\theta\sin\phi\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}
\end{aligned}$$

Prob 6.8. 3D cubic wall(unpertunbated)

微扰：$H'=a^3V_0\delta\left(x-\frac{a}{4}\right)\delta\left(y-\frac{a}{2}\right)\delta\left(z-\frac{3a}{4}\right) \quad \delta(ax)=\frac{1}{a}\delta(x)$

Ground state

$$E_0^{(1)}=\langle\psi_{111}|H'|\psi_{111}\rangle=\left(\frac{2}{a}\right)^3a^3V_0\int_0^a dx\sin\left(\frac{\pi}{a}x\right)\delta\left(x-\frac{a}{4}\right)\int_0^a dy\sin\left(\frac{\pi}{a}y\right)\delta\left(y-\frac{a}{4}\right)\int_0^a dz\sin\left(\frac{\pi}{a}z\right)\delta\left(z-\frac{a}{4}\right)$$

$$E_0^{(1)}=2V_0$$

For 1st excited states

$$\begin{bmatrix} w_{aa} & w_{ab} & w_{ac} \\ w_{ba} & w_{bb} & w_{bc} \\ w_{ca} & w_{cb} & w_{cc} \end{bmatrix} \longrightarrow \begin{cases} E_1^{(1)} & \psi_1 \\ E_2^{(1)} & \psi_2 \\ E_3^{(1)} & \psi_3 \end{cases}$$

6.3 Fine Structure of Hydrogen（氢原子精细结构）

Fine structures = spinless relativitices + spin-orbit coupling(also relastivistic)

Recap Section 4.2 Hydrogen atom

$$H=-\frac{\hbar^2}{2m}\nabla^2-\frac{1}{4\pi\varepsilon_0}\cdot\frac{1}{r}\Rightarrow \text{玻尔能级}-\frac{13.6\text{eV}}{n^2}$$

$-\frac{\hbar^2}{2m}\nabla^2$为动能项$E_k$，$-\frac{1}{4\pi\varepsilon_0}\cdot\frac{1}{r}$为氢原子模型的势能项$V$。

精细结构常数（Fine structure constant）

$$\alpha=\frac{e^2}{4\pi\epsilon\hbar c}\approx\frac{1}{137}$$

因为额外考虑的自旋轨道耦合与不考虑自旋轨道耦合的能量差距较大（约为4个数量级），因此，自旋轨道耦合的影响可以视作对于原来模型的微扰修正。

some hierarchy	
Bohr	α^2mc^2
Fine structure	α^4mc^2
lamb shift（兰姆位移）	α^5mc^2
Hyper fine splitting 超精细结构	$\left(\frac{m}{m_p}\right)\alpha^4mc^2$

Problem 6.11. Express Bohr energy in terms of α and mc^2

$$E_n=-\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{1}{n^2}[4.70]=-\frac{mc^2}{2}\left(\frac{e^2}{4\pi\hbar\varepsilon_0 c}\right)^2\frac{1}{n^2}=-\frac{mc^2}{2}\alpha^2\cdot\frac{1}{n^2}\quad[6.43]$$

6.3.1 Spinless relativistic correction 忽略自旋-轨道耦合的相对论修正

Kinetic energy $T=\frac{p^2}{2m}\longrightarrow -\frac{p^2}{2m}\nabla^2 \qquad (\hat{\vec{p}}=-i\hbar\vec{\nabla},\quad \hat{\vec{p}}e^{i\vec{p}\cdot\vec{x}/\hbar}=-i\hbar\vec{\nabla}\cdot e^{i\vec{p}\cdot\vec{x}/\hbar}=\vec{p}$（包含平面波））

注记. $$\hat{\vec{p}}e^{i\vec{p}\cdot\vec{x}/\hbar}=-i\hbar\vec{\nabla}\cdot e^{i\vec{p}\cdot\vec{x}/\hbar}=-i\hbar\left(\frac{i\vec{p}}{\hbar}\right)\cdot e^{i\vec{p}\cdot\vec{x}/\hbar}=\vec{p}\cdot e^{i\vec{p}\cdot\vec{x}/\hbar}=\vec{p}$$

$\hat{\vec{p}}e^{i\vec{p}\cdot\vec{x}/\hbar}$，的$\hat{\vec{p}}$是动量算符。$\vec{p}\cdot e^{i\vec{p}\cdot\vec{x}/\hbar}$的$\vec{p}$是动量的值，等式最右侧的$\vec{p}$是指动量的波函数。

Relativistic kinetic energy $\boldsymbol{T}=\frac{\boldsymbol{mc^2}}{\sqrt{1-\left(\frac{v}{c}\right)^2}}-\boldsymbol{mc^2}$, v is the speed of reference frame.

In QM, we express T in terms of $\vec{p}$, not $\vec{v}$

$$p=\frac{mv}{\sqrt{1-\left(\frac{v}{c}\right)^2}}$$

Note that

$$\begin{aligned}
p^2c^2+m^2c^4 &= \frac{m^2v^2c^2}{1-\left(\frac{v}{c}\right)^2}+m^2c^4\\
&= \frac{m^2v^2c^2+m^2c^4\left(1-\left(\frac{v}{c}\right)^2\right)}{1-\left(\frac{v}{c}\right)^2}\\
&= \frac{m^2c^4}{1-\left(\frac{v}{c}\right)^2}\\
&= (\|\boldsymbol{T}\|+mc^2)^2
\end{aligned}$$

$$\begin{aligned}
\boldsymbol{T} &= \sqrt{p^2c^2+m^2c^4}-mc^2\\
&= mc^2\left[\sqrt{1+\frac{p^2c^2}{m^2c^4}}-1\right]\\
&= mc^2\left[\sqrt{1+\left(\frac{p}{mc}\right)^2}-1\right]\\
&\approx mc^2\left[1+\frac{1}{2}\cdot\left(\frac{p}{mc}\right)^2-\frac{1}{8}\left(\frac{p}{mc}\right)^4-1\right]\\
&= \frac{p^2}{2m}(\text{Bohr kinetic})-\frac{p^4}{8m^3c^2}(\text{pertubation})
\end{aligned}$$

$\frac{p^2}{2m}(\text{Bohr kinetic, unperturbation})$, $-\frac{p^4}{8m^3c^2}(\text{pertubation, spinless relativistic correction})$

$$H_r{}'=-\frac{(\vec{p})^4}{8m^3c^2}=-\frac{\left(\frac{p^2}{2m}\right)}{2mc^2}\quad\left(\text{数量级为}H\text{的}\frac{10^2\text{eV}}{10^6\text{eV}}\text{的大小，故可以看作微扰}\right)$$

1st order correction to energy (氢原子)能量一阶修正

$$E_r^{(1)}=\langle\psi_{n,l,m}|\widehat{H}_r{}'|\psi_{n,l,m}\rangle$$

$\boldsymbol{n}$ is principle Q number(与算符H相关). $\boldsymbol{l}$ is angular-momentum Q number(与L^2算符相关). $\boldsymbol{m}$ is magnetic Q number(与$\hat{L}_z$算符相关).

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\cdot\frac{1}{r}$$

$$H|\psi_{nlm}\rangle = -\frac{13.6\text{eV}}{n^2}|\psi_{nlm}\rangle$$

$$L^2|\psi_{nlm}\rangle = \hbar^2 l(l+1)|\psi_{nlm}\rangle$$

$$\hat{L}_z|\psi_{nlm}\rangle = \hbar m|\psi_{nlm}\rangle$$

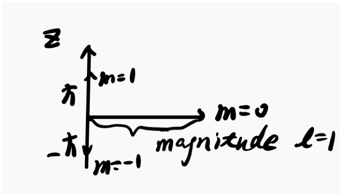


图 1. lm之间的关系

(L_z: projection of the orbital angular momentum along the z direction)

结合$[L^2, H]=0$, $[\hat{L}_z, H]=0$, 说明$L^2, \hat{L}_z, H$三者具有共同的本征态ψ_{nlm}。

$n=1$	$l=0$	$m=0$
$n=2$	$l=0,1$	$m=0,\pm1$
$\ldots$	$\ldots$	$\ldots$

给定$\boldsymbol{n}$，不同的$\boldsymbol{l}, \boldsymbol{m}$所对应的多个态都是简并的(Degenerate states because Bohr energy has notion to do with $\boldsymbol{m}$ or $\boldsymbol{l}$)

我们在利用此微扰时使用的时非简并的理论来计算相同n的态函数（简并的态）

Why use nondegenerate theory?

To explain this, Page 259-260 Theorem

引理. *If we have a Hermiton operator $\hat{A}$ and $[\hat{A}, H^{(0)}]=0, [\hat{A}, H']=0$. If $\psi_a^{(0)}$ and $\psi_b^{(0)}$ (the degnerate eigen states of $H^{(0)}$) are also eigen-states of $\hat{A}$ with distinct eigenvalue.*

$$\hat{A}\psi_a^{(0)} = \mu\psi_a^{(0)} \qquad \hat{A}\psi_b^{(0)} = \nu\psi_b^{(0)} \qquad , \mu \neq \nu$$

then $W_{ab}=0$,i.e. there is no off-digonal form for H'.（因此，$\psi_a^{(0)}$ 和 $\psi_b^{(0)}$）

引理证明. $[A, H']=0 \Rightarrow \langle\psi_a^{(0)}|[AH']|\psi_b^{(0)}\rangle = 0$

$$\langle\psi_a^{(0)}|AH' - H'A|\psi_b^{(0)}\rangle = 0$$

$$\langle\psi_a^{(0)}|AH'|\psi_b^{(0)}\rangle - \langle\psi_a^{(0)}|H'A|\psi_b^{(0)}\rangle = 0$$

$$\langle A\psi_a^{(0)}|H'|\psi_b^{(0)}\rangle - \langle\psi_a^{(0)}|H'|A\psi_b^{(0)}\rangle = 0$$

$$\mu\langle\psi_a^{(0)}|H'|\psi_b^{(0)}\rangle - \nu\langle\psi_a^{(0)}|H'|\psi_b^{(0)}\rangle = 0$$

$$(\mu-\nu)\langle\psi_a^{(0)}|H'|\psi_b^{(0)}\rangle = 0$$

因为$(\mu-\nu)\neq 0, \langle\psi_a^{(0)}|H'|\psi_b^{(0)}\rangle = 0$ $\square$

For Hydrogen atom, 分别由$\hat{L}^2$和$\hat{L}_z$充当定理中的A

$$\text{so } [\hat{p}^4, L_z] = 0 \quad , \quad [\hat{p}^4, L^2] = 0?$$

提醒：$\hat{p}^4$来源于$H' = \frac{p^4}{8m^3c^2}$

- **some tricky.** $[AB, C] = A[B, C] + [A, C]B$

$$[\hat{p}^4, L_z] = [\hat{p}^2\hat{p}^2, L_z] = \hat{p}^2[\hat{p}^2, L_z] + [\hat{p}^2, L_z]\hat{p}^2$$

我们可以先计算$[L_z, \hat{p}^2]$ $(L_z = xp_y - yp_x)$

$$\begin{aligned}
[L_z, \hat{p}^2] &= [L_z, \hat{p}_x^2] + [L_z, \hat{p}_y^2] + [L_z, \hat{p}_z^2] \qquad (L_z, \text{显然与}\hat{p}_z^2\text{对易}) \\
&= [L_z, \hat{p}_x]\hat{p}_x + \hat{p}_x[L_z, \hat{p}_x] + [L_z, \hat{p}_y]\hat{p}_y + \hat{p}_y[L_z, \hat{p}_y] \\
&= [xp_y - yp_x, p_x]\hat{p}_x + \hat{p}_x[p_x, xp_y - yp_x] + \ldots \\
&= p_y\{[x, p_x]\hat{p}_x + p_x[p_x, x]\} + p_x\{[y, p_y]\hat{p}_y + p_y[p_y, y]\}
\end{aligned}$$

利用$[x, p_x] = i\hbar$

$$[L_z, \hat{p}^2] = \; = \; p_y p_x(i\hbar - i\hbar) + p_x p_y(i\hbar - i\hbar) \; = 0$$

同理$[L_y, \hat{p}^2] = 0$, $[L_z, \hat{p}^2] = 0$

$$L^2 = L_x^2 + L_y^2 + L_z^2 \qquad [L^2, p^4] = 0$$

so we have $[p^4, L_z] = 0$, $[p^4, L^2] = 0$

$$\langle\psi_{n\ell m}|H'|\psi_{n\ell' m'}\rangle = 0, \text{for } \ell \neq \ell', m \neq m'$$

now we evaluate $\langle\psi_{n\ell m}|H'|\psi_{n\ell m}\rangle$

$$\frac{p^2}{2m}|\psi\rangle = (E - V)|\psi\rangle$$

$$\begin{aligned}
\langle\psi_{n\ell m}|p^4|\psi_{n\ell m}\rangle &= \langle p^2\psi_{n\ell m}|p^2\psi_{n\ell m}\rangle \\
&= (2m)^2\langle\psi_{n\ell m}|(E - V)^2|\psi_{n\ell m}\rangle \\
&= (2m)^2(E_n^2 - 2E_n\langle\psi_{n\ell m}|V|\psi_{n\ell m}\rangle + \langle\psi_{n\ell m}|V^2|\psi_{n\ell m}\rangle) \\
&= (2m)^2[E_n^2 - 2E_n\langle V\rangle + \langle V^2\rangle]
\end{aligned}$$

这里的$\hat{V}$ 指氢原子势场下电子的势能，即$\hat{V} = -\frac{e^2}{4\pi\epsilon_0}\cdot\frac{1}{r}$

$$E_r^{(1)} = -\frac{1}{8m^3c^2}(2m)^2[E_n^2 - 2E_n\langle V\rangle + \langle V^2\rangle]$$

[tips]:use [Eq:3.97] Stationary Virial theorem

Vivid theorem. *(维里定律)*

1D: $2\langle T\rangle=\left\langle x\frac{dV}{dx}\right\rangle$ *3D:* $2\langle T\rangle=\langle\vec{r}\cdot\nabla V\rangle$

利用球坐标

$$
\begin{aligned}
\nabla V(\vec{r}) &= -\frac{e^2}{4\pi\epsilon_0}\frac{d}{dr}\left(\frac{1}{r}\right)\hat{r}+\ldots\hat{\theta}+\cdots\hat{\varphi}\,(\text{because } V \text{ is not a function of } \theta \text{ or } \varphi)\\
&= \frac{e^2}{4\pi\epsilon_0}\frac{1}{r^2}\hat{r} \quad (\text{与}\hat{\theta}\text{，}\hat{\varphi}\text{相关的项全为0})
\end{aligned}
$$

$$
\begin{aligned}
2\langle T\rangle &= \langle\vec{r}\cdot\nabla V\rangle\\
&= \frac{e^2}{4\pi\epsilon_0}\left\langle\frac{1}{r^2}\vec{r}\cdot\hat{r}\right\rangle\\
&= \frac{e^2}{4\pi\epsilon_0}\left\langle\frac{1}{r}\right\rangle=-\langle V\rangle
\end{aligned}
$$

$$\text{综合}\left\{\begin{array}{l}E_n=\langle T\rangle+\langle V\rangle\\ 2\langle T\rangle=-\langle V\rangle\end{array}\right.,\text{有}\left\{\begin{array}{l}\langle T\rangle=-E_n\\ \langle V\rangle=2E_n\end{array}\right.\quad(\text{For Hydrogen atom only})$$

2023.10.8课堂纪要

Recap of spinless relastic correction to Bohr energy of the Hydrogen atom

$$H=H^0+H',\quad H^{(0)}=-\frac{\hbar^2}{2m}\nabla^2-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r},\quad H'=-\frac{p^4}{8m^3c^2}$$

1st order correction to energy,| 对于Nondegeneration $E_r^{(1)}=\langle\psi_{nlm}|\mathrm{H}'|\psi_{nlm}\rangle$

$$\langle\psi|p^4|\psi\rangle=\langle p^2\psi|p^2\psi\rangle=\langle\psi_{nlm}|(E-V)^2|\psi_{nlm}\rangle$$

$$E_r^1=-\frac{(2m)^2}{8m^3c^2}(E_n-2E_n\langle V\rangle-\langle V^2\rangle)$$

对于中心势场V ,由上面的维里定律，$\langle V\rangle=2E_n$

由Problem 6.33 $\left\langle\frac{1}{r^2}\right\rangle=\frac{1}{(l+\frac{1}{2})n^3a^2}$ where $a=\frac{4\pi\varepsilon_0\hbar^2}{me^2}$ a is Bohr radius. $\langle V^2\rangle=\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{1}{(l+\frac{1}{2})n^3a^2}$.

为简化形式，用玻尔能量(E_n)简化，由式[4.72]

$$E_n=\frac{E_1}{n^2}\qquad E_1=-\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2$$

$$E_n = \underbrace{-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{a}\frac{1}{n^2}}_{\text{Potential like}}=\underbrace{-\frac{\hbar^2}{2m}\frac{1}{a^2}\frac{1}{n^2}}_{\text{Kinetic like}}$$

$$E_r^{(1)}=-\frac{1}{2mc^2}\left[E_n^2-4E_n^2+\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{4n}{4\left(l+\frac{1}{2}\right)n^4a^2}\right]=-\frac{E_n^2}{2mc^2}\left[1-4+\frac{4n}{\left(l+\frac{1}{2}\right)}\right]$$

$$E_r^{(1)}=\frac{E_n^2}{2mc^2}\left[3-\frac{4n}{\left(l+\frac{1}{2}\right)}\right]\qquad[6.57]$$

可以看出，经过相对论修正后，能量不仅与主量子数 n 有关，还与角动量量子数 l 产生联系。

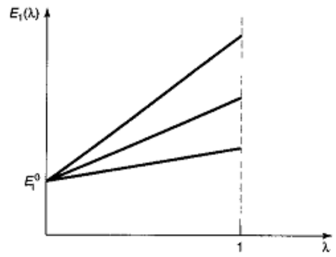


图. 考虑相对论修正后的能级劈裂图

证明. $W \equiv \langle \psi_{nl'm'} | \mathrm{H}_r' | \psi_{nlm} \rangle$的非对角元$(l \neq l', m \neq m')$为零

$$\because [L^2, H_r'] = 0 \qquad [L_z, H_r'] = 0$$

$$\begin{aligned} 0 &= \langle \psi_{nlm} | [L^2, H_r'] | \psi_{nl'm'} \rangle \\ 0 &= \langle \psi_{nlm} | L^2 H_r' | \psi_{nl'm'} \rangle - \langle \psi_{nlm} | H_r' L^2 | \psi_{nl'm'} \rangle \\ 0 &= \hbar^2 \underbrace{[l'(l'+1) - l(l+1)]}_{\neq 0} \langle \psi_{nlm} | H_r' | \psi_{nl'm'} \rangle \end{aligned}$$

$$\therefore \langle \psi_{nlm} | H_r' | \psi_{nl'm'} \rangle = 0\text{，即非对角元为0}$$ □

6.3.2 Fine Structure-spin-orbit coupling 自旋轨道耦合

spin $\rightarrow$ spin angular momentum orbit $\rightarrow$ orbit angular momentum

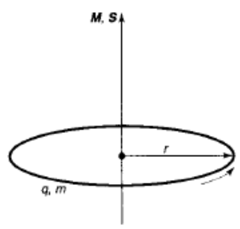


图. 自旋轨道耦合示意图

自旋轨道耦合会形成“Zeeman – like”的能量变化

$$H = -\vec{\mu} \cdot \vec{B} \qquad (6.38)$$

其中H为自旋产生的微扰，$\vec{\mu}$为电子自旋磁矩。该过程为半量子半经典的推导。而纯量子力学的推法为：Dirac equation + potential $\frac{1}{r} \overset{\text{low}-\text{enegy}}{\Longrightarrow}$ Schrodingen equation +自旋轨道耦合。

1、magnetic field of proton

$$B = \frac{\mu_0 I}{2r} (\text{Biot} - \text{Savarrt Law})$$

其中I 为质子"围绕着电子"的转动导致的电流。current of proton $I=\frac{e}{T}$ (e 为proton charge) (tips：此时以电子为参考系，质子在围绕电子旋转)

推导的目的为将$\boldsymbol{B}$ 与角动量$\vec{\boldsymbol{L}}$联系

$$L=\vec{r}\times m\vec{v}=rm\frac{2\pi mr^2}{T}(m\text{为电子质量})$$

$$\frac{1}{T}=\frac{L}{2\pi mr^2}\quad B=\frac{\mu_0}{2r}\frac{e}{T}=\frac{\mu_0}{2r}\frac{e\vec{L}}{2\pi mr^2}=\frac{1}{4\pi\varepsilon_0}\frac{e}{m\,c^2\,r^3}\vec{L}(\vec{L}\text{为电子的轨道角动量})[6.59]$$

2、Magnetic dipole moment of the electron

Angular momentum +charge

Imagine electron e as a ring of charge q and radius r, rotationg with a period of T

Magnetic moment $\mu=\text{current}\times\text{area enclosed by ring}=\frac{q}{T}\pi r^2=q\frac{\pi r^2}{T}$

Mass of the ring m

$$\text{角动量}S=I\omega=mr^2\frac{2\pi}{T}=\frac{2m\pi r^2}{T}$$

$$\therefore\vec{\mu}=\frac{q}{2m}\vec{S},$$

$$|n,l,m\rangle|m_s\rangle$$

其中$|m_s>$为电子自旋产生的磁矩electron spin angular momentum(自旋角动量×磁场),$m_s=\pm\frac{1}{2}$

对于量子磁矩则为$\vec{\mu}=\frac{q}{m}\vec{S}$(6.60) (以下均使用量子磁矩)

$$\overrightarrow{H'_{so}}=-\vec{\mu}\cdot\vec{B}=\frac{e}{m}\vec{S}\cdot\frac{1}{4\pi\varepsilon_0}\frac{e}{mc^2r^3}\vec{L}=\frac{e^2}{4\pi\varepsilon_0}\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}\xlongequal[\text{precession}]{\text{Thomas}}\frac{e^2\vec{S}\cdot\vec{L}}{8\pi\varepsilon_0m^2c^2r^3}$$

where $\vec{S}\cdot\vec{L}=S_xL_x+S_yL_y+S_zL_z=\frac{1}{2}(S_+L_-+S_-L_++S_zL_z)$，其中$\boxed{\begin{array}{ll}S_+=S_x+iS_y & L_+=L_x+iL_y\\ S_-=S_x-iS_y & L_-=L_x-iL_y\end{array}}$

$S_\pm\|m_s>?\|m_{s\pm1}>$	$S_z\|m_s>=\frac{\hbar}{2}m_s\|m_s>$
$L_\pm\|nlm>\to?\|nl(m+1)>$	$L_z\|nml>=m\|nml>$

回顾$J_\pm$, $J_-J_+=J^2-J_z^2-\hbar J_z\Rightarrow\langle j,m|J_-J_+|j,m\rangle=\hbar^2[j(j+1)-m(m+1)]$,$J_+|j,m>=\overline{C_{jm}}|j,m+1>$,thus $|C_{jm}|^2=\hbar^2[j(j+1)-m(m+1)]=\hbar^2(j-m)(j-m+1)$

$$\left\{\begin{array}{l}J_+|j,m>=\sqrt{(j-m)(j+m+1)}\hbar|j,m+1>=\hbar\sqrt{j(j+1)-m(m+1)}|j,m+1>\\ J_-|j,m>=\sqrt{(j+m)(j-m+1)}\hbar|j,m-1>=\hbar\sqrt{j(j+1)-m(m-1)}|j,m-1>\end{array}\right\}$$

with spin-orbit coupling $H=H^{(0)}+H'_r+H'_{so}$,现在有$[H'_{so},L]\neq0$, $[H'_{so},S]\neq0$(部分非对角元项不为0)

$$[\vec{S}\cdot\vec{L},\vec{S}]=i\hbar(\vec{S}\times\vec{L})\neq0$$

定义. 量子力学中的的角动量

[4.99] $[L_x, L_y] = i\hbar L_z \Rightarrow \left\{ \begin{array}{cc} L = \vec{r} \times \vec{p} & \text{classical} \\ [x, p] = i\hbar & \text{uncertainty principle} \end{array} \right\}$

However, spin also has the same definition,but pure Quantum mechanics

In other word,$\hat{L_z}$ and $\hat{S_z}$ are not "good" to be used in the pertubation theory. Instead ,we will use eigenstates of (L^2, S^2, J^2, J_z)

$$\vec{J} \equiv \vec{L} + \vec{S} \quad \text{(Total angular momentum)}$$

$$J^2 = (\vec{L} + \vec{S})(\vec{L} + \vec{S}) = L^2 + S^2 + 2\vec{L} \cdot \vec{S} \quad (\vec{L} \cdot \vec{S} = \vec{S} \cdot \vec{L})$$

$$\vec{L} \cdot \vec{S} = \frac{1}{2}(\vec{J}^2 - \vec{L}^2 - \vec{S}^2)$$

We can show that $[L \cdot S, J^2] = 0 \quad [\vec{L} \cdot \vec{S}, L^2] = 0 \quad [\vec{L} \cdot \vec{S}, S^2] = 0$ (Pro 6.16)

The eigenvalue of $\vec{L} \cdot \vec{S}$:

$$\langle jls_{mJ} | \vec{L} \cdot \vec{S} | jls_{mJ} \rangle = \frac{1}{2} \langle jls_{mJ} | J^2 - L^2 - S^2 | jls_{m_J} \rangle = \frac{1}{2} \left[\hbar^2 j(j+1) - \hbar^2 l(l+1) - \hbar^2 \frac{1}{2} \left(\frac{1}{2} + 1 \right) \right]$$

$$\langle jls_{mJ} | \vec{L} \cdot \vec{S} | jls_{mJ} \rangle = \frac{1}{2} \hbar^2 \left[j(j+1) - l(l+1) - \frac{3}{4} \right]$$

关于$H_{so}^{'}$一阶修正:

[Problem 6.35，6.34] $\Rightarrow \left\langle \frac{1}{r^3} \right\rangle = \frac{1}{l\left(l+\frac{1}{2}\right)(l+1)n^3 a^3}$. $\quad E_n = -\frac{e^2}{8\pi\varepsilon_0 a} \frac{1}{n^2} = -\frac{\hbar^2}{2m} \frac{1}{a^2} \frac{1}{n^2}$, $\quad \frac{1}{a} = E_0 \frac{8\pi\varepsilon_0}{e^2} n^2$

a为玻尔半径 $\quad \frac{1}{a} = -E_n \frac{8\pi\varepsilon_0}{e^2} n^2 \quad \frac{1}{a^2} = -E_n \frac{2m}{\hbar} n^2 \quad \frac{1}{a^3} = \frac{1}{a} \frac{1}{a^2} = E_n^2 \frac{2m}{\hbar^2} \cdot \frac{8\pi\varepsilon_0}{e^2} n^4$,将相应的$a$代入$E_n$

经过以上计算，代入$E_{so}^{(1)}$ （我们选择L^2, S^2, J^2, J_z,因为他们之间可以对易，且为厄密算符，故存在共同的本征态$|nlsjm_j>$进行计算）

$$\begin{aligned} E_{so}^{(1)} &= \langle H_{so}^{(1)} \rangle = \langle nlsjm_j | H_{so}^{'} | nlsjm_j \rangle = \frac{e^2}{8\pi\varepsilon_0 m^2 c^2} \langle \vec{S} \cdot \vec{L} \rangle \left\langle \frac{1}{r^3} \right\rangle \text{（分离变量后}r\text{与}(\theta,\varphi)\text{无关）} \\ &= \frac{e^2}{8\pi\varepsilon_0 m^2 c^2} \frac{1}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)n^3} \cdot E_n^2 \cdot \frac{2m}{\hbar^2} \frac{8\pi\varepsilon_0}{e^2} n^4 \times \frac{1}{2} \hbar^2 \left[j(j+1) - \ell(\ell+1) - \frac{1}{2} s(s+1) \right] \\ &= \frac{E_n^2}{mc^2} n \frac{j(j+1) - \ell(\ell+1) - \frac{3}{4}}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)} \end{aligned}$$

这里补充(复习)一下有关角动量算符可以与$\left\langle \frac{1}{r^n} \right\rangle$分开计算的原因:

$$\boldsymbol{L}\psi = -ir\hat{\mathbf{e}}_r \times \left[\hat{\mathbf{e}}_r \frac{\partial\psi}{\partial r} + \hat{\mathbf{e}}_\theta \frac{1}{r} \frac{\partial\psi}{\partial\theta} + \hat{\mathbf{e}}_\varphi \frac{1}{r\sin\theta} \frac{\partial\psi}{\partial\varphi} \right] = i \left(\hat{\mathbf{e}}_\theta \frac{1}{\sin\theta} \frac{\partial}{\partial\varphi} - \hat{\mathbf{e}}_\varphi \frac{\partial}{\partial\theta} \right) \psi$$

其中，算符L^2, S^2没有与r有相关的项，故有$[L^2, f(r)] = 0, [S^2, f(r)] = 0$

此外，还有$[L^2, p^2] = 0$

Fine Structure（从量子力学的角度来说，自旋轨道耦合本质仍为相对论效应）

$$E_{fs}^{(1)} = E_r^{(1)} + E_{so}^{(1)} = \frac{E_n^2}{2mc^2}\left(3 - \frac{4n}{j+\frac{1}{2}}\right) \quad j\,(\text{总角动量}) = \ell \pm \frac{1}{2}(\text{平行或反向})$$

$$\text{代入} E_n = -\frac{1}{2}mc^2\alpha^2\frac{1}{n^2}$$

$$\Rightarrow E_{fs}^{(1)} = E_n\alpha^2\frac{1}{n^2}\left(\frac{4n}{j+\frac{1}{2}} - 3\right)$$

$$E_{nj} = E_n + E_{fs} = -\frac{13.6\text{eV}}{n^2}\left(1 + \frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)\right)$$

6.4 Zeeman effect

An energy because of the angular momentum of electron charge

$$H_Z' = -(\vec{\mu_l} + \vec{\mu_s}) \cdot \vec{B}_{\text{ext}}$$
$$\qquad\quad \text{orbital}\ \text{spin}\ \text{外加磁场}$$

$$\mu_s = -\frac{e}{m}\vec{S} \qquad \mu_\ell = -\frac{e}{2m}\vec{L}$$

$$H_Z = \frac{e}{2m}(\vec{L} + 2\vec{S}) \cdot \vec{B}_{\text{ext}}$$

Pro 6.20

$$\text{内部磁场} \quad B_{\text{int}} = \frac{1}{4\pi\varepsilon_0}\frac{e}{mc^2r^3}\vec{L} \Longleftarrow H_{so}' \sim \vec{L}\cdot\vec{S} = \vec{B}_{\text{int}} \cdot \vec{\mu_s}$$

Approrimation $\vec{L} \rightarrow \hbar, r \rightarrow \text{Bohr radius}, \ B_{\text{int}} = \frac{(1.6\times10^{-19}C)\,(1.05\times10^{-34}J\cdot s)}{4\pi\,(8.9\times10^{-12}e^2/N\cdot m^2)\,(9.1\times10^{-31}\text{kg})\,(3\times10^8 m/s)^2} \approx 12T$ $(T = \frac{v\cdot s}{m^2})$

现在分情况讨论外部磁场与内部磁场关系对于修正的影响

1. $B_{\text{ext}} \ll B_{\text{int}}$ (weak – field)
2. $B_{\text{ext}} \gg B_{\text{int}}$ (strong - field)
3. $B_{\text{ext}} \approx B_{\text{int}}$ (Intermediate)

6.4.1 Weak - field Zeeman effect

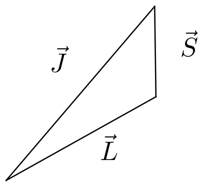
Total H: $H = H_{\text{Bohr}} + H_{fs}'$(非微扰) $+ H_Z'$(微扰部分)

Because of $\vec{L}\cdot\vec{S}$,m_ℓ, m_s are no longer good quantum number, good are n, ℓ, j, m_j, s

The Zeeman correction to the energy

$$E_Z^{(1)} = \langle nljm_j | H_Z' | nljm_j \rangle = \left\langle nljm_j \middle| \frac{e}{2m}\vec{B}_{\text{ext}} \cdot (\vec{L} + 2\vec{S}) \middle| nljm_j \right\rangle$$

为了将H_Z'尽可能转化为“好量子数”的本征态上。$\longrightarrow \vec{L} + 2\vec{S} = \vec{J} + \vec{S}$



$\vec{L}$ and $\vec{S}$ precess about $\vec{J}$

$\Rightarrow$only the average of $\vec{S}$ along the direction of $\vec{J}$ counts

$$\vec{S}_{\text{ave}} = \frac{\vec{S}\cdot\vec{J}}{J}\cdot\frac{\vec{J}}{J} = \frac{\vec{S}\cdot\vec{J}}{J^2}\vec{J}$$

$$\vec{J} + \vec{S} = \vec{J} + \vec{S}_{\text{ave}}$$

$$\vec{L} = \vec{J} - \vec{S} \qquad L^2 = J^2 + S^2 - 2\vec{J}\cdot\vec{S}$$

$$\langle \vec{S}\cdot\vec{J}\rangle = \left\langle \frac{1}{2}(J^2 + S^2 - L^2)\right\rangle = \frac{1}{2}\hbar^2\left[j(j+1) + \frac{3}{4} - \ell(\ell+1)\right]$$

$J^2\vert j> = \hbar j(j+1)\vert j>$	$L^2\vert l> = \hbar^2\ell(\ell+1)\vert l>$	$S^2\vert s> = \hbar^2 s(s+1)\vert s>$

$$\begin{aligned}\langle nljm_j|\vec{L} + 2\vec{S}|nljm_j\rangle &= \left\langle nljm_j\left|\left(1 + \frac{\vec{S}\cdot\vec{J}}{J^2}\right)\vec{J}\right|nljm_j\right\rangle \\ &= \left[1 + \frac{j(j+1) - \ell(\ell+1) + \frac{3}{4}}{2j(j+1)}\right]\langle J\rangle\end{aligned}$$

其中$\left[1 + \frac{j(j+1) - \ell(\ell+1) + \frac{3}{4}}{2j(j+1)}\right]$ 称为朗德g因子

$$\left(\text{for free electron: } \ell = 0, s = \frac{1}{2}, j = \ell + \frac{1}{2} \qquad g = 2\right)$$

$$\therefore E_Z^{(1)} = \frac{e}{2m}\cdot\vec{B}_{\text{ext}}\cdot\langle\vec{L} + 2\vec{S}\rangle = \frac{e}{2m}g_{_J}\vec{B}_{\text{ext}}\langle\vec{J}\rangle$$

$\because$设$\vec{B}_{\text{ext}} = \vec{B}_{\text{ext}}\hat{z}$ field direction define on z axis

$$\begin{aligned}E_Z^{(1)} &= \frac{e}{2m}g_{_J}B_{\text{ext}}\,\hat{z}\cdot\langle J_x\hat{x} + J_y\hat{y} + J_z\hat{z}\rangle \\ &= \frac{e}{2m}g_{_J}B_{\text{ext}}\langle J_z\rangle \\ &= \frac{\hbar e}{2m}g_{_J}B_{\text{ext}}m_j \\ &= \mu_B g_{_J}B_{\text{ext}}m_j \\ &\quad \text{玻尔磁子}\mu_B = \frac{e\hbar}{2m} \approx 5.788\times10^{-5}\text{eV}/T\end{aligned}$$

6.4.2 Strong - field Zeeman effect

Total H $H = H_{\text{Bohr}} + H_r' + H_{so}' + H_Z'$,其中,根据H_{so}'和H_Z'谁小，就把谁看作是微扰。

$H = H^{(0)} + H'$, where $H^{(0)} = H_{\text{Bohr}} + H_Z'$ or $H_{\text{Bohr}} + H_Z' + H_r'$ $\qquad H' = H'_{fs}$ or H_{so}'

Because $H^{(0)}$ include H_Z', we can see m_l,m_s, as "good" quantum numbers.

未微扰能量$E_{n,m_l,m_s} = -\frac{13.6\text{eV}}{n^2} + \mu_B B_{\text{ext}}(m_l + 2m_s)$,其中$L_Z|m_l> = \hbar m_l|m_l>$, $S_Z|m_s> = \hbar m_s|m_s>$

微扰项能量$E_{fs}^{(1)}=\langle nlm_lm_s|H_r^{'}+H_{so}^{'}|nlm_lm_s\rangle$, for $H_r^{'}=\frac{p^4}{8m^3c^2}, E_r^{(1)}=-\frac{E_n^2}{2mc^2}\left(\frac{4n}{\ell+\frac{1}{2}}-3\right)$ (保持不变)

而$H_{so}^{'}\propto\vec{S}\cdot\vec{L}$, $\langle\vec{S}\cdot\vec{L}\rangle=\left\langle nlm_l\,m_s\middle|\frac{1}{2}(S_+L_-+S_-L_+)+S_ZL_Z\middle|nlm_l\,m_s\right\rangle$,

where $\langle m_l\,m_s|S_+L_-|m_l\rangle=\langle m_s|S_+|m_s\rangle\langle m_l|L_-|m_l\rangle=\sim\langle m_s|m_{s+1}\rangle\langle m_l|m_{l-1}\rangle$正交为0.

$$\Longrightarrow\langle\vec{S}\cdot\vec{L}\rangle=\langle m_lm_s|S_ZL_Z|m_l\,m_s\rangle=\hbar m_s\,\hbar m_l=\hbar^2m_sm_l$$

$$E_{so}^{(1)}=\frac{e^2}{8\pi\varepsilon_0}\frac{1}{m^2c^2}\left\langle\frac{1}{r^3}\right\rangle\langle\vec{S}\cdot\vec{L}\rangle$$

6.4.3 Intermediate field

$$\begin{array}{rcl} H & = & H_{\text{Bohr}}+H_r^{'}+H_{so}^{'}+H_Z^{'} \\ & & \text{未微扰} \qquad\quad nljm_j \quad nlm_lm_s \\ & & \qquad\qquad\quad L^2J^2J_Z \quad L_ZS_Z \end{array}$$

$H_{so}^{'}$与$H_Z^{'}$ 在同等地位上。

例. The $n=2$ states of hydrogen atom, how many states(states is a basis of expending the matrix of $H_r^{'}+H_{so}^{'}+H_Z^{'}$). 由于$J^2, J_Z$与$L_Z, S_Z$不对易，不存两组的共同本征态，导致$H_r^{'}+H_{so}^{'}+H_Z^{'}$非对角项不全为0，需要进行对角化。

$$\begin{array}{llll} n=2\quad l=0\quad s=\frac{1}{2} & \text{for } l=0 & j=\frac{1}{2} \qquad m_j=-\frac{1}{2},\frac{1}{2} & 2\,\text{states} \\ \qquad j=l\pm s & \text{for } l=1 & \left\{\begin{array}{ll} j=\frac{1}{2} & m_j=\frac{1}{2},-\frac{1}{2} \\ j=\frac{3}{2} & m_j=\frac{3}{2},\frac{1}{2},-\frac{1}{2},\frac{3}{2} \end{array}\right. & \begin{array}{l} 2\,\text{states} \\ 4\,\text{states}\end{array} \end{array}$$

因此，一共有八个states as basis to express $H_r^{'}+H_{so}^{'}+H_z^{'}$ in terms of matrix for $n=2$

$$l=0\left\{\begin{array}{lll} \psi_1\equiv|\frac{1}{2}\,\frac{1}{2}\rangle & =|0\,0\rangle|\frac{1}{2}\,\frac{1}{2}\rangle, & \\ \psi_2\equiv|\frac{1}{2}\,\frac{-1}{2}\rangle & =|0\,0\rangle|\frac{1}{2}\,\frac{-1}{2}\rangle, & \end{array}\right.$$

$$l=1\left\{\begin{array}{lll} \psi_3\equiv|\frac{3}{2}\,\frac{3}{2}\rangle & =|1\,1\rangle|\frac{1}{2}\,\frac{1}{2}\rangle, & \\ \psi_4\equiv|\frac{3}{2}\,\frac{-3}{2}\rangle & =|1\,-1\rangle|\frac{1}{2}\,\frac{-1}{2}\rangle, & \\ \psi_5\equiv|\frac{3}{2}\,\frac{1}{2}\rangle & =\sqrt{2/3}|1\,0\rangle|\frac{1}{2}\,\frac{1}{2}\rangle & +\sqrt{1/3}|1\,1\rangle|\frac{1}{2}\,\frac{-1}{2}\rangle, \\ \psi_6\equiv|\frac{1}{2}\,\frac{1}{2}\rangle & =-\sqrt{1/3}|1\,0\rangle|\frac{1}{2}\,\frac{1}{2}\rangle & +\sqrt{2/3}|1\,1\rangle|\frac{1}{2}\,\frac{-1}{2}\rangle, \\ \psi_7\equiv|\frac{3}{2}\,\frac{-1}{2}\rangle & =\sqrt{1/3}|1\,-1\rangle|\frac{1}{2}\,\frac{1}{2}\rangle & +\sqrt{2/3}|1\,0\rangle|\frac{1}{2}\,\frac{-1}{2}\rangle, \\ \psi_8\equiv|\frac{1}{2}\,\frac{-1}{2}\rangle & =-\sqrt{2/3}|1\,-1\rangle|\frac{1}{2}\,\frac{1}{2}\rangle & +\sqrt{1/3}|1\,0\rangle|\frac{1}{2}\,\frac{-1}{2}\rangle. \end{array}\right.$$

第一个等号后为以$H_{so}^{'}$的本征态为basis的形式($|j\quad m_j>$),而第二个等号后为$H_{so}^{'}$的本征态在以$H_Z^{'}$的本征态为basis($|lm_l>|sm_s>$)的形式。

而第二个等号中存在一些交叉项，它们前面的系数称为CG系数，以$C_{m_lm_s}^{j\quad m_j}$

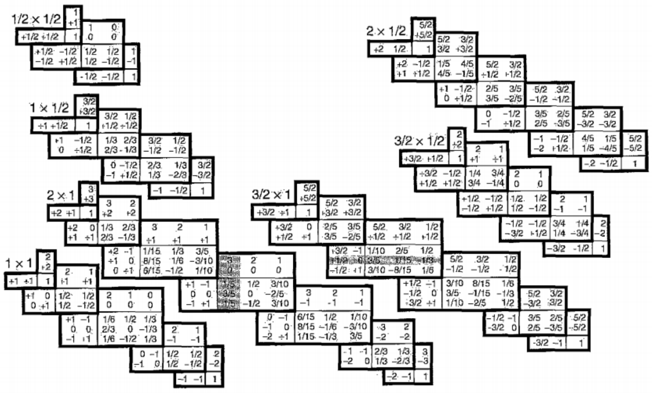
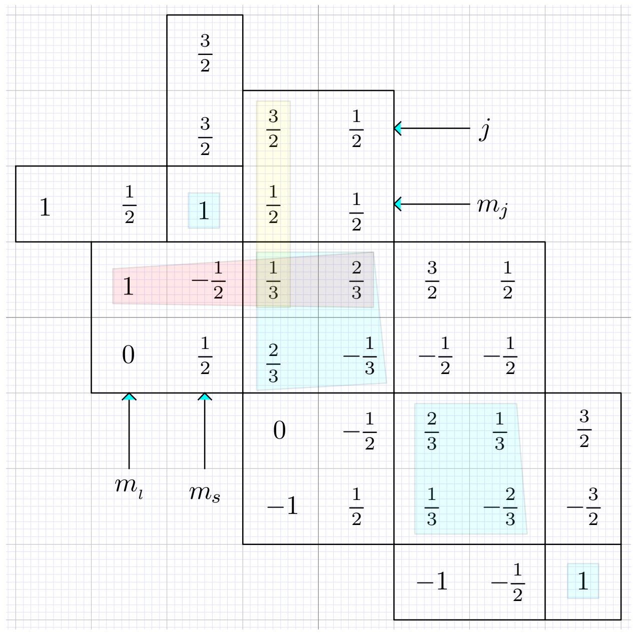


图. Clebsch-Gorden coefficients (P180 Table 4.8)

关于如何读取CG系数，见以下示意图：



as the figure shows $|m_l=1, m_s=-\frac{1}{2}, j=\frac{3}{2}, m_j=\frac{1}{2}> \Leftrightarrow C^{\frac{3}{2}\ \frac{1}{2}}_{1-\frac{1}{2}}=\frac{1}{3}$

为什么使用两种表象

$\mathrm{Eq}[6.67] \Rightarrow$ we need j to evaluate E_{fs}' $\qquad \mathrm{Eq}[6.71] \Rightarrow m_l, m_s \Rightarrow E_z^{(1)}$

Pro 6.25 . Find the matrix of $H_{fs}'+H_z'$ in the basis of $\{\psi_1,\ldots,\psi_8\}$

(1) Fine structure $E_{fs}'=\frac{E_1}{n^2}\frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}}-\frac{3}{4}\right)$

for $\psi_1 | j=\frac{1}{2}, m_j=\frac{1}{2}>$, $\langle\psi_1|H_{fs}'|\psi_1\rangle=\frac{E_1}{2^2}\frac{\alpha^2}{2^2}\left(\frac{2}{\frac{1}{2}+\frac{1}{2}}-\frac{3}{4}\right)=\frac{E_1\alpha^2}{4^2}\cdot 5\equiv 5\gamma$,其中，$\gamma=E_1\left(\frac{\alpha}{8}\right)^2$

$\langle\psi_2|H_{fs}'|\psi_2\rangle=5\gamma\ldots\ldots$

(2) Matrix of Zeeman

$E_Z^{(1)}=\mu_B B_{\mathrm{ext}}(m_l+2m_s)$,$m_l$，$m_s$分别为$L_Z, S_Z$的本征值

$\langle\psi_1|\,H_Z'|\psi_1\rangle=\mu_B B_{\mathrm{ext}}\left(0+2\cdot\frac{1}{2}\right)=\mu_B B_{\mathrm{ext}}=\beta$

$\langle\psi_2|\,H_Z'|\psi_2\rangle=\cdots,$

$\cdots$

$\langle\psi_8|\,H_Z'|\psi_8\rangle=\ldots$

ψ_5会产生两个态：$\psi_5=\sqrt{\frac{2}{3}}\,|10>|\frac{1}{2}\frac{1}{2}>+\sqrt{\frac{1}{3}}\,|11>|\frac{1}{2}-\frac{1}{2}>$

$\langle\psi_5|\,H_Z'\,|\psi_5\rangle=\left\langle\psi_5|\,\mu_B B_{\text{ext}}(\hat{L}_z+2\hat{S}_z)\,|\sqrt{\frac{2}{3}}\,|10>|\frac{1}{2}\frac{1}{2}>+\sqrt{\frac{1}{3}}\,|11>|\frac{1}{2}-\frac{1}{2}>\right\rangle$ 在基$|lm_l>|sm_s>$之间同样存在正交归一关系，即 $\left\{\begin{array}{ll}\langle 10|11\rangle=0 & \left\langle\frac{1}{2}\frac{1}{2}|\frac{1}{2}-\frac{1}{2}\right\rangle=0\\ \langle 10|01\rangle=1 & \left\langle\frac{1}{2}\frac{1}{2}|\frac{1}{2}\frac{1}{2}\right\rangle=0\end{array}\right\}$,而$\hat{L}_z,\hat{S}_z$与其本征态函数作用不会升降阶。故仅余下对应的项。

$$\begin{aligned}\langle\psi_5|\,H_Z'\,|\psi_5\rangle &= \mu_B B_{\text{ext}}\left\{\frac{2}{3}\left\langle 10|\left\langle\frac{1}{2}\frac{1}{2}|\,(\hat{L}_z+2\hat{S}_z)\,|10\right\rangle|\frac{1}{2}\frac{1}{2}\right\rangle+\frac{1}{3}\left\langle 11|\left\langle\frac{1}{2}\quad-\frac{1}{2}|\,(\hat{L}_z+2\hat{S}_z)\,|11\right\rangle|\frac{1}{2}\quad-\frac{1}{2}\right\rangle\right\}\\ &= \mu_B B_{\text{ext}}\left\{\frac{2}{3}\left(0+2\cdot\frac{1}{2}\right)+\frac{1}{3}\left(1-2\cdot\frac{1}{2}\right)\right\}=\frac{2}{3}\beta\end{aligned}$$

$\psi_6=-\sqrt{\frac{1}{3}}\,|10>|\frac{1}{2}\frac{1}{2}>+\sqrt{\frac{2}{3}}\,|11>|\frac{1}{2}-\frac{1}{2}>$ ，

$\langle\psi_6|\,H_z'\,|\psi_6\rangle=\beta\left\{\frac{1}{3}\times\left(1\times 0+2\times\frac{1}{2}\right)+\frac{2}{3}\times\left(1\times 1+2\times\left(-\frac{1}{2}\right)\right)\right\}=\frac{1}{3}\beta$

可以发现ψ_5,ψ_6 share the same basis$\Rightarrow$ H_z' couple ψ_5 and ψ_6

交叉项：

$$\begin{aligned}\langle\psi_5|\,H_z'\,|\psi_6\rangle &= \left[\sqrt{\frac{2}{3}}\langle 10|\langle\frac{1}{2}\frac{1}{2}|+\sqrt{\frac{1}{3}}\langle 11|\left\langle\frac{1}{2}-\frac{1}{2}\right|\right]\mu_B B_{\text{ext}}(\hat{L}_z+2\hat{S}_z)\left[-\sqrt{\frac{1}{3}}|10>|\frac{1}{2}\frac{1}{2}>+\sqrt{\frac{2}{3}}|11>|\frac{1}{2}-\frac{1}{2}>\right]\\ &= \mu_B B_{\text{ext}}\left(-\frac{\sqrt{2}}{3}\times\left(0+2\times\frac{1}{2}\right)+\frac{\sqrt{2}}{3}\times\left(1+2\times-\frac{1}{2}\right)\right)=-\frac{\sqrt{2}}{3}\mu_B B_{\text{ext}}=-\frac{\sqrt{2}}{3}\beta\end{aligned}$$

同理计算所有的$W_{ij}\,(i,j=1,2,\ldots,8)$

$$-W=\begin{bmatrix}5\gamma-\beta &&&&&&&\\ &5\gamma+\beta&&&&&&\\ &&\gamma-2\beta&&&&&\\ &&&\gamma+2\beta&&&&\\ &&&&\gamma-\frac{2}{3}\beta&\frac{\sqrt{2}}{3}\beta&&\\ &&&&\frac{\sqrt{2}}{3}\beta&\gamma-\frac{1}{3}\beta&&\\ &&&&&&\gamma+\frac{2}{3}\beta&\frac{\sqrt{2}}{3}\beta\\ &&&&&&\frac{\sqrt{2}}{3}\beta&5\gamma+\frac{1}{3}\beta\end{bmatrix}$$

下一步对W进行对角化与简并微扰。

6.5 Hyperfine Splitting 超精细能级劈裂

质子自旋S_p,耦合因子g_p(电子自旋 – 质子自旋耦合)

$$\boldsymbol{\mu}_p=\frac{g_p e}{2m_p}\boldsymbol{S}_p,\qquad \boldsymbol{\mu}_e=-\frac{e}{m_e}\boldsymbol{S}_e\qquad[6.85]$$

$$\boldsymbol{B}=\frac{\mu_0}{4\pi r^3}[3(\boldsymbol{\mu}\cdot\hat{r})\hat{r}-\boldsymbol{\mu}]+\frac{2\mu_0}{3}\boldsymbol{\mu}\delta^3(\boldsymbol{r})\qquad[6.86]$$

$$H_{\text{hf}}'=\frac{\mu_0 g_p e^2}{8\pi m_p m_e}\frac{[3(\boldsymbol{S}_p\cdot\hat{r})(\boldsymbol{S}_e\cdot\hat{r})-\boldsymbol{S}_p\cdot\boldsymbol{S}_e]}{r^3}+\frac{\mu_0 g_p e^2}{3m_p m_e}\boldsymbol{S}_p\cdot\boldsymbol{S}_e\delta^3(\boldsymbol{r}).[6.87]$$

$$E_{\text{hf}}^1=\frac{\mu_0 g_p e^2}{8\pi m_p m_e}\left\langle\frac{3(\boldsymbol{S}_p\cdot\hat{r})(\boldsymbol{S}_e\cdot\hat{r})-\boldsymbol{S}_p\cdot\boldsymbol{S}_e}{r^3}\right\rangle+\frac{\mu_0 g_p e^2}{3m_p m_e}\langle\boldsymbol{S}_p\cdot\boldsymbol{S}_e\rangle\,|\psi(0)|^2\qquad[6.88]$$

$$[6.85]-[6.88]\Rightarrow H_{\text{hf}}^{(1)}=\frac{\mu_0 g_p e^2}{3m_p m_e a^3}\langle\vec{\boldsymbol{S}}_p\cdot\vec{\boldsymbol{S}}_e\rangle$$

So its Hamiltonian can be written as

$$H'_{\mathrm{hf}} = \text{Const} \cdot \vec{\boldsymbol{S}}_p \cdot \vec{\boldsymbol{S}}_e \left(\text{both have a spin of} \frac{1}{2}\right)$$

因为 $\vec{S}_p \cdot \vec{S}_e$不再与$\vec{S}_p, \vec{S}_e$ 不再对易(即$[\vec{S}_e, \vec{S}_p \cdot \vec{S}_e] \neq 0, [\vec{S}_p, \vec{S}_p \cdot \vec{S}_e] \neq 0$)，因此$\vec{S}_p, \vec{S}_e$不是好量子数。

$\vec{S}_p \cdot \vec{S}_e = \frac{1}{2}(S_e^+ S_p^- + S_e^- S_p^+) + S_e^z S_p^z$

存疑？	$S_e^{\pm}$，$S_p^{\pm}$，$\vec{S} = \vec{S}_e + \vec{S}_p$之间两两对易，是好量子数

$$S = \left\{ \begin{array}{l} S_e + S_p = \frac{1}{2} + \frac{1}{2} = 1 \\ S_e - S_p = \frac{1}{2} - \frac{1}{2} = 0 \end{array} \right\} \qquad \vec{S}^2 = \vec{S}_e^2 + \vec{S}_p^2 + 2\vec{S}_e \cdot \vec{S}_p \Rightarrow \vec{S}_e \cdot \vec{S}_p = \frac{1}{2}(\vec{S}^2 - \vec{S}_e^2 - \vec{S}_p^2)$$

$$\Rightarrow [\vec{S}_e^2, \vec{S}_p \cdot \vec{S}_e] = 0, [\vec{S}_p^2, \vec{S}_p \cdot \vec{S}_e] = 0$$

$$S = \left\{ \begin{array}{lll} S_e + S_p = \frac{1}{2} + \frac{1}{2} = 1 & \Rightarrow m = 0, \pm 1 & \text{三重态} \\ S_e - S_p = \frac{1}{2} - \frac{1}{2} = 0 & \Rightarrow m = 0 & \text{单态} \end{array} \right\} m\text{为}S\text{的}z\text{分量}$$

$$\begin{aligned} E_{\mathrm{hf}} &= \text{const} \times \langle S^2 - S_e^2 - S_p^2 \rangle \\ &= \text{const} \times \hbar^2 \left\{ \begin{array}{ll} 1(1+1) - \frac{1}{2}\left(1 + \frac{1}{2}\right) - \frac{1}{2}\left(1 + \frac{1}{2}\right) = \frac{1}{2} & \text{三重态} \\ 0(0+1) - \frac{1}{2}\left(1 + \frac{1}{2}\right) - \frac{1}{2}\left(1 + \frac{1}{2}\right) = -\frac{3}{2} & \text{单态} \end{array} \right\} \Longrightarrow \text{Splitting} \equiv \text{const} \times \hbar^2 z \end{aligned}$$

Chapter 7 The Variational Principle 变分原理

7.1 Theory

Given the upper bound for the ground-state Energy (Egs).(Also a approximately), Pick any normalized function(can not be eigenstates, and usually we use the Guassion form) ψ, we can claim that

$$E_{gs} \leqslant \langle \psi | H | \psi \rangle \equiv \langle H \rangle$$

证明. The (unknown) eigenstates of H form a complete set, so ψ can be expressed as a linear combination.

$$\psi = \sum_n C_n \psi_n \quad \text{with} \langle \psi_m | \psi_n \rangle = \delta_{mn} \quad \text{and} \quad H\psi_n = E\psi_n (\psi_n\text{是本征态})$$

since ψ is normalized.

$$1 = \langle \psi | \psi \rangle = \left\langle \sum_m C_m \psi_m \middle| \sum_n C_n \psi_n \right\rangle = \sum_m \sum_n C_m^{\dagger} C_n \langle \psi_m | \psi_n \rangle = \sum_m \sum_n C_m^{\dagger} C_n \delta_{mn} = \sum_n |C_n|^2$$

Meanwhile

$$\langle H\rangle = \left\langle \sum_m C_m\psi_m \,|\, \sum_n C_n\psi_n \right\rangle = \sum_m \sum_n C_m^\dagger C_n \langle \psi_m \,|\, H \,|\, \psi_n\rangle = \sum_n |C_n|^2 E_n$$

由于E_{gs}为基态能量，所以$E_{gs} \leqslant E_n$

$$\langle H\rangle = \sum_n |C_n|^2 E_n \geqslant \sum_n |C_n|^2 E_{gs} = E_{gs} \qquad \square$$

Example 7.1. 1D harmonic oscillator $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$, find E_{gs}.

解答.

Step 1: Pick a normalized trial wave function, usually as Guass form $\psi(x) = Ae^{-bx^2}$ to be determined by using the variational principle. (A will be used for normalization, while b is the Variation parameter)

Normalization: $1 = \int |\psi|^2 dx = |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} = |A|^2 \sqrt{\frac{\pi}{2b}} \Longrightarrow |A| = \left(\frac{2b}{\pi}\right)^{\frac{1}{4}}$

Step 2: Calculate $\langle H\rangle = \langle\psi \,|\, H \,|\, \psi\rangle = \langle T\rangle + \langle V\rangle$

$$\begin{aligned}
\langle T\rangle &= \int_{-\infty}^{\infty} \psi^\dagger \left(-\frac{\hbar^2}{2m}\frac{\partial}{\partial x^2}\right)\psi dx \\
&= -\frac{\hbar^2 |A|^2}{2m}\int_{-\infty}^{\infty} e^{-bx}\frac{\mathrm{d}}{\mathrm{d}x}e^{-bx}dx \\
&= -\frac{\hbar^2 |A|^2}{2m}\int_{-\infty}^{\infty} e^{-2bx^2}(4bx^2 - 2b)\,\mathrm{d}x
\end{aligned}$$

$$由 \int_{-\infty}^{\infty} e^{-ax^2}\mathrm{d}x = \sqrt{\frac{\pi}{a}} \quad , \quad \int_{-\infty}^{\infty} x^2 e^{-ax^2}\mathrm{d}x = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}$$

$$\langle T\rangle = \frac{\hbar^2}{2m}b$$

$$\begin{aligned}
\langle V\rangle &= \int_{-\infty}^{\infty} \psi^* \left(\frac{1}{2}m\omega^2 x^2\right)\psi \mathrm{d}x \\
&= \frac{m\omega^2}{8b}
\end{aligned}$$

$$\Longrightarrow \langle H\rangle = \langle T\rangle + \langle V\rangle = \frac{\hbar^2}{2m}b + \frac{m\omega^2}{8b} \qquad A\,\text{function of the variational parameter}$$

Step 3: Minimize $\langle H\rangle$ as a function of b $\frac{\mathrm{d}}{\mathrm{d}b}\langle H\rangle = 0$, $\frac{\mathrm{d}^2}{\mathrm{d}b^2}\langle H\rangle > 0$

Step 4: At $b = \frac{m\omega}{2\hbar}$, $\langle H\rangle = \frac{1}{2}\hbar\omega$

Example 7.2. Delta potential $H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \alpha\delta(x)$, find E_{gs}.

解答.

Step1: $\psi = \left(\frac{2b}{\pi}\right)^{\frac{1}{4}} e^{-bx^2}$

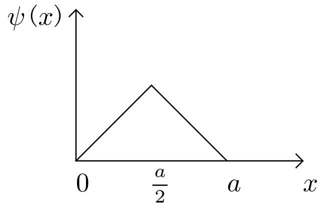
Step2: $\langle T\rangle = \frac{\hbar^2 b}{2m} - \alpha\sqrt{\frac{2b}{\pi}}$

Step3:Minimize $\langle H\rangle$ $\frac{\mathrm{d}}{\mathrm{d}b}\langle H\rangle = 0 \Rightarrow b = \frac{2m^2\alpha^2}{\pi\hbar^4}$ and $\frac{\mathrm{d}^2}{\mathrm{d}b^2}\langle H\rangle > 0$

Step4: $b = \frac{2m^2\alpha^2}{\pi\hbar^4}$ $\quad \langle H\rangle = -\frac{m\alpha^2}{\pi\hbar}$

(exact solution is $-\frac{m\alpha^2}{2\hbar}$)

Example 7.3. 1D infinite square wall + "triangular trail wave funtion"



$$\psi_x = \left\{ \begin{array}{cc} Ax & , x \in \left[0, \frac{a}{2}\right] \\ A(a-x) & , x \in \left[\frac{a}{2}, a\right] \\ 0 & , \text{Elsewhere} \end{array} \right\}$$

Step1: Normalized trial wavefunction $1 = |A|^2 \left[\int_0^{\frac{a}{2}} x^2 \mathrm{d}x + \int_{\frac{a}{2}}^{a} (a-x)^2 \mathrm{d}x\right] = \frac{1}{3}\frac{a^2}{4}|A|^2 \Rightarrow A = \frac{2}{a}\sqrt{\frac{3}{a}}$

$$\langle H \rangle = \langle T \rangle + \langle V \rangle \quad (\langle V \rangle = 0)$$

$\langle T \rangle = \int_0^a \psi^* \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) \psi \mathrm{d}x \quad \frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi = A\left[\delta(x) - 2\delta\left(x - \frac{a}{2}\right) + \delta(x-a)\right]$ as we can check $\int \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}\mathrm{d}x = \frac{\mathrm{d}\psi}{\mathrm{d}x}$

$$\Rightarrow \langle T \rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \mathrm{d}x \psi(x) A^2 \left[\delta(x) - 2\delta\left(x - \frac{a}{2}\right) + \delta(x-a)\right] = -\frac{\hbar^2}{2m}A^2\left[\psi(0) - 2\psi\left(\frac{a}{2}\right) + \psi(a)\right]$$

$$\Rightarrow \langle T \rangle = \frac{6\hbar^2}{ma^2} > \frac{\pi^2\hbar^2}{2ma^2} (\text{exact solution})$$

7.2 Ground-state energy of Helium

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + V$$

$$V = -\frac{e^2}{4\pi\varepsilon_0}\left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\vec{r}_1 - \vec{r}_2|}\right)$$

Goal. To calculate E_{gs} use the variational principle (Experimentally measured to be -78.975eV, the energy to strip off both electrons.

Trouble. Interaction Coulumb potential $V_{ee} = \frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{r}_1 - \vec{r}_2|}$

2023.10.24 课程纪要

当不考虑氦原子两个电子之间的相互作用V_{ee}时，$H = H_{e1} + H_{e2}$

$$\begin{array}{l} H_{e1} = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{e^2}{4\pi\varepsilon_0}\frac{2}{r_1} \\ H_{e2} = -\frac{\hbar^2}{2m}\nabla_2^2 - \frac{e^2}{4\pi\varepsilon_0}\frac{2}{r_2} \end{array}$$ 每一个都是氢原子的计算方式，不过有原子核$e \rightarrow 2e$。

由4.72

$$\begin{array}{rcl} \text{Bohr radius} \quad a & \equiv & \frac{4\pi\varepsilon_0\hbar^2}{me^2} \qquad (\text{分母的}e^2\text{ 出自核}e\text{和电子}e) \\ \text{核电子}e \rightarrow 2e & \Rightarrow & r' = \frac{a}{2} \end{array}$$

4.80 the ground-state wavefunvtion of hydrogen.

$$\psi_{100} = A e^{-r/a} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} \xrightarrow[a\to\frac{a}{2}]{} \psi_{100} = \sqrt{\frac{8}{\pi a^3}} e^{-r/a}$$

当考虑到V_{ee}, the wavefunction is a product of two $\psi_{100}\left(a\to\frac{a}{2}\right)$

$$\psi_0(\vec{r}_1,\vec{r}_2) = \psi_{100}(\vec{r}_1)\,\psi_{100}(\vec{r}_2) = \left(\sqrt{\frac{8}{\pi a^3}}\right)^2 e^{-r_1/\left(\frac{1}{2}a\right)} e^{-r_2/\left(\frac{1}{2}a\right)} = \frac{8}{\pi a^3} e^{-2(r_1+r_2)/a}$$

from 4.72, 4.77

$$-13.6\mathrm{eV} = E_1 = -\frac{\hbar^2}{2m}\frac{1}{a^2} \longrightarrow -\frac{\hbar^2}{2m}\frac{4}{a^2}$$

Two "$2e$ Hydrogen" electron $\Rightarrow 2E_1^{+2e} \approx 8E_1 \approx 8\times(-13.6\mathrm{eV})$ (The free (no V_{ee}) energy)

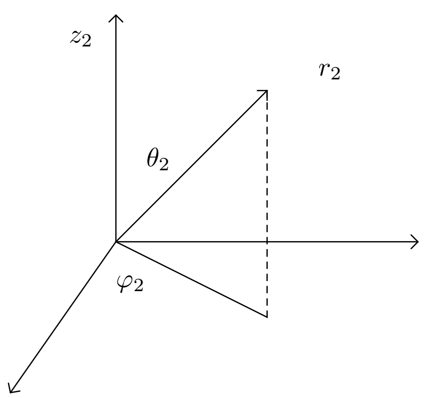
Now we include V_{ee} and then

$$\begin{aligned}\langle\psi(r_1,r_2)|H_{\mathrm{total}}|\psi(r_1,r_2)\rangle &= \langle\psi(r_1,r_2)|H_{e1}+H_{e2}+V_{\mathrm{ee}}|\psi(r_1,r_2)\rangle\\ &= 8E_1 + \langle\psi(r_1,r_2)|V_{\mathrm{ee}}|\psi(r_1,r_2)\rangle\end{aligned}$$

$$\begin{aligned}\langle\psi(r_1,r_2)|V_{\mathrm{ee}}|\psi(r_1,r_2)\rangle &= \int \mathrm{d}^3r_1\mathrm{d}^3r_2\psi^*(r_1,r_2)\frac{e^2}{4\pi\varepsilon_0}\frac{1}{|r_1-r_2|}\psi(r_1,r_2)\\ &= \frac{e^2}{4\pi\varepsilon_0}\left(\frac{8}{\pi a}\right)^2\int \mathrm{d}\vec{r}_1^{\,3}\mathrm{d}\vec{r}_2^{\,3}\frac{e^{-4(r_1+r_2)/a}}{|\vec{r}_1-\vec{r}_2|}\end{aligned}$$

$$\because |\vec{r}_1-\vec{r}_2| = \sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}$$

为积分方便，我们让r_1与z轴平行



$$\langle\psi_{100}|V_{\mathrm{ee}}|\psi_{100}\rangle = \frac{e^2}{4\pi\varepsilon_0}\left(\frac{8}{\pi a^3}\right)^2\int \mathrm{d}^3r_1\, e^{-4r_1/a}\int \mathrm{d}^3r_2\frac{e^{-4r_2/e}}{|r_1-r_2|}$$

先对r_2 进行积分

$$
\begin{aligned}
I_2 &= \int_0^{2\pi} \mathrm{d}\varphi_2 \int_0^{\pi} \sin\theta_2 \mathrm{d}\theta_2 \int_0^{\infty} r_2^2\,\mathrm{d}r_2 \frac{e^{-4r_2/a}}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}} \\
&= 2\pi \int_0^{\infty} r_2^2\, e^{-4r_2/a}\mathrm{d}r_2 \int_0^{\pi} \mathrm{d}\theta_2 \sin\theta_2 \frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}} \\
&= 2\pi \int_0^{\infty} r_2^2\, e^{-4r_2/a}\mathrm{d}r_2 \int_0^{\pi} -1\mathrm{d}\,(\cos\theta_2)\ \frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}}
\end{aligned}
$$

$$\text{令}\ \ x=\cos\theta_2$$

$$
\begin{aligned}
-\int_0^{\pi} \mathrm{d}\,(\cos\theta_2)\ \frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}} &= -\int_{-1}^{1} \mathrm{d}x \frac{1}{\sqrt{2r_1r_2}} \frac{1}{\sqrt{\frac{r_1^2+r_2^2}{2r_1r_2}-x}} \\
&= \frac{-2}{\sqrt{2r_1r_2}} \sqrt{\frac{r_1^2+r_2^2}{2r_1r_2}-x}\ |_{-1}^{1} \\
&= \frac{-2}{\sqrt{2r_1r_2}} \sqrt{\frac{r_1^2+r_2^2}{2r_1r_2}-1} - \frac{-2}{\sqrt{2r_1r_2}} \sqrt{\frac{r_1^2+r_2^2}{2r_1r_2}+1} \\
&= \frac{1}{r_1r_2}\left(\sqrt{r_1^2+r_2^2+2r_1r_2} - \sqrt{r_1^2+r_2^2-2r_1r_2}\right) \\
&= \frac{1}{r_1r_2}(|r_1+r_2| - |r_1-r_2|) \\
&= \begin{Bmatrix} \frac{2}{r_1} & , & r_2<r_1 \\ \frac{2}{r_2} & , & r_2>r_1 \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\therefore I_2 &= 2\pi \int_0^{\infty} r_2^2\, e^{-4r_2/a}\mathrm{d}r_2\ (\theta_2\text{的积分}) \\
&= 2\pi\left[\int_0^{r_1} \mathrm{d}\,(r_2)\ r_2^2\, e^{-4r_2/a} \left(\frac{2}{r_1}\right) + \int_{r_1}^{\infty} \mathrm{d}\,(r_2)\ r_2^2\, e^{-4r_2/a} \left(\frac{2}{r_2}\right)\right] \\
&= 4\pi\left[\frac{1}{r_1}\int_0^{r_1} \mathrm{d}r_2\, r_2^2\, e^{-4r_2/a} + \int_{r_1}^{\infty} \mathrm{d}r_2\, r_2\, e^{-4r_2/a}\right]
\end{aligned}
$$

using
$$\int \mathrm{d}x \quad x e^x = e^x(x-1)$$
$$\int \mathrm{d}x \quad x^2 e^x = e^x(x^2-2x+2)$$

$$
\begin{aligned}
I_2 &= 4\pi\left\{\frac{1}{r_1}\left(\frac{a}{4}\right)^3 e^{-4r_1/a}\left[\left(-\frac{4r_1}{a}\right)^2 - 2\left(-\frac{4r_1}{a}\right) + 2\right] + \left(\frac{a}{4}\right)^2 e^{-4r_1/a}\left(1+\frac{4r_1}{a}\right)\right\} \\
&= \frac{\pi a^3}{8r_1}\left[1-\left(1+\frac{2r_1}{a}\right)e^{-4r_1/a}\right]
\end{aligned}
$$

$$
\begin{aligned}
\langle V_{\mathrm{ee}}\rangle &= \frac{e^2}{4\pi\varepsilon_0}\left(\frac{8}{\pi a^3}\right)^2 \iiint I_2 e^{-4r_1/a} r_1 \sin\theta_1 \mathrm{d}r_1 \mathrm{d}\theta_1 \mathrm{d}\varphi_1 \\
&= \frac{e^2}{4\pi\varepsilon_0}\left(\frac{8}{\pi a^3}\right) 4\pi \int_0^{\infty} \mathrm{d}r_1 \left(r_1 e^{-4r_1/a} - r_1 e^{-8r_1/a} - \frac{2r_1^2}{a} e^{-4r_1/a}\right) \\
&= \frac{e^2}{4\pi\varepsilon_0}\left(\frac{8}{\pi a^3}\right) 4\pi \frac{5}{128} a^2 = \frac{5}{4a}\frac{e^2}{4\pi\varepsilon_0} = -\frac{5}{2}E_1 \left(\text{where } E_1 = -\frac{e^2}{8\pi\varepsilon_0} = -13.6\text{eV}\right)
\end{aligned}
$$

$\langle\psi_0|H_{e1}+H_{e2}+V_{ee}|\psi_0\rangle=8E_1-\frac{5}{2}E_1=75\text{eV}$

注意：到目前为止未使用变分

Due to electron 2, electron 1 sees an effective nuclear charge of z, $(1\leqslant z\leqslant 2)$

“屏蔽效应（z为有效电荷）”

Step 1: rewrite wave function：$\psi_1(\vec{r}_1,\vec{r}_2)\equiv\frac{z^3}{\pi a^3}e^{-z(r_1+r_2)/a}$

Step 2: Calculate $\langle\psi_1|H|\psi_1\rangle$ as a function of z

$$H=-\frac{\hbar^2}{2m}\nabla_1^2-\frac{1}{4\pi\varepsilon_0}\frac{z}{r_1}-\frac{\hbar^2}{2m}\nabla_2^2-\frac{1}{4\pi\varepsilon_0}\left(\frac{z-2}{r_1}+\frac{z-2}{r_2}\right)+\frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{r}_1-\vec{r}_2|}$$

$$\langle H\rangle=2z^2E_1+2(z-2)\frac{e^2}{4\pi\varepsilon_0}\left\langle\frac{1}{r_{1,2}}\right\rangle+\langle V_{ee}\rangle$$

由 [6.55] $\left\langle\frac{1}{r}\right\rangle=\frac{1}{a}$

$$\left\langle\frac{1}{r_1}\right\rangle=\underbrace{\int d^3\vec{r}_2\frac{z^2}{\pi a^3}e^{-2zr_2/a}}_{\text{归一化为1}}\int d^3r_1\frac{z^3}{\pi a^3}e^{-2zr_1/a}\frac{1}{r_1}=\frac{z}{a}=\frac{1}{\text{effective Bohr radius}}$$

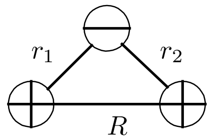
又$\langle V_{ee}\rangle=-\frac{5}{2}E_1=\frac{5}{4a}\frac{e^2}{4\pi\varepsilon_0}=\frac{5}{8}\frac{1}{\frac{a}{2}}\frac{e^2}{4\pi\varepsilon_0}=-\frac{5}{4}zE_1$

put them together

$$\begin{aligned}\langle\psi_1|H|\psi_1\rangle&=2z^2E_1+2(z-2)\frac{e^2}{4\pi\varepsilon_0}\frac{z}{a}-\frac{5}{4}zE_1\\&=2z^2E_1-4(z-2)zE-\frac{5}{4}zE_1\\&=E_1\left[-2z^2+\frac{27}{4}z\right]\ \text{(计算出其极值)}\end{aligned}$$

$$\langle H\rangle=\left[-2\left(\frac{27}{16}\right)^2+\frac{27}{4}\frac{27}{16}\right]\approxeq 77.5\text{eV}$$

7.3 氢分子离子(H_2^+) one-particle wave function



玻恩-奥本海默近似（原子核不动） $\psi=A[\psi_0(r_1)+\psi_0(r_2)]$。（同时处于两个原子的势场中）

$$\psi_0(r)=\frac{1}{\sqrt{\pi a^3}}e^{-r/c}$$

在这里，r 是变量。(前面是r_1, r_2 两个变量)。

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r_1} - \frac{1}{r_2}\right) + \frac{e^2}{4\pi\varepsilon_0}\frac{1}{R}$$

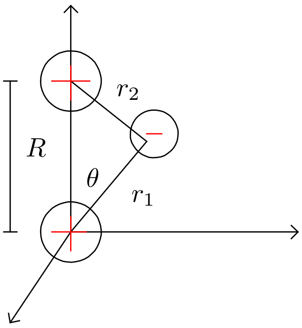
Step 1: 试探函数

one protons : $\psi_0(r) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$

two protons : $\psi = A[\psi_0(r_1) + \psi_0(r_2)]$

归一化： $1 = \int_{-\infty}^{\infty}\psi^2(r)\mathrm{d}r = A^2\left[\int_{-\infty}^{\infty}|\psi_0(r_1)|^2\mathrm{d}r + \int_{-\infty}^{\infty}|\psi_0(r_2)|^2\mathrm{d}r + 2\int_{-\infty}^{\infty}|\psi_0(r_1)||\psi_0(r_2)|\mathrm{d}r\right]$

上述的积分分为三个积分。



(1) (2) 对于氢原子波函数天然有$\int_{-\infty}^{\infty}|\psi_0(r_1)|^2\mathrm{d}r = \int_{-\infty}^{\infty}|\psi_0(r_2)|^2\mathrm{d}r = 1$ （分别选取两个质子为原点）

(3) 对于第三个积分$\int_{-\infty}^{\infty}|\psi_0(r_1)||\psi_0(r_2)|\mathrm{d}r$ ，令其为I

$$\begin{aligned} I &= \frac{1}{\pi a^3}\int e^{-(r_1+r_2)/a}\mathrm{d}^3\vec{r} \quad \text{where } r_1 = |\vec{r}|, r_2 = \sqrt{R^2 + r_1^2 - 2Rr_1\cos\theta} \\ &= \frac{2}{a^3}\int_0^\infty r^2 e^{-r/a}\mathrm{d}r \int_0^\pi \mathrm{d}\theta \sin\theta e^{-\frac{1}{a}\sqrt{R^2+r_1^2-2Rr_1\cos\theta}} \\ &= \qquad\qquad\qquad\qquad I_\theta \end{aligned}$$

令$y = \sqrt{R^2 + r^2 - 2Rr\cos\theta}$, $\mathrm{d}y^2 = 2Rr\sin\theta\mathrm{d}\theta$. $2y\mathrm{d}y = 2Rr\sin\theta\mathrm{d}\theta$ $\sin\theta\mathrm{d}\theta = \frac{y}{Rr}\mathrm{d}y$ $y \in [|r-R|, |R+r|]$

$$\begin{aligned} \therefore I_\theta &= \int_{|r-R|}^{|r+R|}\frac{y}{Rr}e^{-\frac{y}{a}}\mathrm{d}y = -\frac{a}{rR}\left[e^{-\frac{r+R}{a}}(r+R+a) - e^{-\frac{r-R}{a}}(|r-R|+a)\right] \\ &= e^{-\frac{R}{a}}\left[\frac{1}{3}\left(\frac{z}{a}\right)^2 + \frac{R}{a} + 1\right] \qquad (7.42) \end{aligned}$$

归一化 $1 = A^2(1 + 1 + 2I_\theta) \quad \Rightarrow \quad |A|^2 = \frac{1}{2(1+I_\theta)}$

Step 2: 算$\langle H\rangle$ as a function of $\frac{R}{a}$

$$\langle H\rangle = \langle\psi|\hat{H}|\psi\rangle \qquad \psi = A[\psi_0(r_1) + \psi_0(r_2)]$$

Note that: $\begin{array}{l}\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r_1}\right)\psi_0(r_1) = E_1\psi_0(r_1) \\ \left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r_2}\right)\psi_0(r_2) = E_1\psi_0(r_2)\end{array}$ $E_1 = -13.6\mathrm{eV}$

$$\begin{aligned}
\Rightarrow H\psi &= \left[-\frac{\hbar^2}{2m}\nabla^2-\frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r_1}+\frac{1}{r_2}\right)\right]A[\psi_0(r_1)+\psi_0(r_2)] \\
\text{其中 ，} & \left[-\frac{\hbar^2}{2m}\nabla^2-\frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r_1}\right)\right]\psi_0(r_1)=H_0\psi_0=E_0\psi_0 \\
&= E_1\psi - A\left(\frac{e^2}{4\pi\varepsilon_0}\right)\left[\frac{1}{r_1}\psi_0(r_2)+\frac{1}{r_2}\psi_0(r_1)\right]
\end{aligned}$$

$$\begin{aligned}
\langle\psi|H|\psi\rangle &= E_1 + A(\langle\psi_0(r_1)|+\langle\psi_0(r_2)|)\times(\ldots) \\
&= E_1 - A^2\frac{e^2}{4\pi\varepsilon_0}\left[\left\langle\psi_0(r_1)\left|\frac{1}{r_2}\right|\psi_0(r_1)\right\rangle+\left\langle\psi_0(r_2)\left|\frac{1}{r_2}\right|\psi_0(r_1)\right\rangle+\left\langle\psi_0(r_1)\left|\frac{1}{r_1}\right|\psi_0(r_2)\right\rangle+\right. \\
&\quad \left.\left\langle\psi_0(r_2)\left|\frac{1}{r_1}\right|\psi_0(r_2)\right\rangle\right] \\
&= E_1 - 2|A|^2\left(\frac{e^2}{4\pi\varepsilon_0}\right)\left[\left\langle\psi_0(r_1)\left|\frac{1}{r_2}\right|\psi_0(r_1)\right\rangle+\left\langle\psi_0(r_1)\left|\frac{1}{r_1}\right|\psi_0(r_2)\right\rangle\right]
\end{aligned}$$

We define $\begin{aligned} D &\equiv a\left\langle\psi_0(r_1)\left|\tfrac{1}{r_2}\right|\psi_0(r_1)\right\rangle \quad \text{Direct直接积分} \\ X &\equiv a\left\langle\psi_0(r_1)\left|\tfrac{1}{r_1}\right|\psi_0(r_2)\right\rangle \quad \text{Exchange交换积分}\end{aligned}$

from [Problem 7.8] $D=\frac{a}{R}-\left(1+\frac{a}{R}\right)e^{-2R/a}$,$X=\left(1+\frac{R}{a}\right)e^{-R/a}$

Also $E_1=-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{2a}$

$$\Rightarrow\langle H\rangle=\left[1+2\frac{(D+X)}{(1+I)}\right]E_1 \quad \text{（只算了电子的部分）}$$

For the proton-proton repulsion.

$$V_{\mathrm{pp}}=\frac{e^2}{4\pi\varepsilon_0}\frac{1}{R}=-\frac{2a}{R}\left(-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{2a}\right)=-\frac{2a}{R}E_1$$

令 $x=\frac{R}{a}$, E_1为单位

$$F(x)=-1+\frac{2}{a}\left\{\frac{\left(1-\frac{2}{3}x^2\right)e^{-x}+(1+x)e^{-2x}}{1+\left(1+x+\frac{1}{3}x^2\right)e^{-x}}\right\}$$

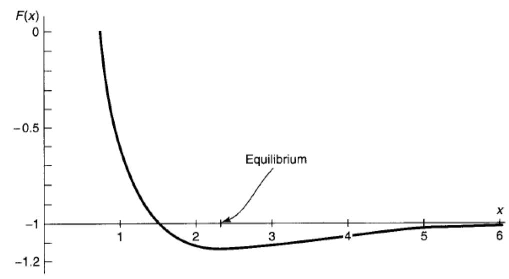


图 7.7 函数 F（x）（7.51 式）的图像，表明束缚态的存在（x 为质子间距，单位为玻尔半径）

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Chapter 8 WKB 近似

WKB is to obtain approximate solution to the 1D time-independent Schrodinger equation, for a "slowly" varying potential $V(x)$ wave length $\lambda = \frac{2\pi}{k}$

$$k = \frac{\sqrt{2m(E-V)}}{\hbar} = \frac{\sqrt{2m(E-V(x))}}{\hbar}$$

Portential　　同时确定了坐标和动量的关系（半经典的理论）

WKB 近似理论根据E 和 V 的关系划分三种情况。

$$\text{3 Region} \begin{Bmatrix} E > V \\ E < V \\ E = V \end{Bmatrix}$$

8.1 $E > V$ 经典区域（The "classical" Region）

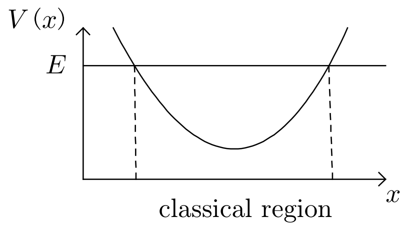
$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi = E\psi$$

$$\Rightarrow \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{2m}{\hbar^2}[E - V(x)]\psi \Rightarrow \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{p^2}{\hbar^2}\psi$$

$$P(x) = \sqrt{2m(E - V(x))}$$ （不是真正的动量，因为没有不确定性关系）

$P(x)$ is a function of x, so it is a semiclassical approximation

$E > V(x)$, $P(x)$ is real



In general, $\psi(x)$ is complex, we can express $\psi(x) = A(x)e^{i\phi(x)}$

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = [A'e^{i\phi} + Ae^{i\phi}i\phi']$$

$$\text{其中}, \quad A' = \frac{\mathrm{d}A}{\mathrm{d}x} \quad \phi' = \frac{\mathrm{d}\psi}{\mathrm{d}x}$$

Approximate both $A(x)$ and $\phi(x)$ are real function of x

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = [A'' + i2A'\phi' + iA\phi'' - A\cdot(\phi')^2]e^{i\phi}$$

$$[A'' + i2A'\phi' + iA\phi'' - A\cdot(\phi')^2]e^{i\phi} = -\frac{P^2}{\hbar^2}Ae^{i\phi}$$

for real part $A'' - A\cdot(\phi')^2 = -\frac{P^2}{\hbar^2}A$ or $A'' = A\left[(\phi')^2 - \frac{p^2}{\hbar^2}\right]$ [8.6] for Im part $2A'\phi'+A\phi''=0$ or $\frac{\mathrm{d}}{\mathrm{d}x}(A^2\phi')=0$ [8.7]

8.6 和8.7式， 与原先的薛定谔方程完全等价， 由第二个等式有$A=\pm\frac{C}{\sqrt{\phi'}}$, 其中$C$ 为常数

假定振幅A 变化缓慢, so that A'' 可忽略的.

$\Rightarrow 0=A\left[(\phi')^2-\frac{p^2}{\hbar^2}\right]\Rightarrow\frac{\mathrm{d}\phi}{\mathrm{d}x}=\pm\frac{p}{\hbar}$, 积分得到$\phi(x)=\pm\frac{1}{\hbar}\int p(x)\,\mathrm{d}x$

The general solution is

$$\psi(x)=\frac{C_+}{\sqrt{p(x)}}e^{\frac{i}{\hbar}\int p(x)\,\mathrm{d}x}+\frac{C_-}{\sqrt{p(x)}}e^{-\frac{i}{\hbar}\int p(x)\,\mathrm{d}x}[8.10]$$

注意到$|\psi(x)|^2\sim\frac{1}{p(x)}$, 概率与“动量”成反比

例. 8.1

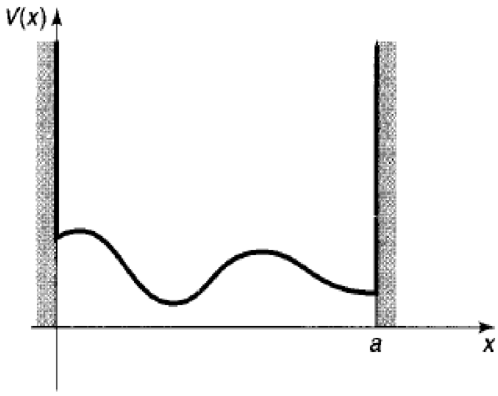


图. $V(x)=\left\{\begin{array}{cc}\text{some function} & , \quad 0<x<a\\ \infty & , \quad \text{otherwise}\end{array}\right\}$

Inside the wall if $E>V(x)$

$$\psi(x)\cong\frac{1}{\sqrt{p(x)}}[C_+e^{i\phi(x)}+C_-e^{-i\phi(x)}]$$

where $\phi(x)=\frac{1}{\hbar}\int_0^x p(x')\,\mathrm{d}x'$ $\quad(\frac{\mathrm{d}\phi}{\mathrm{d}x}=\frac{1}{\hbar}p(x))$, using $e^{ix}=\cos x+i\sin x$

$$\Rightarrow\psi(x)\cong\frac{1}{\sqrt{p(x)}}[C_1\sin\phi(x)+C_2\cos\phi(x)]$$

1. At $x=0,\phi(x)=0$. 且$\psi(x=0)=0$(无限深势阱边界条件) $\Rightarrow C_2=0$

$\Rightarrow\psi(x)=\frac{C_1}{\sqrt{p(x)}}\sin\phi(x)$

2. $\psi(x=a)=0\Rightarrow\phi(x=a)=n\pi$, $\Rightarrow\frac{1}{\hbar}\int_0^a p(x)\,\mathrm{d}x=n\pi\Rightarrow\int_0^a p(x')\,\mathrm{d}x'=n\pi\hbar$

$$\int_0^a p(x')\,\mathrm{d}x'=n\pi\hbar \quad \text{第一量子化条件}(n=1,2,3,\ldots)$$

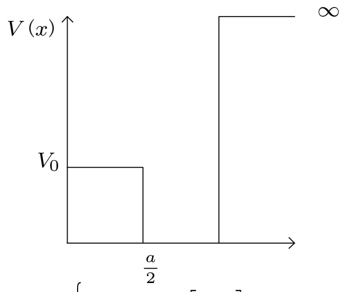
$p(x)=\sqrt{2m(E-V(x))}$ and the E is to find. And $V(x)$ is to be given.

For example: $V(x)=0$ in infinite well.

$$p(x)=\sqrt{2\mathrm{mE}}\Rightarrow\int_0^a\sqrt{2mE}\,\mathrm{d}x=n\pi\hbar\Rightarrow\sqrt{2mE}a=n\pi\hbar,E=\frac{n^2\pi^2\hbar^2}{2ma^2}$$

而这正是无限深方势阱的精确解. 因此可以用WKB近似。

Problem 8.1.



$$V(x)=\begin{cases}V_0 & , \quad x\in\left[0,\frac{a}{2}\right]\\ 0 & , \quad x\in\left[\frac{a}{2},a\right]\\ \infty & , \quad \text{elsewhere}\end{cases}$$

解: 利用量子化条件: $\int_0^{\frac{a}{2}}p(x)\,\mathrm{d}x=n2\hbar,n\in Z \quad p(x)=\sqrt{2m(E-V(x))}$

$$\int_0^{\frac{a}{2}}\sqrt{2m(E-V_0)}\,\mathrm{d}x+\int_{\frac{a}{2}}^a\sqrt{2mE}=n\pi\hbar$$

$$\Rightarrow\sqrt{2m(E-V_0)}\cdot\frac{a}{2}+\sqrt{2mE}\cdot\frac{a}{2}=n\pi\hbar\Rightarrow E_n=E_n^0+\frac{V_0}{2}+\frac{V_0^2}{16E_n^0} \qquad E_n^0 \text{ 为无限深势阱的能量}$$

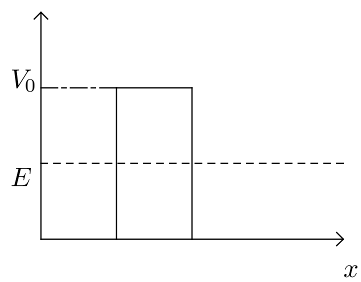
8.2 隧穿效应

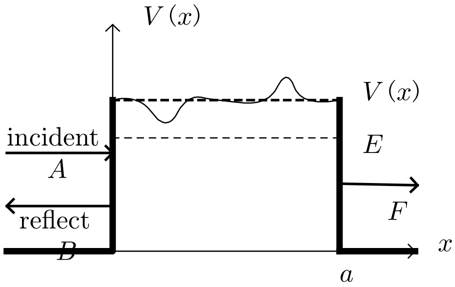
对于$E<V(x)$, $p(x)=\sqrt{2m(E-V)}$ 是一个虚数。

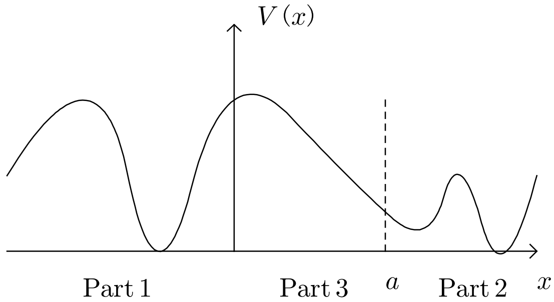
The general solution:

$$\psi(x)\quad\cong\quad\frac{C_+}{\sqrt{|p(x)|}}e^{\frac{1}{\hbar}\int p(x)\,\mathrm{d}x}+\frac{C_-}{\sqrt{|p(x)|}}e^{-\frac{1}{\hbar}\int p(x)\,\mathrm{d}x}$$

指数发散，物理上不合理，舍去 隧穿势垒，decaying







例如，考虑粒子被一个方势垒散射问题，势垒顶部崎岖不平，如上左图。

Part 1. On the left（$x<0$）

$$\psi(x) = \color{red}{Ae^{ikx}} + \color{blue}{Be^{-ikx}}$$

$$k=\sqrt{\frac{2mE}{\hbar}} \qquad \color{red}{\text{incident}} \quad \color{blue}{\text{reflect}}$$

Part 2. On the right（$x>a$）

$$\psi(x) = Fe^{ikx} \quad F\text{为散射振幅}$$

Part 3. 隧穿区间$(0\leqslant x\leqslant a)$： WKB 近似给出$\psi(x)=\frac{D}{\sqrt{p(x)}}e^{-\frac{1}{\hbar}\int_0^x p(x')\mathrm{d}x'}$

Given $E, V(x)$, to find the transmission probability

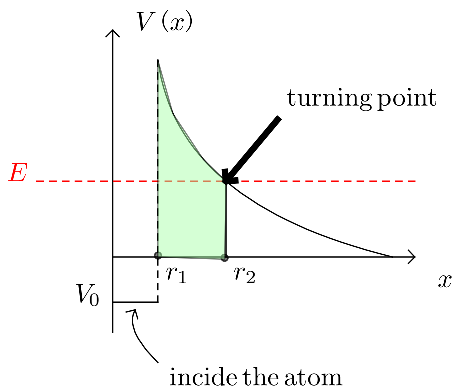
$$\frac{|F|}{|A|}\sim e^{-\frac{1}{\hbar}\int_0^a |p(x')|\mathrm{d}x'}$$

$$T\equiv\left|\frac{F}{A}\right|^2\cong e^{-2\gamma}, \text{where } \gamma=\frac{1}{\hbar}\int_0^a |p(x)|\mathrm{d}x$$

其中，γ is the result after matching bounding condition

We can check $\left\{\begin{matrix} a\to\infty & , & r\to\infty & , & T\to 0 \\ a\to 0 & , & r\to 0 & , & T\to 1\end{matrix}\right\}$

例 8.2 . α decay（α:${}_2^4$He 氦核） α 衰变的伽莫夫（Gamow）理论。



Potential energy has two parts

1. It is repelled by the left over nucleus charge $\frac{Ze}{r}$
2. A potential barrior more than twice. The emitted α particle of E

At the turning point $r_2, V(r_2)=E$

$$\left\{\begin{matrix} \frac{2e\mathrm{Z}e}{4\pi\varepsilon_0}\frac{1}{r_2}=E \\ \\ V(r)=\frac{2eZe}{4\pi\varepsilon_0}\frac{1}{r}\end{matrix}\right\} V(r)=E\frac{r_2}{r}$$ .To find the transmission probability T, we need to know γ

$$\gamma=\frac{1}{\hbar}\int_{r_1\to 0}^{r_2\to a}\sqrt{2m(V(r)-E)}\,\mathrm{d}r=\frac{1}{\hbar}\int_{r_1}^{r_2}\mathrm{d}r\sqrt{2m\left(E\frac{r_2}{r_1}-E\right)}=\frac{\sqrt{2mE}}{\hbar}\int_{r_1}^{r_2}\mathrm{d}r\sqrt{\frac{r_2}{r}-1}$$

计算此积分,

令 $r=r_2\sin^2 u$,

$$\left\{\begin{array}{c} \mathrm{d}r=r_2\sin u\cos u\,\mathrm{d}u=r_2\sin^2 u\mathrm{d}u \\ \sqrt{\frac{r}{r_2}}=\sin u\Rightarrow\left\{\begin{array}{c} u_1=\arcsin\sqrt{\frac{r}{r_2}} \\ u_1=\arcsin\sqrt{\frac{r_1}{r_2}}\ \mathrm{at}\ r=r_1 \\ u_2=\arcsin 1=\frac{\pi}{2}\ \mathrm{at}\ r=r_2 \end{array}\right. \end{array}\right\}\int_{r_1}^{r_2}\mathrm{d}r\sqrt{\frac{r_2}{r}-1}=\int_{\arcsin\sqrt{\frac{r_1}{r_2}}}^{\frac{\pi}{2}}r_2\cos^2 u\mathrm{d}u$$

$$\begin{aligned}\int_{\arcsin\sqrt{\frac{r_1}{r_2}}}^{\frac{\pi}{2}}r_2\cos^2 u\mathrm{d}u &= r_2\int_{\arcsin\sqrt{\frac{r_1}{r_2}}}^{\frac{\pi}{2}}\frac{1+2\cos 2u}{2}\mathrm{d}u \\ &= \frac{1}{2}\times r_2\left(\frac{\pi}{2}-\sin^{-1}\sqrt{\frac{r_1}{r_2}}\right)+\frac{r_2}{2}\frac{1}{2}\sin 2u\,|_{\arcsin\sqrt{\frac{r_1}{r_2}}}^{\frac{\pi}{2}} \\ &= \frac{1}{2}\times r_2\left(\frac{\pi}{2}-\sin^{-1}\sqrt{\frac{r_1}{r_2}}\right)+\frac{r_2}{2}\frac{1}{2}\left(2\sin u\sqrt{1-\sin^2 u}\right)|_{\arcsin\sqrt{\frac{r_1}{r_2}}}^{\frac{\pi}{2}} \\ &= \frac{1}{2}\times\left\{r_2\left(\frac{\pi}{2}-\sin^{-1}\sqrt{\frac{r_1}{r_2}}\right)+r_2\left(0-\sqrt{\frac{r_1}{r_2}}\sqrt{1-\frac{r_1}{r_2}}\right)\right\} \\ &= \frac{1}{2}\times\left\{r_2\left(\frac{\pi}{2}-\sin^{-1}\sqrt{\frac{r_1}{r_2}}\right)-\sqrt{r_1(r_2-r_1)}\right\}\end{aligned}$$

use $E=\frac{1}{4\pi\varepsilon_0}\frac{2eZe}{r_z}=V(r_2)$ at turining point $\Rightarrow r_2=\frac{2ze^2}{4\pi\varepsilon_0}$

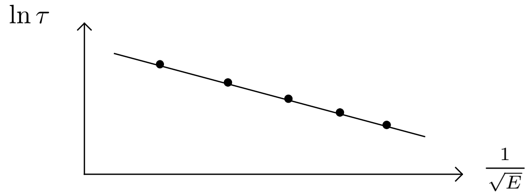
$$\begin{aligned} r &= \frac{\sqrt{2mE}}{\hbar}\left(\frac{\pi}{2}r_2-2\sqrt{r_1r_2}\right) \qquad (代入r_2) \\ &= \frac{\sqrt{2mE}}{\hbar}\frac{\pi}{2}\frac{1}{4\pi\varepsilon_0}\frac{2Ze^2}{E}-\frac{\sqrt{2\mathrm{mE}'}}{\hbar}2\sqrt{r_1\frac{1}{4\pi\varepsilon_0}\frac{2Ze^2}{E'}} \\ &= K_1\frac{Z}{\sqrt{E}}-K_2\sqrt{\mathrm{Zr_1}} \quad \text{where} \quad \begin{array}{c} K_1=\frac{e^2}{4\pi\varepsilon_0}\frac{\pi\sqrt{2m}}{\hbar}\approx 1.98\,(\mathrm{MeV}) \\ K_2=\sqrt{\frac{e^2}{4\pi\varepsilon_0}}\frac{4\sqrt{m}}{\hbar}\approx 1.485\,(fm)^{-1/2} \end{array}\end{aligned}$$

$$T=e^{-2\gamma}$$

Experiment: α 粒子在原子核内的平均速度为v，碰撞频率为$\frac{v}{2r_1}$, 隧穿概率为 $e^{-2\gamma}\Rightarrow$ 每个粒子的隧穿概率为 $\frac{v}{2r_1}e^{-2\gamma}$

$$\text{life time}: \tau=\frac{2r_1}{v}e^{2\gamma}$$

$$\ln\tau=\ln\frac{2r_1}{v}+2\gamma=\ln\frac{2r_1}{v}+2\left[k_1\frac{z}{\sqrt{E}}-k_2\sqrt{zr_1}\right]=C_1+C_1\frac{1}{\sqrt{E}}$$



8.3 Connection formulas

由于在$E>V$，波函数 bound state 含有$\frac{1}{\sqrt{2m(V-E)}}$项。$E<V$，波函数 tunneling state 含有$\frac{1}{\sqrt{2m(V-E)}}$项，而在turning point 二者均发散。

我们考虑在turning point 处的势能线性化，即$V=V_0+\frac{\mathrm{d}V(x=0)}{\mathrm{d}x}|_x$，争取使WKB近似在turning point 连续

[Trick] 线性化：$V(x)=V(x=0)+\frac{\mathrm{d}V}{\mathrm{d}x}|_{x=0}x=E+V'(0)x$

代入薛定谔方程有：

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_p}{\mathrm{d}x^2}+[E-V'(0)x]\psi_{p_p} &= E\psi \\
\Rightarrow\frac{\mathrm{d}^2\psi_p}{\mathrm{d}x^2} &= \alpha^3 x\,\psi_p
\end{aligned}
$$

其中$\alpha\equiv\left[\frac{2m}{\hbar^2}V'(0)\right]^{\frac{1}{3}}$，

Define $z=\alpha\pi$, $x=\frac{z}{\alpha}$ $\Rightarrow\frac{\mathrm{d}^2\psi_p}{\mathrm{d}z^2}=z\psi_p$ 为二阶偏微分方程， Airy Function

two solution $A_i(z)$ and $B_i(z)$ for Airy Function

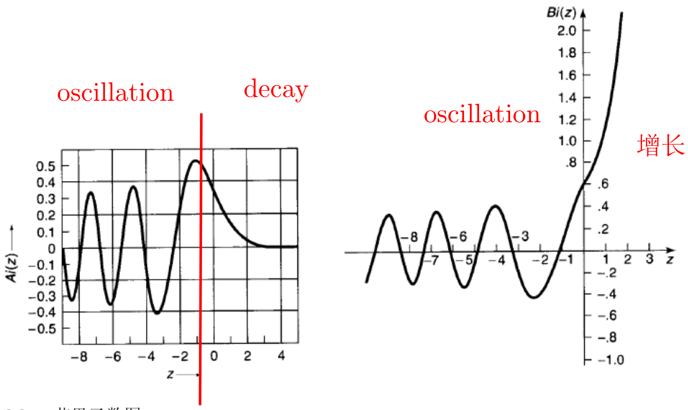


图 8.8: 艾里函数图

通解为两个独立解的线性组合

$$\psi_p(x)=a\,A_i(\alpha x)+b\,B_i(\alpha x)\quad [8.37]$$

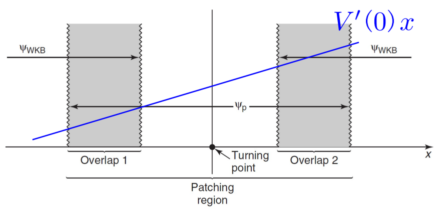


FIGURE 9: Patching region and the two overlap zones.

重叠区域不能距离turning point太近，保证ψ_{WKB}比较符合。也不能太远，保证ψ_p 比较符合

在重叠区域内，用ψ_p分别和两侧的ψ_{WKB}匹配，

在overlap 2 内（右侧$E<V$,非经典区域）

$$\psi_{\mathrm{WKB}}^{(2)}=\frac{D}{\sqrt{|p(x)|}}e^{-\frac{i}{\hbar}\int_0^x|p(x')|\mathrm{d}x'}$$

where $p(x) \cong \sqrt{2m[E-(E+V'(0)x)]} = \hbar\alpha^{\frac{3}{2}}\sqrt{-x}$

$$\int_0^x |p(x')|\,\mathrm{d}x' = \hbar\alpha^{\frac{3}{2}}\int_0^x \sqrt{x'}\,\mathrm{d}x' = \frac{2}{3}\hbar(\alpha x)^{\frac{3}{2}} \quad \left(\text{这里取}\left|i\hbar\alpha^{\frac{3}{2}}\sqrt{x}\right|\text{的模长}\right)$$

$$\Rightarrow \psi_{\mathrm{WKB}}^{(2)} = \frac{D}{\sqrt{\hbar\alpha^{\frac{3}{2}}\sqrt{x}}}e^{-\frac{2}{3}(\alpha x)^{\frac{3}{2}}} \quad [8.39] \left(\text{WKB方程的线性化解，有个}\frac{2}{3}\text{作为常数放进了}D\right)$$

Meanwhile, using the fomula for ψ_p，代入$\psi_p(\alpha x) = \frac{a}{2\sqrt{\pi}(\alpha x)^{\frac{1}{4}}}e^{-\frac{2}{3}(\alpha x)^{\frac{3}{2}}} + \frac{b}{2\sqrt{\pi}(\alpha x)^{\frac{1}{4}}}e^{\frac{2}{3}(\alpha x)^{\frac{3}{2}}}$

Differential Equation: $\quad \frac{d^2y}{dz^2} = zy.$

Solutions: Linear combinations of Airy Functions, $Ai(z)$ and $Bi(z)$.

Integral Representation:

$$Ai(z) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{s^3}{3}+sz\right)ds$$

$$Bi(z) = \frac{1}{\pi}\int_0^\infty \left[e^{-\frac{s^3}{3}+sz} + \sin\left(\frac{s^3}{3}+sz\right)\right]ds$$

Asymptotic Forms:

$$\left.\begin{aligned} Ai(z) &\sim \frac{1}{2\sqrt{\pi}\,z^{1/4}}e^{-\frac{2}{3}z^{3/2}} \\ Bi(z) &\sim \frac{1}{\sqrt{\pi}\,z^{1/4}}e^{\frac{2}{3}z^{3/2}} \end{aligned}\right\} z \gg 0 \qquad \left.\begin{aligned} Ai(z) &\sim \frac{1}{\sqrt{\pi}(-z)^{1/4}}\sin\left[\frac{2}{3}(-z)^{3/2}+\frac{\pi}{4}\right] \\ Bi(z) &\sim \frac{1}{\sqrt{\pi}(-z)^{1/4}}\cos\left[\frac{2}{3}(-z)^{3/2}+\frac{\pi}{4}\right] \end{aligned}\right\} z \ll 0$$

对比
$$\begin{aligned} \psi_{\mathrm{WKB}}^{(2)} &= \frac{D}{\sqrt{\hbar\alpha^{\frac{3}{2}}\sqrt{x}}}e^{-\frac{2}{3}(\alpha x)^{\frac{3}{2}}} \\ \psi_p(\alpha x) &= \frac{a}{2\sqrt{\pi}(\alpha x)^{\frac{1}{4}}}e^{-\frac{2}{3}(\alpha x)^{\frac{3}{2}}} + \frac{b}{2\sqrt{\pi}(\alpha x)^{\frac{1}{4}}}e^{\frac{2}{3}(\alpha x)^{\frac{3}{2}}} \end{aligned}, \Rightarrow \begin{aligned} &b=0 \\ &\frac{a}{2\sqrt{\pi}(\alpha x)^{\frac{1}{4}}} = \frac{D}{\sqrt{\hbar\alpha^{\frac{3}{2}}\sqrt{x}}} \end{aligned} \Rightarrow a = D\sqrt{\frac{4\pi}{\alpha\hbar}}$$

For overlap 1 内(左侧$E>V$,经典区域 $x<0$ $z\ll 0$)

[8.31]$\Rightarrow$ $\int_x^0 p(x')\,\mathrm{d}x' = \int \hbar\alpha^{\frac{3}{2}}\sqrt{-x}\,\mathrm{d}x = \frac{2}{3}\hbar(-\alpha x)^{\frac{3}{2}}$

WKB波函数：$\psi(x) \cong \frac{1}{\sqrt{\hbar}\alpha^{\frac{3}{4}}(-x)^{\frac{1}{4}}}\left[Be^{i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}} + Ce^{-i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}}\right]$ [8.43]

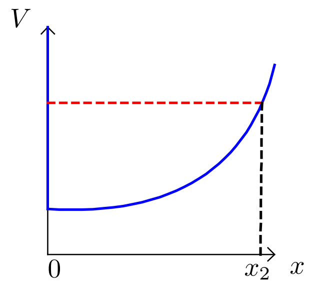
using the asymptotic form of the Airy function for $z\ll 0$, 利用 $\sin x = \frac{1}{2i}(e^{ix}-e^{-ix})$

通过比较
$$\frac{a\cdot e^{i\frac{\pi}{4}}}{\sqrt{\pi}(-\alpha x)^{\frac{1}{4}}2i}\sin\left[\frac{2}{3}(-\alpha x)^{\frac{3}{2}}+\frac{\pi}{4}\right] = \frac{a\cdot e^{i\frac{\pi}{4}}}{\sqrt{\pi}(-\alpha x)^{\frac{1}{4}}2i}\left[e^{i\pi/4}e^{i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}} - e^{-i\pi/4}e^{-i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}}\right]$$
$$\psi_{\mathrm{WKB}} = \frac{1}{\sqrt{\hbar}\alpha^{\frac{3}{4}}(-x)^{\frac{1}{4}}}\left[Be^{i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}} + Ce^{-i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}}\right]$$

$B = \frac{\sqrt{\hbar\alpha}}{2i\sqrt{\pi}}e^{i\frac{\pi}{4}}\cdot D\sqrt{\frac{4\pi}{\alpha\hbar}} = -i\,e^{i\frac{\pi}{4}}D \qquad C = i\,e^{-i\frac{\pi}{4}}D$

$$\psi(x) \cong \left\{\begin{aligned} &\frac{2D}{\sqrt{p(x)}}\sin\left[\frac{1}{\hbar}\int_x^{x_2}p(x')\,\mathrm{d}x' + \frac{\pi}{4}\right], x<x_2 \\ &\frac{D}{\sqrt{|p(x)|}}\exp\left[-\frac{1}{\hbar}\int_{x_2}^x|p(x')|\,\mathrm{d}x'\right], x>x_2 \end{aligned}\right\} \quad [8.46]$$

例 8.3. Potential wall with one vertical wall



$$V(x) = \left\{ \begin{array}{cc} \frac{1}{2}m\omega^2 x^2 & , \ x>0 \\ \infty & , \ x<0 \end{array} \right\}$$

step 1: find turning point $E = \frac{1}{2}m\omega^2 x_2^2$, $x_2 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}$

step 2: 求 $p(x)$ $p(x) = \sqrt{2m(E-V)} = \sqrt{2m\frac{1}{2}m\omega^2(x_2^2 - x^2)} = m\omega\sqrt{x_2^2 - x^2}$

step 3: 量子化条件 $\int_0^a p(x')\,\mathrm{d}x' = \left(n - \frac{1}{4}\right)\pi\hbar$

$$\Rightarrow \int_0^{x_2} p(x')\,\mathrm{d}x' = m\omega\int_0^{x_2}\sqrt{x_2^2 - x^2}\,\mathrm{d}x = m\omega\frac{\pi}{4}x_2^2 = m\omega\,\frac{\pi}{4}\left(\frac{2E}{m\omega^2}\right) = \left(n - \frac{1}{4}\right)\pi\hbar$$

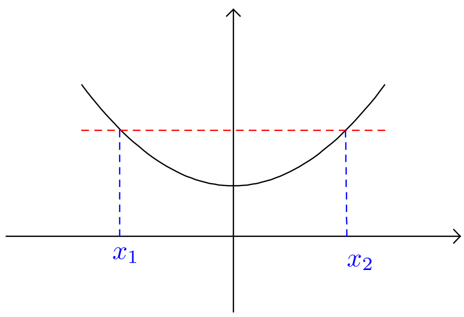
$$\frac{\pi}{2}\frac{E}{\omega} = \left(n - \frac{1}{4}\right)\pi\hbar \Rightarrow E_n = \left(2n - \frac{1}{2}\right)\hbar\omega \qquad n = 1, 2, \ldots$$

$$\{E_n\} = \left\{\frac{3}{2}\hbar\omega, \frac{7}{2}\hbar\omega, \frac{11}{2}\hbar\omega, \ldots\right\}$$

而对于完整的harmonic oscillator

$$\{E_n\} = \left\{\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \ldots\right\}$$

Example 8.4. Potential well with no vertical wall 无垂直墙势阱



$$E = \frac{1}{2}m\omega^2 x_1^2 = \frac{1}{2}m\omega^2 x_2^2 \Rightarrow -x_1 = x_2 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}$$

我们以前已经解决了x_2的问题（线性化时斜率为正），Problem 8.9考虑关于x_1的问题.

解Problem 8.9 有

$$\psi(x) \cong \left\{ \begin{array}{ccc} \frac{D'}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_x^{x_1}|p(x')|\,\mathrm{d}x'} & , & x < x_1 \\ \frac{2D'}{\sqrt{|p(x)|}} \sin\left[\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,\mathrm{d}x' + \frac{\pi}{4}\right] & , & x > x_1 \\ \text{This part should be equivalent to} & [8.46] & \text{for } x < x_2 \end{array} \right\}$$

由[8.46]

$$\psi(x)_{\text{in}}=\frac{2D}{\sqrt{|p(x)|}}\sin\theta_2(x)\quad \theta_2(x)=\frac{1}{\hbar}\int_x^{x_2}p(x')\,\mathrm{d}x'+\frac{\pi}{4}$$

由[8.50]

$$\psi_{\text{in}}=\frac{-2D'}{\sqrt{p(x)}}\sin\theta_1(x)\quad \theta_1(x)=-\frac{1}{\hbar}\int_{x_1}^{x}p(x')\,\mathrm{d}x'-\frac{\pi}{4}$$

内部可有由这两个函数任一表示，所以二者的角度只能相差π的整数倍 $\theta_2=\theta_1+n\pi$（产生的符号可以吸收到因子D里）

$$\int_{x_1}^{x_2}p(x')\,\mathrm{d}x'=n\pi-\frac{\pi}{2}=\left(n-\frac{1}{2}\right)\pi\hbar$$

$$\int_{-x_2}^{x_2}p(x')\,\mathrm{d}x=2m\omega\int_0^{x_2}\sqrt{x_2^2-x^2}\,\mathrm{d}x=\frac{\pi}{2}x_2^2=\frac{\pi}{2}\frac{2E}{\omega}$$

$$\begin{aligned}E_n &= \left(n-\frac{1}{2}\right)\hbar\omega \qquad n=1,2,3,\ldots\\ &= \frac{1}{2}\hbar\omega,\frac{3}{2}\hbar\omega,\ldots\end{aligned}$$

期中复习课

一、Preliminary（基础知识）

1. Infinite square well $E=\frac{(n\pi\hbar)^2}{2ma^2}$ $\quad\psi_n=\sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x$

2. Harmonic oscillator （谐振子）

   $a_\pm=\frac{1}{\sqrt{2\hbar m\omega}}(\mp ip+m\omega x)$ $\qquad\langle n|x|n'\rangle=\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n'}\delta_{n,n'-1}+\sqrt{n}\delta_{n',n-1}\right)$

   $a_+|n>=\sqrt{n+1}|n+1>$ $\qquad a_-|n>=\sqrt{n}|n-1>$

   $x=\sqrt{\frac{\hbar}{2m\omega}}(a_++a_-)$ $\qquad p=i\sqrt{\frac{\hbar m\omega}{2}}(a_+-a_-)$ [2.69]

   $[x,p]=i\hbar$

   $\psi_0(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}e^{-\frac{m\omega}{\pi\hbar}x^2}$[2.59] 基态波函数

   $\psi_n(x)=\frac{1}{\sqrt{n!}}(a_+)^n\psi_0(x)$

3. Hydrogen atom

   $E_n=-\left[\frac{m}{2\hbar^2}\left(\frac{e}{4\pi\varepsilon_0}\right)^2\right]\frac{1}{n^2}=\frac{E_1}{n^2}$ $\quad E_1=-13.6\text{eV}$ $\qquad\psi_{100}(r,\theta,\phi)=\frac{1}{\sqrt{\pi a^3}}e^{-\frac{r}{a}}$[4.80]基态波函数

   氢原子半径$a=\frac{4\pi\varepsilon_0\hbar^2}{me^2}\approx0.529\mathring{\text{A}}$

   角动量算符与氢原子态函数$\vec{L}^2|nlm>=\hbar^2l(l+1)|nlm>$ $\quad L_Z|nlm>=\hbar m|nlm>$

4. Angular momentum

   对于轨道角动量，由经典与量子相对应：$\begin{matrix}\vec{L}=\vec{r}\times\vec{p}\\ [x,p]=i\hbar\end{matrix}\Rightarrow\begin{matrix}[L_x,L_y]=i\hbar Lz\\ [L_y,L_z]=i\hbar Lx\\ [L_z,L_x]=i\hbar Ly\end{matrix}$

对于自旋角动量，仅由 $\begin{array}{l}[S_x, S_y] = i\hbar Sz\\ [S_y, S_z] = i\hbar Sx\\ [S_z, S_x] = i\hbar Sy\end{array}$ 定义

5. δ function

$$\delta(ax) = \frac{1}{a}\delta(x) \qquad \int_{-\infty}^{\infty}\delta(x) = 1 \qquad \int f(x)\,\delta(x - x_0) = f(x_0)$$

6. Varial theorem

$$\text{1D:} \quad 2\langle T\rangle = \left\langle x\frac{\mathrm{d}V}{\mathrm{d}x}\right\rangle \qquad \text{3D:} \quad 2\langle T\rangle = \langle \vec{r}\cdot\nabla V\rangle$$

二、Review of Chapter 6 **Purterbation Theory**

1. how [6.7] [6.8] are deprived?

$$\left\{\begin{array}{c} H^{(0)}\psi_n^{(1)} + H'\psi_n^{(0)} = E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)} \\ H^{(0)}\psi_n^{(2)} + H'\psi_n^{(1)} = E_n^{(0)}\psi_n^{(2)} + E_n^{(1)}\psi_n^{(1)} + E_n^{(2)}\psi_n^{(0)} \end{array}\right\}$$

Assumption $\begin{array}{c} E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \\ \psi_n = \psi^{(0)} + \lambda\psi_n^{(1)} + \cdots \end{array}$

2.

$$\Rightarrow \left\{\begin{array}{c} E_n^{(1)} = \langle\psi_n^0|H'|\psi_n^0\rangle \\ \psi_n^{(1)} = \sum_{m\neq n}\frac{\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}\psi_m^0 \\ E_n^{(2)} = \sum_{m\neq n}\frac{|\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}} \end{array}\right\}$$

3. Theorem P260 $[A, H^{(0)}] = 0$ $[A, \mathrm{H}'] = 0$,则$A\psi_\mu = \mu\psi_\mu, A\psi_\gamma = \gamma\psi_\gamma$(即使存在简并的态，仍然可以使用非简并的近似方法，因为W中的非零元素全在对角上。

需要会推导的对易关系

$$[H^0, L^2] = 0, \quad [H^{(0)}, L_z] = 0 \quad [p^4, L^2] = 0 \quad [p^4, L_z] = 0$$

$$[\vec{S}\cdot\vec{L}, \vec{L}] \neq 0 \quad [\vec{S}\cdot\vec{L}, \vec{S}] \neq 0 \quad [\vec{S}\cdot\vec{L}, \vec{J}] = 0 \quad [\vec{S}\cdot\vec{L}, L^2] = 0$$

4. 2×2 Matrix $= c_0\sigma_0 + c_x\sigma_x + c_y\sigma_y + c_z\sigma_z$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

5. $H = \begin{bmatrix} w_{aa} & w_{ab} \\ w_{ba} & w_{ba} \end{bmatrix} \Rightarrow \text{eigen value} = c_0 \pm \sqrt{c_x^2 + c_y^2 + c_z^2} = \frac{w_{aa} + w_{bb}}{2} \pm \sqrt{\left(\frac{w_{aa} - w_{bb}}{2}\right)^2 + w_{ba}\cdot w_{ab}}$

$$\psi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}, \psi_- = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} = \begin{pmatrix} \sin\frac{\theta}{2}e^{-i\phi} \\ -\cos\frac{\theta}{2} \end{pmatrix}$$

$$\cos\theta = \frac{\frac{w_{aa} - w_{bb}}{2}}{\sqrt{\left(\frac{w_{aa} - w_{bb}}{2}\right)^2 + w_{ab}w_{ba}}} \qquad w_{ab} = |w_{ab}|e^{i\phi}$$

6. some hierarchy of Hydrogen atom

Bohr	$\alpha^2 mc^2$
Fine structure	$\alpha^4 mc^2$
lamb shift (兰姆位移)	$\alpha^5 mc^2$
Hyper fine splitting 超精细结构	$\left(\frac{m}{m_p}\right)\alpha^4 mc^2$

7. $$\alpha \equiv \frac{e^2}{4\pi\varepsilon_0 \hbar c} \approx \frac{1}{137}$$

8. Fine Structure = spinless Relativistic相对论效应 $+\vec{S}\cdot\vec{L}$ 自旋轨道耦合

9. Dirac equation

10. ...

Chapter 9 含时微扰论

$$\text{含时薛定谔方程} H(r,t)\Psi(r,t) = i\hbar\frac{\partial}{\partial t}\Psi(r,t)$$

where $H(r,t) = -\frac{\hbar^2}{2m}\nabla^2 + V(r,t)$ 含时， 如果$V(r,t)$如果没有与 t 相关的量， 则还能转换为非含时解。

我们可以对$\Psi(r,t)$进行分离变量，即$\Psi(\vec{r},t) = \psi(\vec{r})\varphi(t) \rightarrow \left\{\begin{array}{c} \frac{\partial}{\partial t}\Psi = \psi(r)\frac{\partial\varphi}{\partial t} \\ \nabla^2\Psi = (\nabla^2\psi)\varphi \end{array}\right\}$

$$\Rightarrow -\frac{\hbar^2}{2m}(\nabla^2\psi)\varphi + V\psi\varphi = i\hbar\psi\frac{\partial\varphi}{\partial t}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{1}{\psi}(\nabla^2\psi) + V = i\hbar\frac{1}{\varphi}\frac{\partial\varphi}{\partial t} = \text{Constant} = E$$

$$\Rightarrow \left\{\begin{array}{ccc} \frac{1}{\varphi}\frac{\mathrm{d}\varphi}{\mathrm{d}t} = -i\frac{E}{\hbar} & \Rightarrow & \varphi = \varphi(0)e^{-i\frac{E}{\hbar}t} \\ -\frac{\hbar^2}{2m}\frac{1}{\psi}(\nabla^2\psi) = E & \Rightarrow & \text{非简并微扰论} \end{array}\right\}$$

Wave function $\Psi(\vec{r},t) = \sum_n C_n\psi_n(\vec{r})e^{-\frac{iE_nt}{\hbar}}$,C_n归一化系数 (where $H\varphi_n(r) = E_n\psi_n(r)$)

$\psi(0) = C_1\begin{pmatrix}1\\0\end{pmatrix} + C_2\begin{pmatrix}0\\1\end{pmatrix}$,and $V(r)$ has no time independent,

find $\Psi(t) = C_1\begin{pmatrix}1\\0\end{pmatrix}e^{-iE_1t/\hbar} + C_2\begin{pmatrix}0\\1\end{pmatrix}e^{-iE_2t/\hbar}$ E_1, E_2为H的本征值

如果$V(r,t)$ has a weak time dependent, 可以看作微扰计算能量。

9.1 二能级系统

未微扰时

$$H^{(0)}\psi_a = E_a\psi_a \qquad H^{(0)}\psi_b = E_b\psi_b \qquad \langle\psi_a|\psi_b\rangle = \delta_{ab}$$

s任意波函数可以表现为这两个态的线性叠加：$\Psi(t=0)=C_a\psi_a+C_b\psi_b$

含时解$\Psi(t)=C_a\psi_a e^{-iE_at/\hbar}+C_b\psi_b e^{-iE_bt/\hbar}$ $(\|C_a\|^2+\|C_b\|^2=1)$ C_a,C_b目前不含时。

9.1.1 Perturbation 微扰

$H'(t)$ time-dependent,假设$\Psi(\vec{r},t)=C_a(t)\,\psi_a e^{-iE_at/\hbar}+C_b(t)\,\psi_b e^{-iE_bt/\hbar}$ (需要解出$C_a(t)$和$C_b(t)$)

将$\Psi(r,t)$代入$H\Psi(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\Psi(r,t)$ $(H=H^{(0)}+H'(t))$

$$\begin{aligned}
\text{左边}H\Psi(\vec{r},t) &= [H^{(0)}+H'(t)][C_a(t)\,\psi_a e^{-iE_at/\hbar}+C_b(t)\,\psi_b e^{-iE_bt/\hbar}]\\
&= H'[C_a(t)\,\psi_a e^{-iE_at/\hbar}+C_b(t)\,\psi_b e^{-iE_bt/\hbar}]\\
&\quad +E_aC_a(t)\,e^{-iE_at/\hbar}+E_bC_b(t)\,e^{-iE_bt/\hbar}\\
\text{右边}i\hbar\frac{\partial}{\partial t}\Psi(r,t) &= i\hbar\left[\frac{\partial C_a(t)}{\partial t}\psi_a e^{-iE_at/\hbar}+\frac{\partial C_b(t)}{\partial t}\psi_b e^{-iE_bt/\hbar}\right]\\
&\quad +i\hbar\left[C_a(t)\,\psi_a e^{-iE_at/\hbar}\times\left(-i\frac{E_a}{\hbar}\right)+C_b(t)\,\psi_b e^{-iE_bt/\hbar}\left(-i\frac{E_b}{\hbar}\right)\right]\\
&= i\hbar[\dot{C}_a\psi_a e^{-iE_at/\hbar}+\dot{C}_b\psi_b e^{-iE_bt/\hbar}]\\
&\quad +E_aC_a(t)\,\psi_a e^{-iE_at/\hbar}+E_bC_b(t)\,\psi_b e^{-iE_bt/\hbar}
\end{aligned}$$

$$\Rightarrow H'[C_a(t)\,\psi_a e^{-iE_at/\hbar}+C_b(t)\,\psi_b e^{-iE_bt/\hbar}]=i\hbar[\dot{C}_a\psi_a e^{-iE_at/\hbar}+\dot{C}_b\psi_b e^{-iE_bt/\hbar}]$$

[Trick]: 左乘$<\psi_a|$

$$C_a\langle\psi_a|H'|\psi_a\rangle e^{-iE_at/\hbar}+C_b\langle\psi_a|H'|\psi_b\rangle e^{-iE_bt/\hbar}=i\hbar[\dot{C}_a\langle\psi_a|\psi_a\rangle e^{-iE_at/\hbar}+\dot{C}_b\langle\psi_a|\psi_b\rangle e^{-iE_bt/\hbar}]$$

$$C_a\langle\psi_a|H'|\psi_a\rangle e^{-iE_at/\hbar}+C_b\langle\psi_a|H'|\psi_b\rangle e^{-iE_bt/\hbar}=i\hbar\dot{C}_a e^{-iE_at/\hbar}$$

define $H_{ij}=\langle\psi_i|H'(t)|\psi_j\rangle$

$$C_aH'_{aa}e^{-iE_at/\hbar}+C_bH'_{ab}e^{-iE_bt/\hbar}=i\hbar\dot{C}_a e^{-iE_at/\hbar}$$

左右同乘以$-\frac{i}{\hbar}e^{-iE_at/\hbar}$：

$$\dot{C}_a=-\frac{i}{\hbar}[C_aH'_{aa}+C_bH'_{ab}e^{-i(E_b-E_a)t/\hbar}]$$

同理，

$$\dot{C}_b=-\frac{i}{\hbar}[C_bH'_{bb}+C_aH'_{ba}e^{-i(E_a-E_b)t/\hbar}]$$

[Approximation]: $H'_{aa}=H'_{bb}=0$ $\Leftarrow(H'\sim\overrightarrow{E(t)}\cdot\vec{r})$类似于电磁场中的什么？？

$$\left\{\begin{array}{c}\dot{C}_a=-\frac{i}{\hbar}H'_{ab}e^{-i(E_b-E_a)t/\hbar}C_b\\ \dot{C}_b=-\frac{i}{\hbar}H'_{ba}e^{i(E_b-E_a)t/\hbar}C_a\end{array}\right\}\Longrightarrow\left\{\begin{array}{c}\dot{C}_a=-\frac{i}{\hbar}H'_{ab}e^{-i\omega_0t}C_b\\ \dot{C}_b=-\frac{i}{\hbar}H'_{ba}e^{i\omega_0t}C_a\end{array}\right\}[9.13]$$

其中$\omega_0\equiv\frac{E_b-E_a}{\hbar}$

E_b

不妨设 $E_b>E_a$ E_a ,此时并未引入任何微扰。

9.1.2 Time-dependent Pertunbation 含时微扰

Initial conditions $C_a(t=0)=1$, $C_b(t=0)=0$

存在微扰的情况下：

零阶：$C_a^{(0)}=1,\ C_b^{(0)}=0,$

一阶情形时： 由[9.13] $\dot{C}_a=-\frac{i}{\hbar}H_{ab}^{'}e^{-i\omega_0 t}C_b$ （代入$C_b^{(0)}=0$）$\Rightarrow \frac{\mathrm{d}C_a^{(1)}}{\mathrm{d}t}=0\Rightarrow C_a^{(1)}=C_a^{(0)}=1$

而$\dot{C}_b=-\frac{i}{\hbar}H_{ba}^{'}e^{i\omega_0 t}C_a,\quad \mathrm{d}C_b^{(1)}=-\frac{i}{\hbar}H_{ba}^{'}e^{i\omega_0 t}C_a\mathrm{d}t\Rightarrow C_b^{(1)}(t)-C_b^{(1)}(t=0)=-\frac{i}{\hbar}\int_0^t\mathrm{d}t'H_{ba}^{'}(t')e^{i\omega_0 t'}$

$\Rightarrow C_b^{(1)}(t)=-\frac{i}{\hbar}\int_0^t\mathrm{d}t'\,H_{ba}^{'}(t)\,e^{i\omega_0 t'}$[9.17]

二阶：$\dot{C}_a^{(2)}=-\frac{i}{\hbar}H_{ab}^{'}e^{i\omega_0 t}C_b^{(1)}=-\frac{i}{\hbar}e^{i\omega_0 t}\left(-\frac{i}{\hbar}\int_0^t\mathrm{d}t'H_{ba}^{'}e^{i\omega_0 t'}\right)$ 同理$\dot{C}_a^{(2)}=\frac{\mathrm{d}C_a^{(2)}}{\mathrm{d}t}$

$C_a^{(2)}=\int_0^t-\frac{1}{\hbar^2}\mathrm{d}t'\,H_{ab}^{'}(t)\,e^{-i\omega_0 t'}\int_0^{t'}\mathrm{d}t''\,H_{ba}^{'}e^{i\omega_0 t'}+C_a^2(0)$

9.1.3 正弦微扰

$$H'(r,t)=V(\vec{r})\,\cos\omega t$$

So that $H_{ab}^{'}(t)=\langle\psi_a(\vec{r})\,|\,H'(r,t)\,|\,\psi_b(\vec{r})\rangle$

$$\Rightarrow H_{ab}^{'}(t)=\langle\psi_a\,|\,V(r)\,|\,\psi_b\rangle\cos\omega t=V_{ab}\cos\omega t=V_{ab}\frac{(e^{i\omega t}+e^{-i\omega t})}{2}$$

from 9.17 $\Rightarrow C_b^{(1)}(t)\cong-\frac{i}{\hbar}\int_0^t\mathrm{d}t'V_{ba}\cos(\omega t)\,e^{i\omega_0 t}=-\frac{i}{2\hbar}V_{ba}\int_0^t\mathrm{d}t'\,(e^{i\omega t}+e^{-i\omega t})\,e^{i\omega_0 t}$

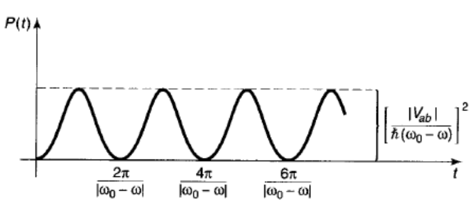
$$C_b^{(1)}(t)=-\frac{i}{2\hbar}V_{ba}\frac{1}{i(\omega+\omega_0)}e^{i(\omega+\omega_0)t'}\Big|_0^t+\frac{1}{i(\omega-\omega_0)}e^{i(\omega+\omega_0)t'}\Big|_0^t$$

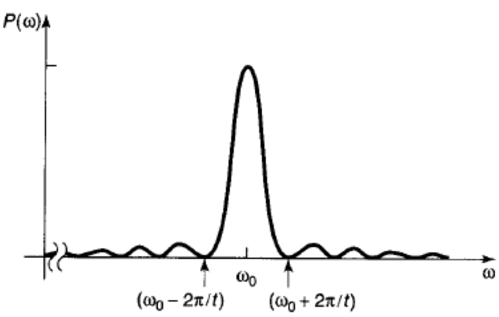
近似：$\omega\sim\omega_0\Rightarrow\omega+\omega_0\gg|\omega-\omega_0|$，可以舍去第一项。

$$\begin{aligned}C_b^{(0)}(t)&\approx-\frac{V_{ba}}{2\hbar}\frac{e^{i(\omega_0-\omega)t}-1}{\omega_0-\omega}\\ \text{跃迁系数}&=-\frac{V_{ba}}{2\hbar}\frac{e^{i(\omega_0-\omega)t/2}}{\omega_0-\omega}\underbrace{[e^{i(\omega_0-\omega)t/2}-e^{-i(\omega_0-\omega)t/2}]}_{2i\sin\frac{(\omega_0-\omega)t}{2}}\\ &=i\frac{V_{ba}}{\hbar}\frac{e^{i(\omega_0-\omega)t/2}}{\omega_0-\omega}\sin\frac{(\omega_0-\omega)t}{2}\end{aligned}$$

$$\text{跃迁概率：}\lim_{x\to0}P(t)=\frac{|V_{ab}^2|}{\hbar^2}\frac{\sin^2\left[\frac{(\omega_0-\omega)t}{2}\right]}{(\omega_0-\omega)^2}\ [9.28]$$

令$\omega_0-\omega=x,\frac{t}{2}=a\ \lim_{x\to0}\frac{\sin^2(ax)}{x^2}=a^2=\frac{t^2}{4}\quad\Longrightarrow P=\left|\frac{V_{ab}^2}{\hbar^2}\right|\frac{t^2}{4}.$





Problem 9.7 (Rotating-Wave approximation and Rabi oscillation)

9.2 Emission and Absorption of Radiation

9.2.1 电磁波

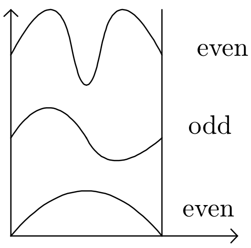
当电磁波波长很长(远大于原子尺度)，我们可以忽略场随空间变化：即粒子处在正弦震荡的电场中

$$E = E_0 \cos\omega t\, \hat{k} \quad (\hat{k}\text{为微扰方向，微扰大小为}H'(t) = -qE_0 z\, \boldsymbol{\cos\omega t}\ \text{Time dependent})$$

Then $H'_{\rm bc} = \langle \psi_b \,|\, H'(t) \,|\, \psi_a \rangle$,其中ψ_a, ψ_b为未微扰时的波函数

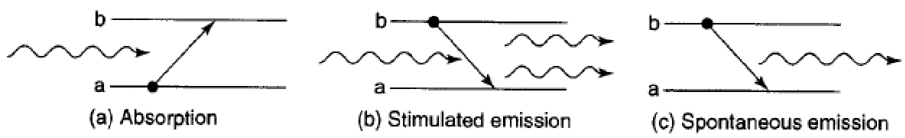
$$\begin{aligned} H'_{ba} &= \langle \psi_b \,|\, H'(t) \,|\, \psi_a \rangle \\ &= -qE_0 \langle \psi_b \,|\, \hat{z} \,|\, \psi_a \rangle \cos\omega t \\ &= -\mathcal{R} E_0 \cos\omega t \\ \text{其中}\quad , &\quad \mathcal{R} \equiv q \langle \psi_b \,|\, z \,|\, \psi_a \rangle \end{aligned}$$

infinite wall



而$z\,|\,\psi\,|^2$为奇函数， 对空间积分为0。 即满足H'的对角元矩阵元为0的通常假设。 而对应非对角元有：$V_{ba} = -\mathcal{R} E_0$

9.2.2 吸收、受激辐射、自发辐射



由[9.28]在正弦微扰下，跃迁几率为

$$P_{a\to b}(t) = |\,c_b(t)\,|^2 \cong \frac{|V_{ab}|^2}{\hbar^2} \frac{\sin^2[(\omega_0 - \omega)t/2]}{(\omega_0 - \omega)^2} = \left(\frac{|\mathcal{R}|E_0}{\hbar}\right)^2 \frac{\sin^2[(\omega_0 - \omega)t/2]}{(\omega_0 - \omega)^2}$$

a) Absorption

   the probability of a transition from "low" state to the high "state"

   $\Rightarrow P_{b\to a}(t) = \left(\frac{|\mathcal{R}|E_0}{\hbar}\right)^2 \frac{\sin^2[(\omega_0 - \omega)t/2]}{(\omega_0 - \omega)^2}$ [9.36]

   注意，此时吸收一个光子，但光仍看作经典光（光子属于量子电动力学）

b) Stimulated emission

   We can solve Eq[9.13] using the initial conditions $c_a(t=0) = 0 \quad c_b(t=0) = 1$,

   then $P_{b\to a}(t) = |\,c_a(t)\,|^2 = [9.28]$ predicted by Einstein

   Laser:通过受激辐射发射出来的光。

c) Spontaneous Emission

   no need external perturbation

9.2.3 Incoherent pertubation 非相干微扰

相干	coherent	$\lvert\psi_a+\psi_b\rvert^2=\lvert\psi_a\rvert^2+\lvert\psi_b\rvert^2+\boldsymbol{\psi_1^*\psi_2+\psi_2^*\psi_1}$ **(Interference)**
非相干	incoherent	$\lvert\psi_1\rvert^2+\lvert\psi_2\rvert^2$

We need a distribution of light as a function of frequency consider the energy density of the EM field.

$$u=\frac{\varepsilon_0}{2}E_0^2$$

E_0是电场的振幅。而跃迁概率于场的能量密度成正比。$P_{b\to a}(t)=\frac{2u}{\varepsilon_0\hbar^2}\lvert\mathcal{R}\rvert^2\frac{\sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2}$

上式只对单一频率ω的单色光成立。实际上很多体系处于一个有完整频谱的电磁波场中，此时 $u\to\rho(\omega)\mathrm{d}\omega$,$\rho(\omega)\mathrm{d}\omega$为频率在$\mathrm{d}\omega$范围时的能量密度。

$$P_{b\to a}(t)=\frac{2\lvert\mathcal{R}\rvert^2}{\hbar^2\varepsilon_0}\int\mathrm{d}\omega\rho(\omega)\frac{\sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2}$$

[Approximation]:$\frac{\sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2}$ 有类似于δ函数类似的性质，因此 $\rho(\omega)\to\rho(\omega_0)$ $\quad\hbar\omega_0=E_a-E_b$

$$P_{b\to a}(t)=\frac{2\lvert\mathcal{R}\rvert^2}{\hbar^2\varepsilon_0}\rho(\omega_0)\int_0^\infty\mathrm{d}\omega\frac{\sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2}$$

关于积分

令$x=\frac{\omega_0-\omega}{2}t\Rightarrow\left\{\begin{array}{l}\mathrm{d}\omega=-\frac{2}{t}\mathrm{d}x\\ \omega_0-\omega=\frac{2x}{t}\end{array}\right\}$,并把积分上下限拓展为$x\equiv\pm\infty$(在额外的区域内积分基本为0)

$$\int_0^\infty\mathrm{d}\omega\frac{\sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2}=\int_0^\infty\mathrm{d}x\left(-\frac{2}{t}\right)\frac{\sin^2x}{x^2\left(\frac{2}{t}\right)^2}=-\frac{t}{2}\int_{-\infty}^\infty\mathrm{d}x\left(\frac{\sin x}{x}\right)^2=\frac{\pi}{2}t$$

$\left(\int_{-\infty}^\infty\mathrm{d}x\left(\frac{\sin x}{x}\right)^2=\pi\right)$

$$\int_0^\infty\mathrm{d}\omega\frac{\sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2}=\frac{\pi}{2}t$$

$$P_{b\to a}(t)=\frac{2\lvert\mathcal{R}\rvert^2}{\hbar^2\varepsilon_0}\rho(\omega_0)\frac{\pi}{2}t=\frac{\pi\lvert\mathcal{R}\rvert^2}{\hbar^2\varepsilon_0}\rho(\omega_0)t$$

Transition Probability: $P_{b\to a}(t)=\frac{\pi\lvert\mathcal{R}\rvert^2}{\hbar^2\varepsilon_0}\rho(\omega_0)t$

跃迁速率$R_{b\to a}(t)\equiv\frac{\mathrm{d}P}{\mathrm{d}t}=\frac{\pi}{\varepsilon_0\hbar^2}\lvert\mathcal{R}\rvert^2\rho(\omega_0)$ [9.43] 跃迁速率为常数

到这里只考虑了y方向$\Rightarrow$拓展到所有方向,不同方向的入射光对场的能量$\rho(\omega)$的贡献相同，用$\lvert\vec{\mathcal{R}}\cdot\hat{n}\rvert^2$的平均值代替$\lvert\mathcal{R}\rvert^2$， 平均值是对所有极化和入射方向求平均。

$$\text{where }\boldsymbol{\mathcal{R}}\equiv q\langle\psi_b\lvert\boldsymbol{r}\rvert\psi_a\rangle$$

求取平均值的步骤：

选择球坐标系，使z轴沿着波的传播方向（极化方向在 $x-y$ 平面）矢量$\mathcal{R}$位于$y-z$平面

$$\hat{n}=\cos\phi\hat{i}+\sin\phi\hat{j}\qquad\boldsymbol{\mathcal{R}}=\mathcal{R}\sin\theta\hat{j}+\mathcal{R}\cos\theta\hat{k}\Longrightarrow\boldsymbol{\mathcal{R}}\cdot\hat{n}=\mathcal{R}\sin\theta\sin\phi$$

$$\lvert\boldsymbol{\mathcal{R}}\cdot\hat{n}\rvert_{\text{average}}=\frac{1}{4\pi}\int\lvert\boldsymbol{\mathcal{R}}\rvert^2\sin^2\theta\sin^2\phi\sin\theta\mathrm{d}\theta\mathrm{d}\phi=\frac{\lvert\mathcal{R}\rvert^2}{4\pi}\int_0^\pi\sin^3\theta\mathrm{d}\theta\int_0^{2\pi}\sin^2\phi\mathrm{d}\phi=\frac{1}{3}\lvert\boldsymbol{\mathcal{R}}\rvert^2$$

综上在所有方向入射的非相干，非极化光的作用下，从b态到a态受激发射的跃迁速率为

$$R_{b\to a}(t) \;=\; \frac{\pi}{3\varepsilon_0\hbar^2}|\mathcal{R}|^2\rho(\omega_0) \qquad [9.47]$$

Matrix element of the electric dipole moment

energy density at $\omega_0 = \dfrac{E_b - E_a}{\hbar}$

9.3 Spontaneous emission （自发辐射）

goal：To derive the transition rate of the spontaneous emission

9.3.1 Einstein's A and B coefficients爱因斯坦发射与吸收系数

$$R_{\substack{b\to a\\ a\to b}} = \frac{\pi}{3\varepsilon_0\hbar^3}|\mathcal{R}|^2\rho(\omega_0) \equiv B_{\substack{ba\\ ab}}\rho(\omega_0) \quad \text{Rate}$$

为 b 能级的粒子数随时间变化的速率。

$$\frac{\mathrm{d}N_b}{\mathrm{d}t} \;=\; \underbrace{-N_bA}_{\text{spontaneous}} \underbrace{- N_bB_{ba}\rho(\omega_0)}_{\text{stimulated}} + \underbrace{N_aB_{ab}\rho(\omega_0)}_{\text{Absorption}}$$

达到热力学平衡时（粒子数不发生变化）：$\frac{\mathrm{d}N_b}{\mathrm{d}t} = 0$

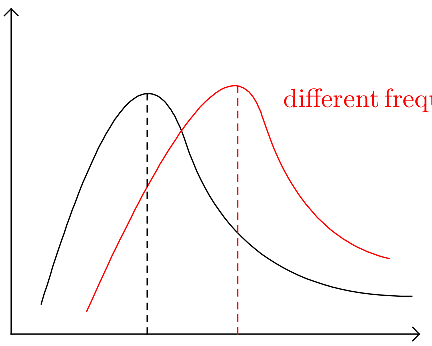
$$\Rightarrow N_bA = \rho(\omega_0)\,(N_aN_{ab} - N_bB_{ba})$$

$$\rho(\omega_0) = \frac{N_bA}{N_aB_{ab} - N_bB_{ba}} = \frac{A}{(N_a/N_b)\,B_{ab} - B_{ba}}$$

由统计力学，当处于温度T的热平衡时，能量E对应的粒子数与玻尔兹曼因子$\exp(-E/k_BT)$,成正比

$$\frac{N_a}{N_b} = \frac{e^{-E_a/k_bt}}{e^{-E_b/k_{\mathrm{B}t}}} = e^{\hbar\omega_0/k_Bt}$$

$$\rho(\omega_0) = \frac{A}{e^{\hbar\omega_0/k_BT}B_{ab} - B_{ba}}$$



Recall 普朗克黑体辐射公式$\rho(\omega) = \frac{\hbar}{\pi^2c^3}\frac{\omega_0^3}{e^{\hbar\omega/k_Bt} - 1}$

通过比较：$\rho(\omega) = \frac{\hbar}{\pi^2c^3}\frac{\omega_0^3}{e^{\hbar\omega/k_Bt} - 1}$ 与 $\rho(\omega_0) = \frac{A}{e^{\hbar\omega/k_BT}B_{ab} - B_{ba}}$ $\Rightarrow \left\{ \begin{array}{c} B_{ab} = B_{ba} \\ A = \frac{\omega_0^3\hbar}{\pi^2c^3}B_{ba} \end{array} \right\}$

$$\text{又因为}B_{ba} = \frac{\pi}{3\varepsilon_0\hbar^2}|\mathcal{R}|^2 \Rightarrow \text{自发发射速率}A = \frac{\omega_0^3\hbar}{\pi^2c^3}B_{ba} = \frac{\omega_0^3|\mathcal{R}|^2}{3\pi\varepsilon_0\hbar c^3} \quad [9.56]$$

9.3.2 Life time

$$\text{No radiation} \Rightarrow \text{only spontaneous emission}$$

$$\Rightarrow \frac{\mathrm{d}N_b}{\mathrm{d}t} = -AN_b \quad \Rightarrow \quad \frac{\mathrm{d}N_b}{N_b} = -A\mathrm{d}t$$

$$\Rightarrow N_b(t) = Ce^{-At} = N_b(0)\,e^{-At}$$

处于激发态的粒子数目按照指数减少，定义时间常数 $\tau = \frac{1}{A}$,为 life time.N_b 变为额原来的$\frac{1}{e}$倍。

$$\frac{1}{\tau} = \frac{1}{\tau_1} + \frac{1}{\tau_2} + \cdots \text{(许多种衰变方式)}$$

例. 1 电荷q 与弹簧链接，电荷沿着x轴方向震荡，设初始态$|n>$,通过自发衰减到态$|n'>$

$$\boldsymbol{\mathcal{R}} = q\langle n|x|n'\rangle\hat{i}$$

from [3.33] $\langle n|x|n'\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n'}\delta_{n,n'-1} + \sqrt{n}\delta_{n',n-1}\right)$

我们只考虑 $n' < n$时的情况

$$\vec{\mathcal{R}} = q\sqrt{\frac{n\hbar}{2m\omega}}\delta_{n',n-1}\hat{i} \text{ (即，只有}n' = n-1\text{时才能跃迁)}$$

跃迁速率：$A = \frac{\omega^2|\mathcal{R}|^2}{3\pi\varepsilon_0\hbar c^3} = \frac{\omega^3 q^2 n\hbar}{3\pi\varepsilon_0\hbar c^3 2m\omega} = \frac{nq^2\omega^2}{6\pi\varepsilon_0 mc^3}$, 第n阶定态寿命：$\tau_n = \frac{6\pi\varepsilon_0 mc^3}{nq^2\omega^2}$

辐射功率：$P = A\hbar\omega = \frac{nq^2\omega^2}{6\pi\varepsilon_0 mc^3}\hbar\omega = \frac{q^2\omega^2}{6\pi\varepsilon_0 mc^3}\left(E_n - \frac{1}{2}\hbar\omega\right)$, $\quad E_n = \left(\frac{1}{2} + n\right)\hbar\omega$

与经典相比较$P_{\text{classical}} = \frac{q^2\omega^2}{6\pi\varepsilon_0 mc^3}E$ （没有零能态）

而量子公式防止了基态辐射：如果$E = \frac{1}{2}\hbar\omega$, 振子不辐射。

9.3.3 Select Rules 选择定则

The calculation of spantaneous emission rate is about evalution $\langle\psi_b|\vec{r}|\psi_a\rangle$, most of them are Zero.

The **select rules** helps us to know which states can be coupled by light.

(选择定则告诉我们光能够把哪些能级耦合起来)

氢原子模型具有球对称性（哈密顿量只与 r 有关，与φ,θ无关）

$$H = -\frac{\hbar^2}{2m}\nabla - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$$

The matrix elements $\langle\psi_b|\underbrace{\vec{r}}_{\text{light}}|\psi_a\rangle \to \langle n'l'm'|(x,y,z)|nlm\rangle$(将$r$转换为$x,y,z$坐标进行后来的计算)

n principle $\ell \to \hat{L}^2, m \to \hat{L}_z$ Selection rules: involving m and m'

Selection Rules for m

Noted that $\hat{L}_z|nlm\rangle = \hbar m|nlm\rangle$

$$\vec{L} = \vec{r} \times \vec{p} \quad L_z = xP_y - yP_x$$

$$\begin{aligned}
[L_z, z] &= 0 \\
[L_z, x] &= [xP_y - yP_x, x] = -[yP_x, x] = i\hbar y \\
[L_z, y] &= [xP_y - yP_x, y] = [xP_y, y] = -i\hbar x
\end{aligned}$$

Using $0=[L_z,z]\Rightarrow$

$$\begin{aligned}\langle n'l'm'|0|nlm\rangle &= \langle n'l'm'|[L_z,z]|nlm\rangle\\ 0 &= \langle n'l'm'|L_z z - zL_z|nlm\rangle\\ 0 &= \langle n'l'm'|m' z - zm|nlm\rangle\\ 0 &= (m'-m)\langle z\rangle\end{aligned}$$

因此，除非$m=m'$, the matrix element of z is 0. 判断极化方向是否有 z 分量。

同理，Using$[L_z,x]=i\hbar y$ and $[L_z,y]=-i\hbar x$

$$\begin{aligned}\langle n'l'm'|[L_z,x]|nlm\rangle &= \langle n'l'm'|i\hbar y|nlm\rangle\\ \langle n'l'm'|L_z x - xL_z|nlm\rangle &= i\hbar\langle y\rangle\\ \hbar(m'-m)\langle x\rangle &= i\hbar\langle y\rangle\\ (m'-m)\langle x\rangle &= i\langle y\rangle\\ \text{同理}\qquad (m'-m)\langle y\rangle &= -i\langle x\rangle\end{aligned}$$

$$\Rightarrow (m'-m)^2\langle x\rangle=\langle x\rangle \qquad \text{and} \qquad (m'-m)^2\langle y\rangle=\langle y\rangle$$

$$\Rightarrow [(m'-m)^2-1]\left\langle \begin{matrix} x\\ \text{or}\\ y\end{matrix}\right\rangle=0$$

因此除非$m'=m\pm 1$, 否则不会有x,y分量上的辐射。

[Summary] Selection Rules for m

$$\Delta m=m'-m \qquad \text{no transition unless } \Delta m=\underset{z}{0},\ \underset{x,y}{\pm 1}$$

Selection Rules for l

Problem [9.12] $\Rightarrow$ $[L^2,[L^2,\hat{r}]]=2\hbar^2(\vec{r}L^2+L^2\vec{r})$

Sandwich it between $\langle n'l'm'|$ and $|nlm\rangle$

$$\begin{aligned}\langle n'l'm'|[L^2,[L^2,\hat{r}]]|nlm\rangle &= \langle n'l'm'|2\hbar^2(\vec{r}L^2+L^2\vec{r})|nlm\rangle\\ \langle n'l'm'|L^2[L^2,\hat{r}]-[L^2,\hat{r}]L^2|nlm\rangle &= 2\hbar^2\hbar^2[(\ell+1)\ell+(\ell'+1)\ell']\langle\vec{r}\rangle\\ \hbar^2[\ell'(\ell'+1)-\ell(\ell+1)]\langle[L^2,\hat{r}]\rangle &= 2\hbar^4[(\ell+1)\ell+(\ell'+1)\ell']\langle\vec{r}\rangle\\ \hbar^2[\ell'(\ell'+1)-\ell(\ell+1)]\langle L^2\hat{r}-\hat{r}L^2\rangle & \\ \hbar^4[\ell'(\ell'+1)-\ell(\ell+1)]^2\langle\hat{r}\rangle &= 2\hbar^4[(\ell+1)\ell+(\ell'+1)\ell']\langle\vec{r}\rangle\\ \{[\ell'(\ell'+1)-\ell(\ell+1)]^2-2[(\ell+1)\ell+(\ell'+1)\ell']\}\langle\hat{r}\rangle &= 0\end{aligned}$$

第一项

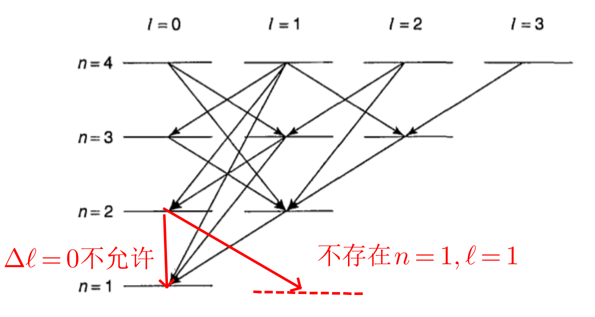
$$\begin{aligned}[\ell'(\ell'+1)-\ell(\ell+1)] &= \ell'(\ell'+1)+\ell'\ell-[\ell(\ell+1)+\ell'\ell]\\ &= \ell'(\ell'+1+\ell)-\ell(\ell+1+\ell')\\ &= (\ell'-\ell)(\ell'+\ell+1)\end{aligned}$$

第二项

$$\begin{aligned}2[(\ell+1)\ell+(\ell'+1)\ell'] &= 2[\ell^2+\ell+\ell'^2+\ell']\\ &= (\ell'+\ell+1)^2+(\ell'-\ell)^2-1\end{aligned}$$

$$\begin{aligned}\{[\ell'(\ell'+1)-\ell(\ell+1)]^2-2[(\ell+1)\ell+(\ell'+1)\ell']\}\langle\hat{r}\rangle &= 0\\ [(\ell'-\ell)(\ell'+\ell+1)-(\ell'+\ell+1)^2+(\ell'-\ell)^2-1]\langle\hat{r}\rangle &= 0\end{aligned}$$

$$\underset{\ell'-\ell=\pm1}{[(\ell-\ell')^2-1]}\ \underset{\text{cannot be 0, unless }\ell'=\ell=0}{[(\ell+\ell'+1)]} = 0$$



Chapter 10 Adiabatic Aprroximation 绝热近似

微扰随时间变化非常缓慢

10.1 Adiabatic Theorem 绝热定理

10.1.1 Adiabatic Process

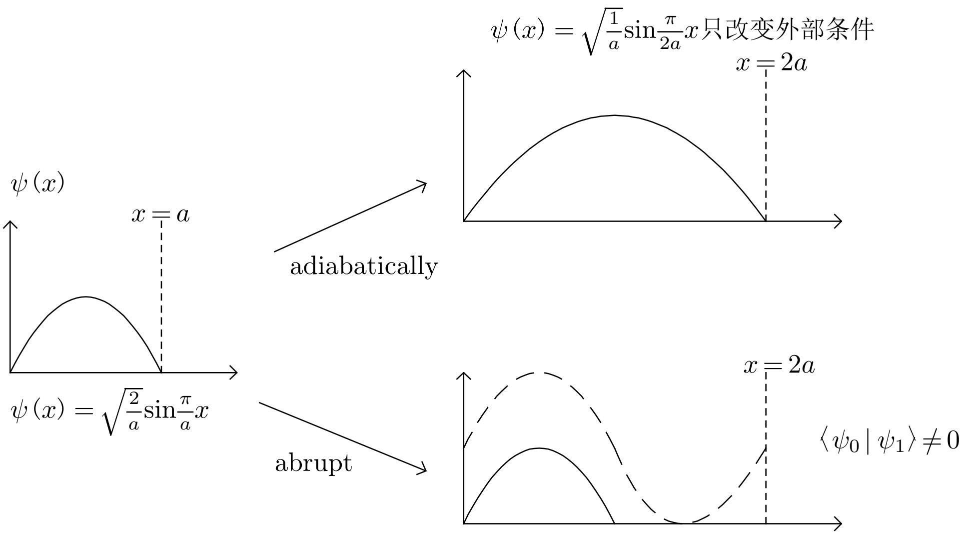
单摆： $T=2\pi\sqrt{\frac{L(t)}{g}}$

单摆所在的箱子也在发生震动。

T_i: Internal time : Period （单摆的固有周期）

T_e: External time : Time scale of changing the length L gradual change of the external can be definss an adiabatic process.（“箱子”的震动频率）

Infinite square well



10.1.2 Adiabtic theorem

如果哈密顿量不依赖时间，则在开始时满足：$H\psi_n=E_n\psi_n$.

第 n 本征态ψ_n 的一个粒子以后将仍然处在第n 本征态，只是具有了一个相因子$\Psi_n(t)=\psi_n e^{-iE_n t/\hbar}$

如果哈密顿随时间变化，则本征函数和本征值也随时间变化：

We solve $H(t)\,\psi_n(t)=E_n(t)\,\psi_n(t)$, instead of solve $\mathrm{i}t\frac{\partial}{\partial t}\psi(t)=H\psi(t)$ we deal t as a parameter not a variable.

能这么做的原因是①$\psi_n(t)$是空间中一组完备的基底，②$\langle\psi_n(t)\,|\,\psi_m(t)\,\rangle=\delta_{mn}$ 要求：t变化的特别缓慢.

$$\text{含时薛定谔方程：}i\hbar\frac{\partial}{\partial t}\Psi(t)=H(t)\Psi(t)\quad[10.11]$$

$$\Psi(t)=\sum_n c_n(t)\,\psi_n(t)\,e^{i\theta_n(t)}\qquad[10.12]$$

$$\text{where}\quad\theta_n(t)=-\frac{1}{\hbar}\underbrace{\int_0^t E_n(t')\,\mathrm{d}t'}_{\text{在}t\to t+\mathrm{d}t\text{内相位积累}}\xrightarrow{\text{if }E_n\text{ is constant}}-\frac{1}{\hbar}E_n t$$

将[10.12] 代入[10.11]得到：

$$i\hbar\frac{\partial}{\partial t}\sum_n c_n(t)\,\psi_n(t)\,e^{i\theta_n(t)}=H(t)\sum_n c_n(t)\,\psi_n(t)\,e^{i\theta_n(t)}$$

$$\text{右边}=\sum_n c_n(t)\,E_n(t)\,\psi_n(t)\,e^{i\theta_n(t)}$$

$$\text{左边}\Rightarrow i\hbar\sum_n[\dot{c}_n(t)\,\psi_n(t)+c\dot{\psi}_n(t)+i\,\dot{\theta}_n(t)\,c_n(t)\,\psi_n(t)\,]e^{i\theta_n(t)}$$

where $\dot{\theta}=\left(-\frac{1}{\hbar}\right)\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t\mathrm{d}t'\,E_n(t)=-\frac{1}{\hbar}E_n(t)$,

第三项：$i\hbar\sum_n-\frac{i}{\hbar}E_n(t)\,c_n(t)\,\psi_n(t)\,e^{i\theta_n(t)}=\sum_n E_n(t)\,c_n(t)\,\psi_n(t)\,e^{i\theta_n(t)}$,与右边相等

$$\therefore i\hbar\sum_n[\dot{c}_n(t)\,\psi_n(t)+c\dot{\psi}_n(t)\,]e^{i\theta_n(t)}=0$$

inner product $\langle\psi_m(t)\,|\;\Rightarrow$

$$\begin{aligned}\sum_n\dot{c}_n\underbrace{\langle\psi_m\,|\,\psi_n\rangle}_{\delta_{mn}}e^{i\theta_n}&=-\sum_n c_n\underbrace{\langle\psi_m(t)\,|\,\dot{\psi}_n(t)\,\rangle}_{\text{new thing}}e^{i\theta_n}\\ \dot{c}_m e^{i\theta_m}&=-\sum_n c_n\langle\psi_m\,|\,\dot{\psi}_n\rangle e^{i\theta_n}\\ \dot{c}_m&=-\sum_n c_n\langle\psi_m\,|\,\dot{\psi}_n\rangle e^{i(\theta_n-\theta_m)}\quad[10.16]\end{aligned}$$

To calculate $\langle\psi_n\,|\,\dot{\psi}_m\rangle\Rightarrow\frac{\mathrm{d}}{\mathrm{d}t}[H_n(t)\,\psi_n(t)\,]=\frac{\mathrm{d}}{\mathrm{d}t}[E_n(t)\,\psi_n(t)\,]\quad\Rightarrow\dot{H}\psi_n+H\dot{\psi}_n=\dot{E}_n\psi_n+E_n\dot{\psi}_n$

Inner product $\langle\psi_m|$

$$\Rightarrow\langle\psi_m\,|\,\dot{H}\,|\,\psi_n\rangle+\langle\psi_m\,|\,H\,|\,\dot{\psi}_n\rangle=\dot{E}_n\langle\psi_m\,|\,\psi_n\rangle+E_n\langle\psi_m\,|\,\dot{\psi}_n\rangle$$

For $m\neq n$ $\langle\psi_m\,|\,\dot{H}\,|\,\psi_n\rangle=(E_n-E_m)\langle\psi_m\,|\,\dot{\psi}_n\rangle$

$$\langle\psi_m\,|\,\dot{\psi}_n\rangle=\frac{1}{E_n-E_m}\langle\psi_m\,|\,\dot{H}\,|\,\psi_n\rangle$$

代入[10.16]得

$$\dot{c}_m = -c_m\langle\psi_m\,|\,\dot{\psi}_m\rangle - \sum_{m\neq n} c_n\langle\psi_m\,|\,\dot{\psi}_n\rangle e^{i(\theta_m-\theta_n)}$$

$$\dot{c}_m = -c_m\langle\psi_m\,|\,\dot{\psi}_m\rangle - \sum_{m\neq n} c_n\frac{\langle\psi_m\,|\,\dot{H}\,|\,\psi_n\rangle}{E_n-E_m}e^{\left(-\frac{i}{\hbar}\right)\int_0^t[E_n(t')-E_m(t')]\mathrm{d}t'}$$

[Approximation]: $\langle\psi_m\,|\,\dot{H}\,|\,\psi_n\rangle = 0$, H的变化特别缓慢,即$\dot{H}$非常小。舍弃第二项$\langle\psi_m\,|\,\dot{\psi}_n\rangle = 0$（$m\neq n$时）

对于 $\dot{c}_m = -c_m\langle\psi_m\,|\,\dot{\psi}_m\rangle$,

$$\frac{\mathrm{d}c_m}{c_m} = -\langle\psi_m\,|\,\dot{\psi}_m\rangle\mathrm{d}t$$

$$\begin{aligned}
c_m(t) &= c_m(0)\exp\left(-\int_0^t\mathrm{d}t'\left\langle\psi_m(t)\,\middle|\,\frac{\mathrm{d}}{\mathrm{d}t}\,\middle|\,\psi_m(t)\right\rangle\right)\\
&= c_m(0)\,e^{i\gamma_m(t)}\\
\Psi_n(t) &= e^{i\theta_n(t)t}e^{i\gamma_n(t)}\psi_n(t)\\
\text{其中}\quad, &\quad \gamma_m(t) = i\int_0^t\langle\psi_m\,|\,\nabla\,|\,\psi_m\rangle\mathrm{d}t \quad \text{几何相位}\\
&\quad \theta_m(t) = \frac{-1}{\hbar}\int_0^t E_n^{'}(t')\,\mathrm{d}t \qquad \text{动力学相位}
\end{aligned}$$

例. 10.1 Electron spin in a slow- rotating magnetic field

假设一个电子（带电荷$-e$, 质量 m）在强度B_0的磁场中静止在原点，磁场的方向与z轴夹角α,并以角速度 ω 绕 z 轴转动

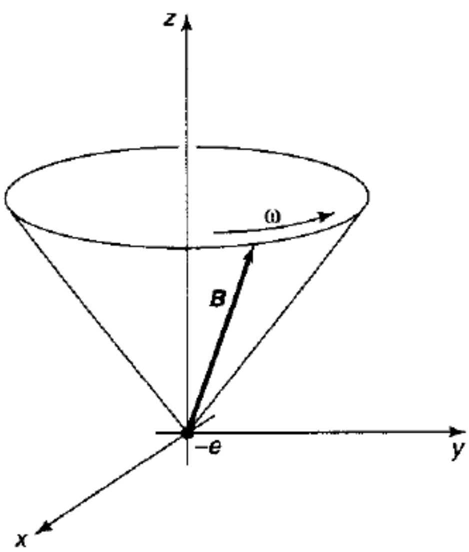


图. 磁场方向沿着一个圆锥面以角速度ω扫动

$$B(t) = B_0[\sin\alpha\,\cos\omega t\hat{i} + \sin\alpha\,\cos\omega t\hat{j} + \cos\alpha\hat{k}]$$

$$\begin{aligned}
H(t) &= \frac{e}{m}\vec{B}\cdot\vec{S}\\
&= \frac{e\hbar B_0}{2m}[\sin\alpha\,\cos\omega t\,\sigma_x + \sin\alpha\,\sin\omega t\,\sigma_y + \cos\alpha\,\sigma_z] \qquad (\sigma_x,\sigma_y,\sigma_z\ \text{为泡利矩阵})
\end{aligned}$$

不妨设 $\omega_1 = \frac{eB_0}{m}$

$$H(t) = \frac{\hbar\omega_1}{2}\begin{bmatrix} \cos\alpha & \sin\alpha\cos\omega t - i\sin\alpha\sin\omega t \\ \sin\alpha\cos\omega t + i\sin\alpha\sin\omega t & -\cos\alpha \end{bmatrix}$$
$$= \frac{\hbar\omega_1}{2}\begin{bmatrix} \cos\alpha & \sin\alpha e^{-i\omega t} \\ \sin\alpha e^{i\omega t} & -\cos\alpha \end{bmatrix}$$

$\uparrow$ ———————— $\frac{\hbar\omega_1}{2} = E$

$\downarrow$ ———————— $\frac{\hbar\omega_1}{2} = E_2$

The "instantaneous" normalized. "spinor" eigen states of $H(t)$

$$\begin{matrix} H(t)\chi_+(t) = E_+\chi_+(t) \\ H(t)\chi_-(t) = E_-\chi_-(t) \end{matrix} \Rightarrow \begin{matrix} \chi_+(t) = \begin{bmatrix} \cos\left(\frac{\alpha}{2}\right) \\ e^{i\omega t}\sin\left(\frac{\alpha}{2}\right) \end{bmatrix} & [10.27] \\ \chi_-(t) = \begin{bmatrix} e^{-i\omega t}\sin\left(\frac{\alpha}{2}\right) \\ -\cos\left(\frac{\alpha}{2}\right) \end{bmatrix} & [10.28] \end{matrix}$$

$$\text{相应的本征值：} E_\pm \equiv \pm\frac{\hbar\omega_1}{2}$$

假设开始时，电子自旋方向沿着$\vec{B}(0)$的瞬时方向(自旋向上)：$\chi(0) = \begin{pmatrix} \cos\left(\frac{\alpha}{2}\right) \\ \sin\left(\frac{\alpha}{2}\right) \end{pmatrix}$

精确解(Problem 10.2) 解 $H(t)\psi(t) = i\hbar\frac{\partial}{\partial t}\psi(t)$ + 初始时 $\psi(0) = \chi_+(0)$

$$\chi(t) = \begin{pmatrix} \left[\cos\left(\frac{\lambda t}{2}\right) - i\frac{(\omega_1-\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\cos\left(\frac{\alpha}{2}\right)e^{-\frac{i\omega t}{2}} \\ \left[\cos\left(\frac{\lambda t}{2}\right) - i\frac{(\omega_1+\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\sin\left(\frac{\alpha}{2}\right)e^{\frac{i\omega t}{2}} \end{pmatrix} \qquad [10.31]$$

其中， $\lambda = \sqrt{\omega^2 + \omega_1^2 - 2\omega\omega_1\cos\alpha}$.

或者用两个态的线性叠加表示精确解：$\chi(t) = (|\chi_+(t)\rangle\langle\chi_+(t)|\chi(t)\rangle + |\chi_-(t)\rangle\langle\chi_-(t)|\chi(t)\rangle)$

$$\langle\chi_+(t)|\chi(t)\rangle = \begin{bmatrix} \cos\frac{\alpha}{2} & \sin\frac{\alpha}{2}e^{-i\omega t} \end{bmatrix} \times [10.31]$$
$$= \left[\cos\left(\frac{\lambda t}{2}\right) - i\frac{(\omega_1-\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]e^{-\frac{i\omega t}{2}}$$

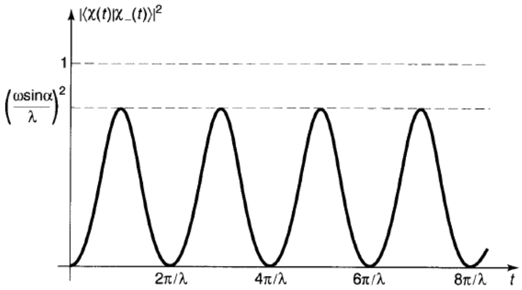
$$\langle\chi_-(t)|\chi(t)\rangle = \begin{bmatrix} \sin\frac{\alpha}{2}e^{-i\omega t} & -\cos\frac{\alpha}{2} \end{bmatrix} \times [10.31]$$
$$= i\left[\frac{\omega}{\lambda}\sin\alpha\sin\left(\frac{\lambda t}{2}\right)\right]e^{\frac{i\omega t}{2}}$$

可以将$\chi(t)$表示为χ_+和χ_-的线性叠加：

$$\chi(t) = \left[\cos\left(\frac{\lambda t}{2}\right) - i\frac{(\omega_1-\omega)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]e^{-\frac{i\omega t}{2}}\chi_+(t) + i\left[\frac{\omega}{\lambda}\sin\alpha\sin\left(\frac{\lambda t}{2}\right)\right]e^{\frac{i\omega t}{2}}\chi_-(t)$$

由此，由自旋向上向自旋向下的跃迁几率时：

$$|\langle\chi_-(t)\,|\,\chi(t)\rangle|^2=\left(\frac{\omega}{\lambda}\sin\alpha\sin\frac{\lambda t}{2}\right)^2$$



在非绝热区域($\omega\gg\omega_1$)的跃迁几率图

接下来我们使用绝热近似的条件:

$$\begin{aligned}\text{External}\quad\text{time}\qquad & T_e\ \sim\ \frac{1}{\omega}\\ \text{Internal time}\qquad & T_i\ \sim\ \frac{1}{\omega_1}\end{aligned}$$

$$T_e\gg T_i\quad\Rightarrow\omega\ll\omega_1\quad\Rightarrow\frac{\omega}{\omega_1}\longrightarrow 0$$

$$\lambda\equiv\sqrt{\omega^2+\omega_1^2-2\omega\omega_1\cos\alpha}=\omega_1\sqrt{1+\left(\frac{\omega}{\omega_0}\right)^2-2\frac{\omega}{\omega_0}\cos\alpha}\approx\omega_1$$

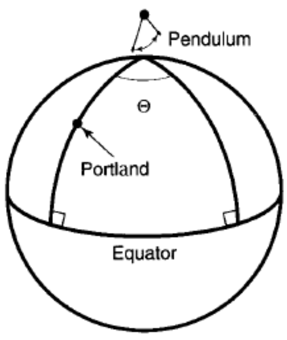
$$\Rightarrow|\langle\chi_-(t)\,|\,\chi(t)\rangle|^2\approx\left(\frac{\omega}{\omega_1}\sin\alpha\sin\frac{\omega t}{2}\right)^2\longrightarrow 0\quad\text{no transition from }\chi_+\text{ to }\chi_-(t)$$

即，如果$\vec{B}$ 的旋转足够慢(adiabtically), 自旋保持初始状态，即仍保持spin-up $\chi_+(t)$，但当$\omega\gg\omega_1$时，体系将在自旋向上和自旋向下的态之间来回振荡。

10.2 Berry 相

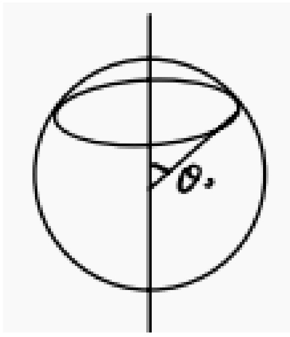
10.2.1 不完全过程 Nonholonomic process

如果单摆在自发摆动的同时，对单摆的支撑物依照下图路径进行缓慢的移动，发现单摆会偏离原来的平面进行运动。因为该闭合路径的面积为北半球面积的$\frac{\Theta}{2\pi}$，面积为$A=\frac{1}{2}\left(\frac{\Theta}{2\pi}\right)4\pi R^2=\Theta R^2$



$$\therefore\Theta=\frac{A_{\text{area}}}{R^2}=\Omega$$

体系的某些参数以某种方式变化并最终回到它们的初始值,但回不到最初状态， 成为不完全体系（变换量与路径有关）Its state depends on the path, taken in order to achieve it. A system does not return to its original state when transported around a loop classical geometric phase.



The rotation of earch carries a pedulum to do an transport around a loop

The change of the angle of the pendulum plane = solid angle of the closed loop

10.2.2 Quantum Geometric phase 几何相

For an adiabatic process, if we start from the state $H(t=0)$, we arrive at the state of $H(t)$, pick up only a time-depend phase factor.

$$\Psi_n(t) = e^{i[\theta(t)+\gamma_n(t)]}\psi_n(t)$$

其中，$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\,\mathrm{d}t'$　被称为动力学相,

$\gamma_n(t) = i\int_0^t \left\langle \psi_n(t') \,|\, \frac{\partial}{\partial t'}\psi_n(t') \right\rangle \mathrm{d}t'$　　[10.40]被称为几何相。

因为哈密顿量中的一些参数$R(t)$时随时间变化的，所以$\psi_n(t)$也是随时间变化的。

$\psi_n(t)$ depends on t because some paramaters $R(t)$ in the $H(t)$ is changing with time

using chain rule $\frac{\partial\psi_n}{\partial t} = \frac{\partial\psi_n}{\partial R}\frac{\partial R}{\partial t}$

$$\gamma_n(t) = i\int_0^t \left\langle \psi_n \,|\, \frac{\partial\psi_n}{\partial R} \right\rangle \frac{\partial R}{\partial t'}\mathrm{d}t' = i\int_{R_i}^{R_f} \left\langle \psi_n \,|\, \frac{\partial\psi_n}{\partial R} \right\rangle \mathrm{d}R \qquad (R_f = R(t), R_i = R(t=0))$$

如果经过时间 T,哈密顿量回到初始形式$R_i = R_f$, $\Rightarrow \gamma_n(T) = 0$,不会有任何有关几何相的事情出现。

以上是假设了哈密顿量中只有一个参数是变化的，如果有N个参数随着 t 变化：

if there are N parameters: $\vec{R}(t) = [R_1(t), R_2(t), \ldots, R_N(t)]$

$$\frac{\partial\psi_n}{\partial t} = \frac{\partial\psi_n}{\partial R_1}\frac{\partial R_1}{\partial t} + \frac{\partial\psi_n}{\partial R_2}\frac{\partial R_2}{\partial t} + \cdots + \frac{\partial\psi_n}{\partial R_N}\frac{\mathrm{d}R_N}{\mathrm{d}t} = (\nabla_R\psi_n)\cdot\frac{\mathrm{d}\boldsymbol{R}}{\mathrm{d}t}$$

这里$\boldsymbol{R} \equiv (R_1, R_2, \ldots, R_N)$,$\nabla_R$则是对这些参量求梯度。我们有：

$$\therefore \gamma_n(t) = i\int_{\vec{R}_i}^{\vec{R}_f} \langle \psi_n \,|\, \nabla_R\psi_n \rangle \cdot \mathrm{d}\vec{\boldsymbol{R}} \qquad [10.44]$$

Berry phase = the geometric phase of a complete cycle (closed loop)

经过时间T之后，哈密顿量回到初始形式，最终的几何相是

$$\gamma_n(T) = i\oint \langle \psi_n | \nabla_R \psi_n \rangle \cdot \mathrm{d}\vec{\boldsymbol{R}} \qquad [10.45]$$

以上是在参数空间中闭合路径的线积分，$\gamma_n(T)$称为**Berry 相**，一般情况下并不为0.

注意$\gamma_n(T)$仅仅依赖所选择的路径，而不依赖在这个路径运动的快慢（当然，只要它需要慢到足以使绝热过程有效）。而动力学相$\theta_n(T) \equiv -\frac{1}{\hbar}\int_0^T E_n(t')\,\mathrm{d}t'$ 则会更显著的依赖时间。

物理量与$|\psi|^2$有关（大部分情况相因子会被抵消），但如果把一束都处在Ψ态的粒子分为两束，一部分经历绝热变化的势，另一束不经历。

当这两束粒子重新合并在一起时，总的波函数形式为$\Psi = \frac{1}{2}\Psi_0 + \frac{1}{2}\Psi_0 e^{i\Gamma}$，其中$\Gamma$是经历绝热变化$H$ 的那束粒子获得的额外的相（包含动力学相和几何相）

此时$|\Psi|^2 = \frac{1}{4}|\Psi_0|^2(1+e^{i\Gamma})(1+e^{-i\Gamma}) = \frac{1}{2}|\Psi_0|^2(1+\cos\Gamma) = |\Psi_0|^2\cos^2\left(\frac{\Gamma}{2}\right)$

通过找到干涉相增或干涉相消位置测量Γ.

当参数空间是三维时，我们可以考虑类比使用矢势$\boldsymbol{A}$来表示**磁通量**。改写Berry phase

Berry connection $\vec{A}$, Berry curcture $\vec{B}$, Berry phase

Recall $\vec{B} = \nabla\times\vec{A}$. Magnetic flux Φ

$$\begin{aligned}\Phi &= \int_s \vec{B}\cdot\mathrm{d}\vec{a} \xrightarrow[\text{stokes}']{} \oint_c \vec{A}\cdot\mathrm{d}\vec{r} \\ &= \int_s (\nabla\times\vec{A})\cdot\mathrm{d}\vec{a}\end{aligned}$$

we can define $\vec{B} = \nabla\times\vec{A} = i\nabla_R\langle\psi_n|\nabla_R\psi_n\rangle$ a magnetic field

$\Rightarrow$ Berry Phase[10.51]

$$\gamma_n(T) = \oint_{\text{loop}} \vec{A}\mathrm{d}\vec{R} = \int_{\text{area}} \vec{B}\cdot\mathrm{d}\vec{a} = i\oint\langle\psi_n|\nabla_R\psi_n\rangle\cdot\mathrm{d}\vec{\boldsymbol{R}} = i\int \underbrace{[\nabla_R\times\langle\psi_n|\nabla_R\psi_n\rangle]}_{\text{magnetic field}}\cdot\mathrm{d}\vec{a}$$

例. 10.2 Berry phase of spin in adiabatically ratating maganetic field

原点处一个电子在一个方向变化的恒定磁场中，假设磁场$\boldsymbol{B}(t)$以恒定的角速度ω进动，且与 z 轴夹角恒为α. [10.33] 给出了电子初态为沿$\boldsymbol{B}$方向自旋向上的精确解。 adiabatic limit $\rightarrow \frac{\omega}{\omega_1}\rightarrow 0$，

对$\lambda = \omega_1\sqrt{1-2\frac{\omega}{\omega_1}\cos\alpha + \left(\frac{\omega}{\omega_1}\right)^2}$，泰勒展开$\approx\omega_1\left(1-\frac{\omega}{\omega_1}\cos\alpha\right) = \omega_1 - \omega\cos\alpha$

$$\begin{aligned}[10.33]\Rightarrow\chi(t) &\cong e^{-i\omega_1 t/2}e^{i(\omega\cos\alpha)t/2}e^{-i\omega t/2}\chi_+(t) + i\left[\frac{\omega}{\omega_1}\sin\alpha\sin\left(\frac{\omega_1 t}{2}\right)\right]e^{i\omega t/2}\chi_-(t) \\ \text{当}\frac{\omega}{\omega_1}\rightarrow 0\text{时} \quad , & \quad \text{第二项可以舍去，结果与[10.23]一致} \\ &= \underbrace{e^{\frac{it}{2}\omega(\cos\alpha-1)}}_{\text{Geometric phase}}\underbrace{e^{-\frac{i\omega_1 t}{2}}}_{\text{Dynamic phase}}\chi_+(t) \\ &= e^{i\theta_n(t)}e^{i\gamma_n(t)}\psi_n(t)\end{aligned}$$

Dynamic phase [10.54] $\theta_+(t) = -\frac{1}{\hbar}\int_0^\theta E_+(t')\,\mathrm{d}t' = -\frac{1}{\hbar}\frac{\hbar}{2}\omega_1 t = -\frac{\omega t}{2}$

Berry phase[10.56]: $\gamma_+(t) = \frac{\omega t}{2}(\cos\alpha - 1)$ $\quad\longleftarrow$解法一：通过含时薛定谔方程

对于完整周期$T = \frac{2\pi}{\omega}$, Berry phase: $\gamma_+(t) = \pi(\cos\alpha - 1)$

现在考虑更一般的境况，磁场矢量的顶端为$r=B_0$的球面上扫过一个任意形状的闭合曲线

代表沿着$\boldsymbol{B}$方向自旋向上的本征态形式为：$\chi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}$,这里$\theta$,$\phi$($B$的球坐标)都是时间的函数

$$\nabla\chi_+ = \frac{\partial\chi_+}{\partial r}\hat{r}\,(\text{无}r\text{方向分量}) + \frac{1}{r}\frac{\partial\chi_+}{\partial\theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial\chi_+}{\partial\phi}\hat{\phi} = \frac{1}{r}\begin{pmatrix} -\frac{1}{2}\sin\frac{\theta}{2} \\ \frac{1}{2}e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}\hat{\theta} + \frac{1}{r\sin\theta}\begin{pmatrix} 0 \\ i\,e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}\hat{\phi}$$

$$\langle\chi_+|\nabla\chi_+\rangle = \frac{1}{2r}\left[-\sin\frac{\theta}{2}\cos\frac{\theta}{2}\hat{\theta} + \sin\frac{\theta}{2}\cos\frac{\theta}{2}\hat{\theta} + 2i\frac{\sin^2\left(\frac{\theta}{2}\right)}{\sin\theta}\hat{\phi}\right] = i\frac{\sin^2\left(\frac{\theta}{2}\right)}{r\sin\theta}\hat{\phi}$$

$$\nabla\times\langle\chi_+|\nabla\chi_+\rangle = \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\left(\frac{i\sin^2\left(\frac{\theta}{2}\right)}{r\sin\theta}\right)\right]\hat{r} = \frac{i}{2r^2}\hat{r}$$

$$|\gamma_+(T)| = i\int_s \nabla_R\times\langle\chi_+|\nabla_R\chi_+\rangle\cdot d\vec{a} = -\frac{1}{2}\int_s\frac{1}{r^2}\hat{r}\cdot r^2 d\Omega\,\hat{r} = -\frac{1}{2}\Omega$$

(积分区域为$\boldsymbol{B}$在球面上扫过一周所围成的面积 $d\boldsymbol{a} = r^2 d\Omega\,\hat{r}$)

$$\gamma_+(T) = -\frac{1}{2}\int d\Omega = -\frac{1}{2}\Omega$$

10.2.3 Aharonor - Bohr effect

scalar φ and vector potential $\vec{A}$, $\vec{E} = -\nabla\varphi - \frac{\partial\vec{A}}{\partial t}$ $\quad\vec{B} = \nabla\times\vec{A}$

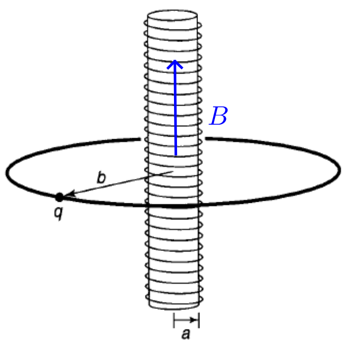
Gauge Invariance 规范不变

We can do a gauge transformation $\left\{\begin{array}{l} \varphi\rightarrow\varphi' = \varphi - \frac{\partial\Lambda}{\partial t'} \\ \vec{A}\rightarrow\vec{A}' = \vec{A} + \nabla\Lambda \end{array}\right\}$,Λ可以是任何函数，而对于$\vec{E}$ 和 $\vec{B}$ 不会产生任何影响。

在经典力学中，$\vec{E}$ 和 $\vec{B} = 0$,不会有任何影响(矢势不能被直接检测到)

而在量子力学中，我们会观察到 **AB effect**

Example: A charge constrained to move in a ring around a solenoid



假设螺线管无限长，螺线管外的磁场为0。但是螺线管外部的矢势 $\vec{A}$ 不为0.

以下为推导$\vec{A}$:

（假设螺线管的单位长度有 n 匝，半径为 a，电流为 I）

$$\oint \vec{B}\cdot \mathrm{d}l = \mu_0 n I$$

Note that $\oint_c \vec{A}\cdot \mathrm{d}\vec{l} = \int_s (\nabla\times\vec{A})\,\mathrm{d}\vec{a} = \int_s \vec{B}\cdot \mathrm{d}\vec{a} = \Phi$ (magnetic flux)

Inside solenoid	Outside solenoid
$A\cdot 2\pi s = \mu_0 n I\cdot \pi s^2$ $\vec{A} = \frac{\mu_0 n I}{2} s\vec{\phi} \quad \text{for} \quad s<a$	The flux is $\Phi = \mu_0 n I \pi a^2 = A\cdot 2\pi s$,$s>a$ $\vec{A} = \frac{\mu_0 n I \pi a^2}{2\pi s}\hat{\phi} \quad \text{for } s>a \quad [10.66]$ shows outside solenoid: $\vec{B}=0 \quad \vec{A}\neq 0$

Hamiltonian in magnetic field

$$H = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\vec{A}\right)^2 = \frac{1}{2m}[-\hbar^2\nabla^2 + q^2A^2 + i\hbar q\nabla\cdot\vec{A} + iq\hbar\vec{A}\cdot\nabla]$$

其中，$(\nabla\cdot\vec{A})\,\varphi = \nabla\cdot\vec{A}\varphi = \vec{A}\cdot\nabla\varphi$ （因为$\nabla\cdot(f\vec{A}) = \vec{A}\cdot\nabla f + f(\nabla\cdot\vec{A})$，而$f(\nabla\cdot\vec{A})$在库伦规范下为0）

在柱坐标下：

$$\begin{aligned}
\nabla\cdot\vec{A} &= \frac{1}{r}\frac{\partial}{\partial r}(rA_r) + \frac{1}{r}\left(\frac{\partial A_\phi}{\partial\phi}\right) + \frac{\partial A_z}{\partial z} \\
H &= \frac{1}{2m}[-\hbar^2\nabla^2 + q^2A^2 + i2q\hbar\vec{A}\cdot\nabla] \quad (\vec{A}\text{只有}\phi\text{方向}) \\
\nabla^2\psi &= \frac{1}{r}\frac{\partial}{\partial r}\underbrace{\left(r\frac{\partial\psi}{\partial r}\right)}_{=0} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2} + \underbrace{\frac{\partial^2\psi}{\partial z^2}}_{=0} \\
\nabla\psi &= \underbrace{\frac{\partial\psi}{\partial r}}_{=0}\hat{r} + \frac{1}{r}\frac{\partial\psi}{\partial\phi}\hat{\phi} + \underbrace{\frac{\partial\psi}{\partial z}}_{=0}\hat{z}
\end{aligned}$$

$$\Rightarrow H\psi = \frac{1}{2m}\left[-\hbar^2\frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2} + q^2\underbrace{\left(\frac{\Phi}{2\pi r}\right)}_{\text{磁矢势}A}{}^2\psi + i2\hbar q\frac{\Phi}{2\pi r}\frac{1}{r}\frac{\partial\psi}{\partial\phi}\right] = E\psi$$

$$\Rightarrow \frac{\mathrm{d}^2\psi}{\mathrm{d}\phi^2} - i2\beta\frac{\mathrm{d}\psi}{\mathrm{d}\phi} + \varepsilon\psi = 0 \qquad \text{where } \beta = \frac{q\Phi}{2\pi\hbar} \quad \varepsilon = \frac{2mb^2E}{\hbar^2} - \beta^2$$

设$\psi = Ae^{i\lambda\phi}$，$\Rightarrow \frac{\mathrm{d}}{\mathrm{d}\phi^2}(Ae^{i\lambda\phi}) - i2\beta\frac{\mathrm{d}}{\mathrm{d}\phi} + \varepsilon\psi = 0 \quad \Rightarrow (-\lambda^2 + 2\beta\lambda + \varepsilon)(Ae^{i\lambda\phi}) = 0$

$$\lambda = \beta \pm \sqrt{\beta^2 + \varepsilon}$$

周期性边界条件：$e^{i\lambda\phi} = e^{i\lambda\phi}\cdot e^{i\lambda\phi\cdot 2\pi} \Rightarrow \beta \pm \sqrt{\beta^2 + n} = n$

$$E_n = \frac{\hbar^2}{2mb^2}(\beta - n)^2, n = 0, \pm 1, \pm 2\cdots$$

注意：此时能量与磁通（Φ）有关（尽管此时外面没有磁场）

$$E_n = \frac{\hbar^2}{2mb^2}\left(\frac{q\Phi^2}{2\pi\hbar} - n\right)^2$$

Effect of magnetic field on the wave function

$$\left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\vec{A}\right)^2 + V(\vec{r})\right]\psi = i\frac{\partial}{\partial t}\psi \quad [10.75]$$

结论：$\psi = e^{ig}\psi'$ where $i\frac{\partial}{\partial t}\psi' = H\psi'$, $g(\vec{r}) = \frac{g}{\hbar}\int_0^{\vec{r}} \vec{A}(\vec{r}')\cdot \mathrm{d}\vec{r}'$

[Proof]: put $\psi = e^{ig}\psi'$ into [10.75]

$$\begin{aligned}\nabla\psi &= \nabla(e^{ig}\psi')\\ &= e^{ig}(i\nabla g)\psi' + e^{ig}(\nabla\psi')\\ &= e^{ig}\left(i\frac{q}{\hbar}\vec{A}(r)\right)\psi' + e^{ig}(\nabla\psi')\\ &= i\frac{q}{\hbar}\vec{A}(r)\psi + e^{ig}(\nabla\psi')\end{aligned}$$

$$\Rightarrow \frac{\hbar}{i}\nabla\psi = q\vec{A}\psi + \frac{\hbar}{i}e^{ig}(\nabla\psi')$$

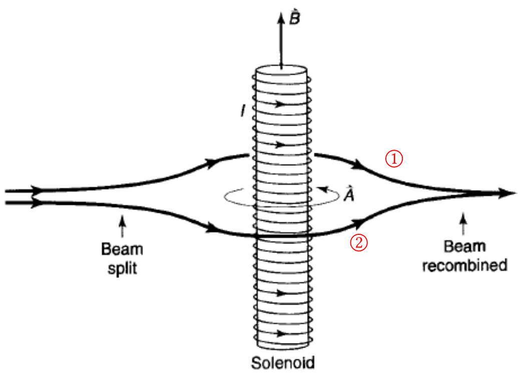
Act $\left(\frac{\hbar}{i}\nabla - q\vec{A}\right)$ on [10.78] $\Rightarrow$

$$\begin{aligned}\left[\frac{\hbar}{i}\nabla - q\vec{A}\right]\frac{\hbar}{i} &= \left(\frac{\hbar}{i}\nabla - q\vec{A}\right)\frac{\hbar}{i}e^{ig}\nabla\psi'\\ &= -\hbar^2\nabla(e^{ig}\nabla\psi') - \frac{q\hbar}{i}\vec{A}e^{ig}\nabla\psi'\\ &= -\hbar^2[ie^{ig}\nabla g\nabla\psi' + e^{ig}\nabla^2\psi'] - \frac{q\hbar}{i}\vec{A}e^{ig}\nabla\psi'\\ &= -\hbar^2 e^{ig}\nabla^2\psi'\end{aligned}$$

$\therefore \left(\frac{\hbar}{i}\nabla\cdot q\vec{A}\right)^2 = -\hbar^2 e^{ig}\nabla^2\psi'$ [10.79] put 10.79 → 10.75

$$\begin{aligned}-\frac{\hbar^2}{2m}e^{ig}\nabla^2\psi' + V\psi' &= i\hbar\frac{\partial}{\partial t}\psi' e^{ig}\\ -\frac{\hbar^2}{2m}\nabla^2\psi' + V\psi' &= i\hbar\frac{\partial}{\partial t}\psi' \qquad \text{No } \vec{A} \text{ here}\end{aligned}$$

AB phase



$$\vec{A} = \frac{\Phi}{2\pi r}\hat{\phi} \qquad g = \frac{q}{\hbar}\int \vec{A}\cdot \mathrm{d}\vec{r} = \frac{q\Phi}{2\pi\hbar}\int \frac{1}{r}\hat{\phi}\cdot r\hat{\phi} = \frac{q\Phi}{2\pi\hbar}\int \mathrm{d}\phi$$

- for ① $g = \frac{q\Phi}{2\pi\hbar}\int_\pi^0 \mathrm{d}\phi = -\frac{q\Phi}{2\hbar}$

- for ② $g=\frac{q\Phi}{2\pi\hbar}\int_{\pi}^{2\pi}\mathrm{d}\phi=\frac{q\Phi}{2\hbar}$

Phase difference: ②-①：$\Delta g=\frac{q\Phi}{2\pi\hbar}\int_0^{2\pi}\mathrm{d}\phi=\frac{q\Phi}{\hbar}=2\pi\frac{\Phi}{\frac{\hbar}{q}}$ This is the A-Bphase $\frac{h}{q}$:量子磁矩

$$\gamma_n(T)=i\oint\underbrace{\langle\psi_n|\nabla_R\psi_n\rangle}_{\text{Berry phase}}\cdot\mathrm{d}\vec{R}=i\int\underbrace{\nabla\times\langle\psi_n|\nabla_n\psi_n\rangle}_{\text{Berry Curvature}}\mathrm{d}\vec{a}$$

证明略。

【朗道能级】2D Electron gas

$$H=\frac{p^2}{2m}=\frac{p_x^2+p_y^2}{2m}\xrightarrow{\text{add}\quad B}H=\frac{\hbar^2}{2m}\left(\vec{k}-\frac{q}{\hbar}\vec{A}\right)^2-\mu\cdot\vec{B}$$

charge $q\to-e$ for electron $\vec{A}$ vector potential $\vec{B}=\nabla\times\vec{A}$

Assume $\vec{B}=(0,0,B)$ (方向沿着 z 轴)

对于$\vec{A}$ 方向的选取，常有的有朗道规范和平均规范

Landau 规范	平均规范
$\vec{A}=(-yB,0,0)$ 或 $(0,xB,0)$	$\vec{A}=\left(-\frac{yB}{2},\frac{xB}{2},0\right)$
即，有x方向无y方向，有y方向无x方向	即，x,y方向二者各占一半

我们将选用$\vec{A}=(-yB,0,0)$进行以后的计算：

$$\nabla\times\vec{A}=\begin{vmatrix}\hat{x} & \hat{y} & \hat{z}\\ \partial_x & \partial_y & \partial_z\\ -yB & 0 & 0\end{vmatrix}=\hat{z}(-\partial_y(yB))=B\hat{z}$$

$$\begin{aligned}\Rightarrow H &= \frac{\hbar^2}{2m}\left(\vec{k}+\frac{e}{\hbar}\vec{A}\right)^2\\ &= \frac{\hbar^2}{2m}\left[\left(k_x-\frac{e}{\hbar}y_B\right)^2+k_y^2\right]\end{aligned}$$

因为波矢k_y和y不是一组好量子数（因为$p=-i\hbar\nabla=\hbar k,\Rightarrow k=-i\nabla,\Rightarrow[y,k_y]\neq0$）

$$H=\frac{\hbar^2}{2m}\left[\left(k_x-\frac{e}{\hbar}yB\right)^2-\partial_y^2\right]$$

定义磁极长度（magnetic length）:$\boldsymbol{\ell_B=\sqrt{\frac{\hbar}{eB}}=\frac{25.6\mathrm{nm}}{\sqrt{B}}}$

H 中含有 y 且$[y,k_y]=i$, 因此，$\left(k_x-\frac{e}{\hbar}By\right)=\left(k_x-\frac{1}{\ell_B^2}y\right)=\frac{1}{\ell_B^2}(\ell_B^2k_x-y)$

$$H=\frac{\hbar^2}{2m}\left[\frac{1}{\ell_B^2}(y_0-y)^2-\partial_y^2\right]=\frac{1}{2}m\frac{\hbar^2}{m^2\ell_B^4}\ell_B^2(y_0-y)^2+\frac{(i\hbar\partial_y)^2}{2m}$$

而在之前的谐振子势场中$H=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2$

where $\boldsymbol{y_0=\ell_B^2k_x}$ **(guiding centre)**

$\omega'=\frac{\hbar}{m\ell_B^2}$, $x'=(y_0-y)$

我们可以定义Ladder operator

$$a=-\frac{1}{\sqrt{2}}\left(\frac{y-y_0}{\ell_B}+\ell_B\partial_y\right)\qquad a^\dagger=-\frac{1}{\sqrt{2}}\left(\frac{y-y_0}{\ell_B}-\ell_B\partial_y\right)$$

可以计算出$[a,a^\dagger]=1$.

$$\begin{aligned}\left[-\frac{1}{\sqrt{2}}\left(\frac{y-y_0}{\ell_B}+\ell_B\partial_y\right),\ -\frac{1}{\sqrt{2}}\left(\frac{y-y_0}{\ell_B}-\ell_B\partial_y\right)\right] &= \frac{1}{2}\left\{\left[\frac{y-y_0}{\ell_B},-\ell_B\partial_y\right]+\left[\ell_B\partial_y,\frac{y-y_0}{\ell_B}\right]\right\}\\ &= \frac{1}{2}\times\frac{\ell_B}{\ell_B}\{[y,-\partial_y]+[\partial_y,y]\}\\ &= \frac{1}{2}\{1+1\}\\ &= 1\end{aligned}$$

$$\therefore\frac{1}{\sqrt{2}}=(a+a^\dagger)=-\frac{y-y_0}{\ell_B},\qquad \frac{1}{\sqrt{2}}(a-a^\dagger)=-\ell_B\partial_y$$

$$H=\frac{\hbar^2}{2m}\frac{1}{\ell_B^2}\cdot\frac{1}{2}[(a+a^\dagger)^2-(a-a^\dagger)^2]=\frac{\hbar^2}{2m}\frac{1}{\ell_B^2}[a\,a^\dagger+a^\dagger a]=\frac{\hbar^2}{2m}(2a^\dagger a+1)=\frac{\hbar^2}{m}\left(a^\dagger a+\frac{1}{2}\right)$$

$$\omega\equiv\frac{eB}{m}=\frac{\hbar}{m}\frac{eB}{\hbar}=\frac{\hbar}{m}\frac{1}{\ell_B^2}\Rightarrow H=\hbar\left(\frac{\hbar}{m}\frac{1}{\ell_B^2}\right)\left(a\,a^\dagger+\frac{1}{2}\right)=\hbar\omega\left(a^\dagger a+\frac{1}{2}\right)$$

$$E=\left(n+\frac{1}{2}\right)\hbar\omega$$

$$\begin{aligned}\psi_n(x) &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^n n!}}H_n(\xi)\,e^{-\frac{\xi^2}{2}}=\left(\frac{e^{ik_x x}}{\sqrt{L_x}}\right)\frac{1}{\sqrt{n!2^n\ell_B\sqrt{\pi}}}e^{-\frac{\xi^2}{2}}H(\xi)\\ \xi &= \sqrt{\frac{m\omega}{\hbar}}x\end{aligned}$$

review 厄密特多项式$H(\xi)$

$$\begin{aligned}H_0(\xi)&=1\\ H_1(\xi)&=2\xi\\ H_2(\xi)&=4\xi^2-2\\ &\cdots\cdots\end{aligned}$$

递推公式：$H_n(x)-2xH_{n-1}(x)+2(n-1)H_{n-2}(x)=0$

Landau能级

在没有磁场时，$E=\frac{\hbar^2}{2m}(k_x^2+k_y^2)$

朗道能级的能量为$E_n=\hbar\omega\left(n+\frac{1}{2}\right),n=0,1,2\ldots$

$$\psi_{n,k_x}(x,y) = \left(\frac{e^{ik_x x}}{\sqrt{L_x}}\right)\frac{1}{\sqrt{n!2^n\ell_B\sqrt{\pi}}}e^{-\frac{\xi^2}{2}}H_n(\xi)$$

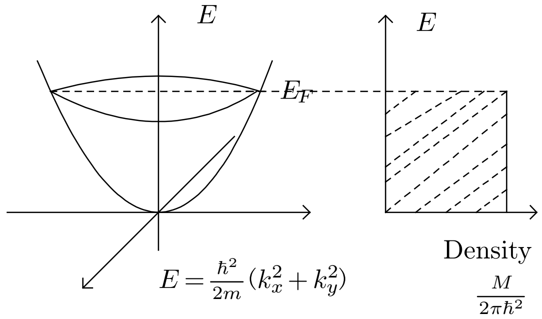
plane wave 沿着x方向是因为使用了朗道gauge$(-yB,0,0)$

no x have $[k_x,H]=0$

$$\xi = \frac{y-\ell_B^2k_x}{\ell_B}$$

当$\vec{A}=(0,xB,0)$时，只需要对调 x ,y 即可

Degeneracy of landau levels

<table>
<tr><th>No magnetic field</th><th>In strong magnetic field</th></tr>
<tr><td>


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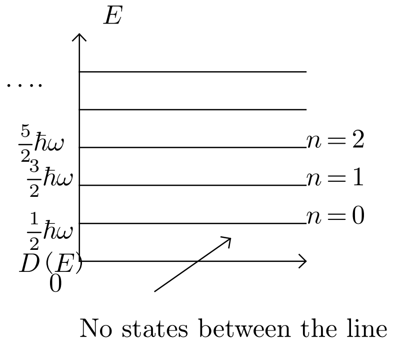

$$\begin{aligned}\text{Number of state on a landau level} &= \hbar\omega\frac{m}{2\pi\hbar^2}\\ &= \hbar\frac{eB}{m}\frac{m}{2\pi\hbar^2}\\ &= \frac{eB}{2\pi\hbar}\\ &= \frac{1}{2\pi\ell_B^2}\end{aligned}$$
</td></tr>
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$\int \mathrm{d}ED(E)=\int\frac{k\mathrm{d}k\mathrm{d}\varphi}{(2\pi)^2}=\int\frac{k\mathrm{d}k}{2\pi}$

where $E=\frac{\hbar^2}{2m}k^2$， $k^2=k_x^2+k_y^2\Rightarrow \mathrm{d}E=\frac{\hbar^2}{2m}2k\mathrm{d}k=\frac{\hbar^2}{m}k\mathrm{d}k$

$$\left\{\begin{array}{c}\mathrm{d}ED(E)=\dfrac{k\mathrm{d}k}{2\pi}\\ \mathrm{d}E=\dfrac{\hbar^2}{m}k\mathrm{d}k\end{array}\right\},\text{上式除以下式，}D(E)=\frac{m}{2\pi\hbar^2}$$

$D(E)=\frac{m}{2\pi\hbar^2}$ is the density of states of $H=\frac{\hbar^2}{2m}(k_x^2+k_y^2)$,可以看出无磁场情况下态密度与能量无关，是一个常数。

3D eletron gas

$$\begin{aligned}H &= \frac{\hbar^2}{2m}\left(\vec{k}+\frac{e}{\hbar}\vec{A}\right)^2\\ &= \frac{\hbar^2}{2m}\left[\left(k_x-\frac{y}{\ell_B^2}\right)^2-\partial_y^2+k_z^2\right]\end{aligned}$$

2D Electron gas in $z-$direction magentic field

wave vector along $z-$direction is still a good quantum number

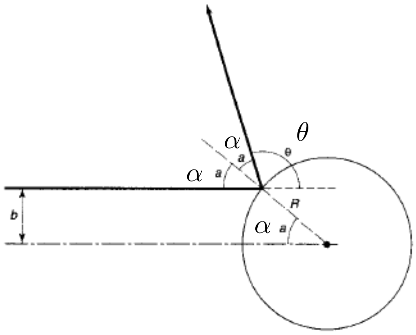
$$E_{n,k,z} = \hbar\omega\left(n+\frac{1}{2}\right)+\frac{\hbar^2}{2m}k_z^2c \qquad \text{plane wave in the } z \text{ direction}$$

cyclotron motion in the $x-y$ plane

Chapter 11 scattering 散射

11.1 引言

11.1.1 classical scattering



11.1. b 为撞击参数(impact parameter)/瞄准距离， 偏转角度θ(scattering angle)

Definition of the proble: Given the b, calculate the θ.

$$b = R\sin\alpha = R\sin\left(\frac{\pi}{2} - \frac{\theta}{2}\right) = R\cos\frac{\theta}{2}$$

$$\theta = \pi - 2\alpha$$

$$\theta = \begin{cases} 2\cos^{-1}\left(\dfrac{b}{R}\right) & , \ b < R \\ 0 & , \ b > R \end{cases}$$

拓展到三维： 定义微分散射界面：$D(\theta) = \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$

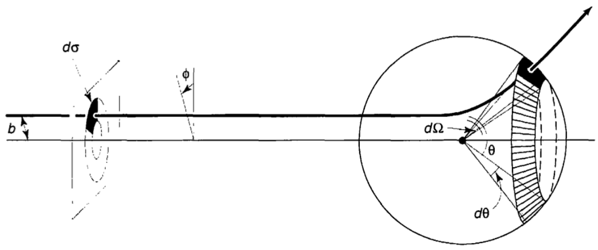


FIGURE 11.3: Particles incident in the area $d\sigma$ scatter into the solid angle $d\Omega$.

$$\boxed{d\sigma = D(\theta)\, d\Omega.} \qquad [11.3]$$

$$\because \begin{cases} \mathrm{d}\sigma = b\mathrm{d}b\mathrm{d}\phi \\ \mathrm{d}\Omega = \sin\theta\mathrm{d}\theta\mathrm{d}\phi \end{cases}$$

$$\Rightarrow D(\theta) = \frac{b}{\sin\theta}\left|\frac{\mathrm{d}b}{\mathrm{d}\theta}\right|$$

例 11.2. 将$b = R\cos\frac{\theta}{2}$, 代入$D(\theta) = \frac{b}{\sin\theta}\left|\frac{\mathrm{d}b}{\mathrm{d}\theta}\right|$

$$\Rightarrow D(\theta) = \frac{b}{\sin\theta}\left(\frac{1}{2}R\sin\frac{\theta}{2}\right) = \frac{R\cos\left(\frac{\theta}{2}\right)}{2\sin\frac{\theta}{2}\cos\frac{\theta}{2}}\left(\frac{1}{2}R\sin\frac{\theta}{2}\right) = \frac{R^2}{4}$$

总的散射截面面积为

$$\sigma \equiv \int D(\theta)\,\mathrm{d}\Omega \qquad [11.7]$$

It is total area of incident beam that is scattered by the target, For the hard sphere:

$$\sigma \equiv \int D(\theta)\,\mathrm{d}\Omega = \frac{R^2}{4} \times 4\pi = \pi R^2$$

假定有一束具有均匀强度的入射粒子$\mathcal{L} \equiv$单位时间内通过单位面积的入射粒子数目。在单位时间内通过面积$\mathrm{d}\sigma$(散射到立体角$\mathrm{d}\Omega$内)的粒子数目是 $\mathrm{d}N = \mathcal{L}\mathrm{d}\sigma = \mathcal{L}D(\theta)\,\mathrm{d}\Omega$, 因此，

$$D(\theta) = \frac{1}{\mathcal{L}}\frac{\mathrm{d}N}{\mathrm{d}\Omega} \qquad [11.10]$$

11.1.2 Quantum Scattering theory

$$\text{Wave function} \begin{cases} \text{Incident plane wave } \psi(z) = Ae^{ikz} \\ \text{Scattering spherical wave } \sim \frac{e^{ikr}}{r} \end{cases}$$

$$\begin{aligned} \psi(r,\theta) &= A\left[e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right] \quad \text{for large} \quad r \\ &= \quad z\text{方向} \quad \text{任意方向}\left(\text{make } |\psi|^2 \propto \left|\frac{1}{r^2}\right|\right) \end{aligned}$$

$f(\theta)$ 为散射振幅，表示θ 方向上的散射几率进而与微分截面联系。

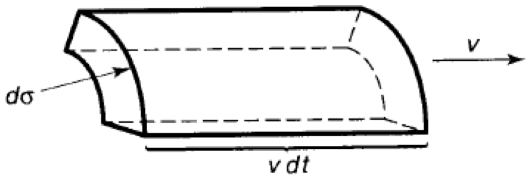


图 11.5：在时间 dt 内通过面积 $d\sigma$ 的入射束体积 dV。

以速度 v 运行的入射粒子在时间 $\mathrm{d}t$ 内通过无穷小面积 $\mathrm{d}\sigma$ 的几率为:

$$\mathrm{d}p = |\psi_{\text{incident}}|^2 \mathrm{d}V = |A|^2 v\,\mathrm{d}t\,\mathrm{d}\sigma \quad ①$$

which is equal to the probability that the scatter into the $\mathrm{d}\Omega$

$$\mathrm{d}p = |\psi_{\text{scattering}}|^2 \mathrm{d}V = \frac{|A|^2 f^2}{r^2} v\mathrm{d}t\mathrm{d}r^2\mathrm{d}\Omega = |A|^2 f^2 v\mathrm{d}t\mathrm{d}\Omega \quad ②$$

$$\text{由}① = ② \Rightarrow \mathrm{d}\sigma = |f|^2 \mathrm{d}\Omega \quad \Rightarrow D(\theta) = \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\theta)|^2$$

两种计算$f(\theta)$的方法：

1. Particle wave analysis
2. Born approximation (Green function)

11.2 Particle wave analysis 分波法

11.2.1 理论表述

由 第四章 中关于氢原子核外电子的波函数 $\psi(r,\theta,\phi) = R(r)Y_\ell^m(\theta,\phi)$

令 $u(r)=rR(r)$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2u}{\mathrm{d}r^2}+\left[V(r)+\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]u=Eu$$

1. Radiation zone (at long r, $V(r)\to 0$, $\frac{1}{r^2}\to 0$)

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2u}{\mathrm{d}r^2}\approx Eu \qquad \frac{\mathrm{d}^2u}{\mathrm{d}r^2}=-k^2u \qquad k=\frac{\sqrt{2mE}}{\hbar}$$

assume $u=e^{\lambda r}\Rightarrow\lambda^2e^{\lambda r}=-k^2e^{\lambda r}\quad\lambda=\pm ik$

$\Rightarrow u(r)=\underbrace{Ce^{ikr}}_{\text{出射球面波}}+\underbrace{De^{-ikr}}_{\text{入射球面波}}$

r 非常大时，$u(r)\sim e^{ikr}\Rightarrow R(r)\sim\frac{e^{ikr}}{r}$

2. 中间情况(仅有$V(r)\to 0$)

$$\frac{\mathrm{d}^2u}{\mathrm{d}r^2}-\frac{\ell(\ell+1)}{r^2}u=-k^2u \qquad [11.17]$$

通解： 球贝塞尔函数的线性组合

$$rR(r)=u(r)=Arj_r(k_r)+Brn_l(k_r)$$

use Hankel 函数

$$h_l^{(1)}(x)\equiv j_l(x)+in_l(x) \qquad h_1^{(2)}\equiv j_l(x)-in_l(x)$$

$h_0^{(1)}=-\frac{i}{x}e^{ikx}$	$h_0^{(2)}=\frac{i}{x}e^{-ikx}$
$h_1^{(1)}=-\left(\frac{i}{x^2}-\frac{1}{x}\right)e^{ikx}$	$h_1^{(2)}=\left(\frac{i}{x^2}-\frac{1}{x}\right)e^{-ikx}$
$h_2^{(1)}=\left(-\frac{3i}{x^3}-\frac{3}{x^2}+\frac{i}{x}\right)e^{ix}$	$h_2^{(2)}=\left(\frac{3i}{x^3}-\frac{3}{x^2}+\frac{i}{x}\right)e^{-ikx}$
当$x\gg 1$时，$\begin{cases}h_1^{(1)}\to\frac{1}{x}(-i)^{l+1}e^{ix}\\h_1^{(2)}\to\frac{1}{x}(i)^{l+1}e^{-ix}\end{cases}$	

r很大时，$h_l^1(kr)=\frac{e^{ikr}}{r}\qquad h_l^2(kr)\to\frac{e^{-ikr}}{r}$, 对于出射波，$h_l^1(kr)$满足 $h_l^{(1)}(kr)\sim R(r)$

$$V(r)=0\text{时，}\psi(r,\theta,\phi)=A\left[e^{ikz}+\sum_{l,m}C_{l,m}h_l^1(kr)Y_l^m(\theta,\phi)\right] \qquad [11.21]$$

由于球对称性，ψ 不依赖于ϕ, Y_l^m中仅有$m=0$ 项存在$Y_l^m\propto e^{im\phi}$

$$Y_l^0(\theta,\phi)=\sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta) \qquad [11.22]$$

令$C_{l_0}=i^{k+1}k\sqrt{4\pi(2l+1)}a_l$, 将[11.22]代入[11.21]

$$\psi(r,\theta)\;=\;A\left[e^{ikz}+k\sum_{l=0}^{\infty}i^{l+1}(2l+1)\underbrace{a_l}_{\text{第}l\text{个分波振幅}}h_l^{(1)}(kr)P_1(\cos\theta)\right] \qquad [11.23]$$

而当r很大时，$h_l^{(1)}(kr)\to(-i)^{k+1}\frac{e^{ikr}}{kr}$,

$$\psi(r,\theta)=A\left[e^{\mathrm{ikz}}+f(\theta)\frac{e^{ikr}}{r}\right] \qquad [11.24]$$

其中，$f(\theta)=\sum\limits_{l=0}^{\infty}(2l+1)a_l p_l(\cos\theta)$ [11.25]

$$D(\theta)=|f(\theta)|^2=\sum_{l}\sum_{l'}(2l+1)(2l'+1)a_l^{\star}a_l^{'}P_l(\cos\theta)P_l^{'}(\cos\theta)$$

$$\begin{aligned}\sigma &= \int D(\theta)\,\mathrm{d}\Omega\\ &= \int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\sin\theta\sum_{l,l'}(2l+1)(2l'+1)a_l^{\star}a_l^{'}P_l(\cos\theta)P_l^{'}(\cos\theta)\\ &= \sum_{l,l'}(2l+1)(2l'+1)a_l^{\star}a_l^{'}\times 2\pi\int_0^{\pi}\mathrm{d}\theta\sin\theta P_l(\cos\theta)P_l^{'}(\cos\theta)\end{aligned}$$

由正交归一性$\int_{-1}^{1}P_l(x)P_l^{'}(x)\,\mathrm{d}x=\frac{2}{2l+1}\delta_{ll'}$

$$\begin{aligned}\sigma &= \sum_{l,l'}(2l+1)(2l'+1)a_l^{\star}a_l^{'}\cdot 2\pi\cdot\frac{2}{2l+1}\delta_{ll'}\\ &= \sum_{l}(2l+1)|a_l|^2 2\pi\cdot 2\\ &= 4\pi\sum_{l}^{\infty}(2l+1)|a_l|^2 \qquad [11.27]\end{aligned}$$

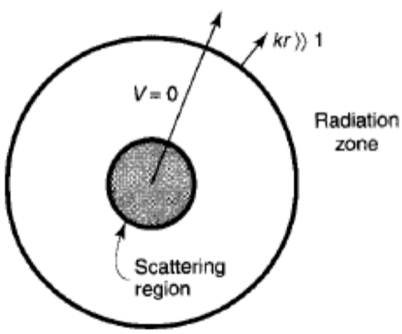
11.2.2 计算 a_l

在前面的计算中，散射波用球坐标，而入射波用笛卡尔坐标，接下来我们需要统一记号。将e^{ikz}用球坐标表示， 利用Rayleigh's formula

$$e^{ikz}=\sum_{l=0}^{\infty}i^l(2l+1)j_l(kr)P_l(\cos\theta) \qquad [11.25]$$

联立[11.23] + [11.28]

$$\psi(r,\theta)=A\sum_{l=0}^{\infty}i^l(2l+1)[j_l(kr)+ika_l h_l^{(1)}(kr)]P_1(\cos\theta)$$



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$$\psi(r,\theta) = A\left\{e^{ikz}+f(\theta)\frac{e^{ikr}}{r}\right\}$$

incident waves outgoing wave

Differenctial cross-section $D(\theta)=|f(\theta)|^2$

Total cross-section: $\sigma=\int f(\theta)\,\mathrm{d}\Omega=\sum_l(2l+1)^2|\sigma_l|^2\cdot 2\pi\cdot\frac{2}{2\rho+1}=4\pi\sum_{l=0}^{\infty}(2l+1)|a_l|^2$[11.27]

$$f(\theta)=\sum_{l=0}^{\infty}(2l+1)a_lP_l(\cos\theta)$$

$$e^{ikz}=\sum_{l=0}^{\infty}i^l(2l+1)j_l(kr)P_l(\cos\theta)\quad[11.28]$$

$J_l(kr)$ Bessel function

$$\psi(r,\theta)=A\sum_{l=0}^{\infty}i^l(2l+1)[j_l(kr)+ika_l(kl)]P_l(\cos\theta)\qquad[11.29]$$

例11.3. 量子硬球散射

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

Boundary condition : $\psi(r=R,\theta)=0$

$$由\sum_{l=0}^{\infty}i^l(2l+1)[j_l(kR)+ika_lh_l^{(1)}(kR)]\cdot\underbrace{\int_0^{\pi}\mathrm{d}\theta\sin\theta P_l(\cos\theta)P_l'(\cos\theta)}_{\frac{2}{2l+1}}=0$$

$$\Rightarrow j_{l'}(kR)+ika_lh_{l'}^{(1)}(kR)=0\Rightarrow a_l=i\frac{j_l(kR)}{kh_l(kR)}$$

由 11.27 $\sigma=\frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\left|\frac{j_r(kR)}{h_l(kR)}\right|^2$ [11.34]

在长波极限下（能量极低的极限下）$\Leftrightarrow kR\ll1$ or $\frac{2\pi}{\lambda}R\ll1$ or $\lambda\gg R$

In [11.34] we need to evaluate

$$\frac{j_l(kR)}{h_l(kR)}=\frac{j_l(z)}{j_l(z)+in_l(z)}\approx-i\frac{j_l(z)}{n_l(z)}\approx z^{2l+1}$$

For $l=0$, $\frac{j_l(z)}{n_l(z)}\sim z$ 0.1 for example

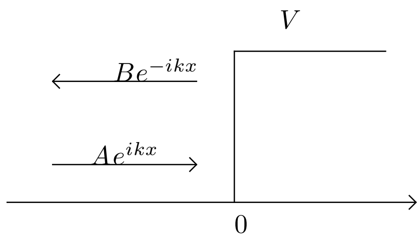
For $l=1$, $\frac{j_l(z)}{n_l(z)}\sim z^3$ 0.001 $\ll$ 故只取零级近似

$\therefore$ 由11.34 得到

$$\begin{aligned}\sigma &\cong \frac{4\pi}{k^2}\left|\frac{j_0(kR)}{h_0(kR)}\right|^2 \qquad \left(h_0^{(1)}=-i\frac{e^{ix}}{x},j_0^{(1)}=\frac{h^{(1)}+h^{(0)}}{2}=\frac{-ie^{ix}+ie^{-ix}}{2}=\frac{\sin x}{x}\right)\\ &\cong \frac{4\pi}{k^2}\left|\frac{\frac{\sin kR}{kR}}{-i\frac{e^{ikR}}{kR}}\right|^2\\ &= \frac{4\pi}{k^2}\sin^2 kR\\ &\approx \frac{4\pi}{k^2}(kR)^2=\underbrace{4\pi}_{\text{solid angle}}R^2=\sigma\ (\text{total cross}-\text{section})\end{aligned}$$

由z轴入射到球中，球在各个方向均有散射，而不是classical中的只有πR^2的面积。

11.3 phase shift 相移



Incident $\psi_i = Ae^{ikx}$
Reflect $\psi_r = Be^{-ikx}$

Total wave function $\psi(x) = Ae^{ikx} + Be^{-ikx}$, $\psi(x=0) = 0 \Rightarrow A + B = 0$

$$\Rightarrow \psi(x) = A(e^{ikx} - e^{-ikx}) = A(e^{ikx} + \underbrace{e^{i\pi}}_{\text{Phase shift}} e^{-ikx})$$

in general:

$$\Rightarrow \psi(x) = A[e^{ikx} + e^{i(2\delta - kx)}]$$

For spherical waves: $a_l = \frac{1}{2ik}(e^{2i\delta_l} - 1) = \frac{1}{k}e^{i\delta_l}\sin\delta_l$

将a_l代入到 [11.25] 和 [11.27]

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin(\delta_l)\,p_l(\cos\theta) \qquad [11.47]$$

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \qquad [11.48]$$

11.4 Born approximation 玻恩近似（格林函数法解 $f(\theta)$）

11.4.1 Intefral form of Schrödinger Equation

time - independent function can be written as:

$$\begin{aligned} -\frac{\hbar^2}{2m}\nabla^2\psi - E\psi &= -V\psi \\ \left(\nabla^2\psi + \frac{2mE}{\hbar^2}\psi\right) &= \frac{2mV}{\hbar^2}\psi \qquad \text{（亥姆霍兹方程，球坐标形式）} \\ (\nabla^2 + k^2)\psi &= Q \end{aligned}$$

$Q \equiv \frac{2m}{\hbar^2}V(r)\psi(r)$ 非齐次项，$k \equiv \frac{\sqrt{2mE}}{\hbar}$。

定义. *Green function: suppose we could find a function $G(r)$ that solves the Helmholtz equation with a delta function "source"*

$$(\nabla^2 + k^2)G(r) = \delta^3(r) \qquad \text{where } \delta^3(r) = \delta(x)\delta(y)\delta(z)$$

Then we could express ψ as a Integral (卷积)

$$\psi(r) = \int G(r - r_0)\,Q(r_0)\,\mathrm{d}^3 r_0$$

$$\begin{aligned} (\nabla^2 + k^2)\psi(r) &= (\nabla^2 + k^2)\int G(r - r_0)\,Q(r_0)\,\mathrm{d}^3 r \\ \updownarrow \quad &= \int \delta(\vec{r} - \vec{r}_0)\,Q(\vec{r}_0)\,\mathrm{d}^3\vec{r}_0 \\ Q(\vec{r}) &= Q(\vec{r}) \end{aligned}$$

$G(r)$: Green's function for the Helmholtz equation. Our task is to find $\boldsymbol{G(\vec{r})}$

傅里叶变化:

$$G(r) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int e^{is\cdot r} g(s)\,\mathrm{d}^3 s \quad [11.54]$$

δ function 定义式：$\delta^3(r) \equiv \frac{1}{(2\pi)^3}\int e^{is\cdot r}\mathrm{d}^3 s$，而

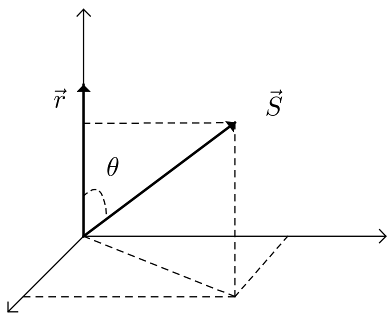
$$\delta^3(r) = (\nabla^2 + k^2)G(r) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int (\nabla^2 + k^2)e^{is\cdot r} g(s)\,\mathrm{d}^3 s = \frac{1}{(2\pi)^{\frac{3}{2}}}\int (-s^2 + k^2)e^{is\cdot r} g(s)\,\mathrm{d}^3 s$$

$$\frac{1}{(2\pi)^3}\int e^{is\cdot r}\mathrm{d}^3 s = \frac{1}{(2\pi)^{\frac{3}{2}}}\int (-s^2 + k^2)e^{is\cdot r} g(s)\,\mathrm{d}^3 s$$

$$\Rightarrow \frac{1}{(2\pi)^{\frac{3}{2}}} = (-s^2 + k^2)\,g(s)$$

$$g(s) = \frac{1}{(2\pi)^{\frac{3}{2}}(k^2 - s^2)} \qquad [11.57]$$

Bring back we find:



$$\begin{aligned}
G(r) &= \frac{1}{(2\pi)^3}\int e^{is\cdot r}\cdot\frac{1}{k^2\cdot s^2}\mathrm{d}^3 s \\
&= \frac{1}{(2\pi)^3}\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\,\sin\theta\int_0^{\infty}\mathrm{d}s\, s^2 e^{is\cdot r}\frac{1}{k^2 - s^2} \\
&= \frac{1}{(2\pi)^3}\cdot 2\pi\int_0^{\infty}\mathrm{d}s\cdot s^2\frac{1}{k^2 - s^2}\int_0^{\pi}\mathrm{d}\theta\,\sin\theta e^{isr\cos\theta} \\
&= \frac{1}{4\pi^2}\int_0^{\infty}\mathrm{d}s\cdot s^2\frac{1}{k^2 - s^2}\frac{1}{i\,sr}(e^{isr} - e^{-isr})\ (\text{even function}) \\
&= -\frac{1}{2}\frac{i}{4\pi^2 r}\int_{-\infty}^{\infty}\mathrm{d}s\,\frac{s}{k^2 - s^2}(e^{isr} - e^{-isr})
\end{aligned}$$

这里利用偶函数进行积分范围的扩充，是为了后面使用留数定理。

解析延拓：

$$G(\vec{r}) = -\frac{i}{8\pi^2 r}\int_{-\infty}^{\infty}\frac{s(e^{isr} - e^{-isr})}{k^2 - s^2 + i0^+}$$

$i0^+$是一个无穷接近0的复数（为了把奇点全包含或者全排除）

$$G(\vec{r}) = \frac{i}{8\pi^2 r}\int_{-\infty}^{\infty}\frac{s(e^{isr} - e^{-isr})}{(s + k + i0^+)(s - k - i0^+)}$$

$$
\begin{aligned}
&= \frac{i}{8\pi^2 r}\left[\int_{-\infty}^{\infty}\frac{s e^{is\cdot r}\mathrm{d}s}{(s+k+i0^+)\,(s-k-i0^+)}-\int_{-\infty}^{\infty}\frac{s\cdot e^{-is\cdot r}\mathrm{d}s}{(s+k+i0^+)\,(s-k-i0^+)}\right]\\
&= \frac{i}{8\pi^2 r}[I_1-I_2]
\end{aligned}
$$

Turn $\int_{-\infty}^{\infty}\mathrm{d}s$ to a complex phase $(s=\operatorname{Re}z,\operatorname{Im}(z))$

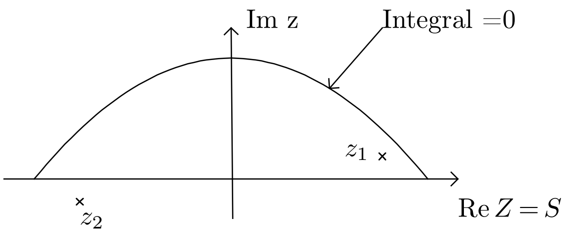
then we use 留数定理。

定理. *Residue theorem:*

$$\oint\frac{f(z)}{z-z_0}=2\pi i f(z_0)$$

We need to choose a contour so that the intefrand goes to 0 as z goes to infinity.

$\text{Counter}=I_1+\operatorname{Im}\text{path}=I_1$

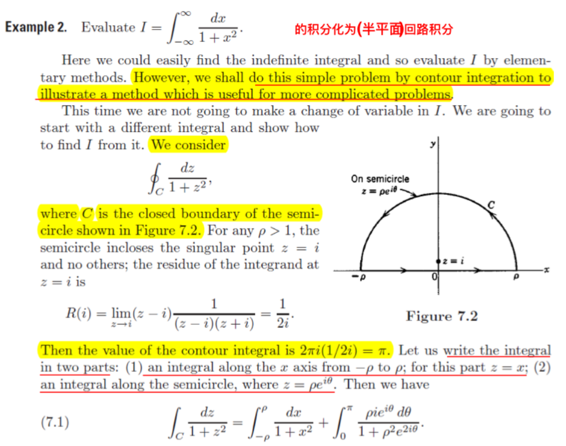


1. For I_1: $I_1=\int_{-\infty}^{\infty}\mathrm{d}s\frac{s\cdot e^{is\cdot r}}{(s-k-i0^+)\,(s+k+i0^+)}$, where $e^{is\cdot r}\rightarrow e^{i(\operatorname{Re}z+\operatorname{Im}z)r}=e^{i\operatorname{Re}zr}e^{-\operatorname{Im}zr}$

   if $\operatorname{Im}z\rightarrow 0$, then the Integral $\rightarrow 0$

2. For I_2: $I_2=-i\pi e^{ikr}$

Some material about residue theorem:



Example 2. Evaluate $I=\int_{-\infty}^{\infty}\frac{dx}{1+x^2}$. 的积分化为(半平面)回路积分

Here we could easily find the indefinite integral and so evaluate I by elementary methods. However, we shall do this simple problem by contour integration to illustrate a method which is useful for more complicated problems.

This time we are not going to make a change of variable in I. We are going to start with a different integral and show how to find I from it. We consider

$$\oint_C\frac{dz}{1+z^2},$$

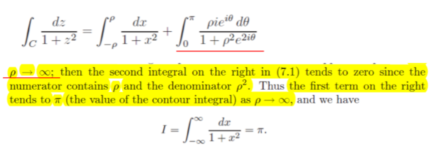
where C is the closed boundary of the semicircle shown in Figure 7.2. For any $\rho>1$, the semicircle incloses the singular point $z=i$ and no others; the residue of the integrand at $z=i$ is

$$R(i)=\lim_{z\to i}(z-i)\frac{1}{(z-i)(z+i)}=\frac{1}{2i}.$$

Figure 7.2

Then the value of the contour integral is $2\pi i(1/2i)=\pi$. Let us write the integral in two parts: (1) an integral along the x axis from $-\rho$ to ρ; for this part $z=x$; (2) an integral along the semicircle, where $z=\rho e^{i\theta}$. Then we have

$$\int_C\frac{dz}{1+z^2}=\int_{-\rho}^{\rho}\frac{dx}{1+x^2}+\int_0^{\pi}\frac{\rho i e^{i\theta}\,d\theta}{1+\rho^2e^{2i\theta}}. \tag{7.1}$$



$$\int_C\frac{dz}{1+z^2}=\int_{-\rho}^{\rho}\frac{dx}{1+x^2}+\int_0^{\pi}\frac{\rho i e^{i\theta}\,d\theta}{1+\rho^2e^{2i\theta}}$$

$\rho\to\infty$; then the second integral on the right in (7.1) tends to zero since the numerator contains ρ and the denominator ρ^2. Thus the first term on the right tends to π (the value of the contour integral) as $\rho\to\infty$, and we have

$$I=\int_{-\infty}^{\infty}\frac{dx}{1+x^2}=\pi.$$

$$G(\boldsymbol{r})=\frac{i}{8\pi^2 r}[\,(i\pi e^{ikr})-(-i\pi e^{ikr})\,]=-\frac{e^{ikr}}{4\pi r}$$

以上为特解，通解由$(\nabla^2+k^2)\,G_0(\boldsymbol{r})=0\Rightarrow\psi_0$，$\psi_0$为无势场存在的通解。

薛定谔方程的一般解(薛定谔方程的积分形式)为

$$\psi(r)=\psi_0(r)-\frac{m}{2\pi\hbar}\int\frac{e^{ik|\boldsymbol{r}-\boldsymbol{r_0}|}}{|\boldsymbol{r}-\boldsymbol{r_0}|}V(r_0)\,\psi(r_0)\,\mathrm{d}^3r_0 \quad [11.67]$$

其中ψ_0满足自由粒子薛定谔方程$(\nabla^2+k^2)\,\psi_0=0$

11.4.2 一阶玻恩近似

假设$V(r_0)$ 是在$r_0=0$（原子附近)的局部势，我们想计算远离散射中心的$\psi(\boldsymbol{r})$。在[11.67]中对积分有贡献的所有区域都有 $|r|\gg|r_0|$

$$|r-r_0|^2=r^2+r_0^2-2\boldsymbol{r}\cdot\boldsymbol{r_0}\cong r^2\left(1-2\frac{\boldsymbol{r}\cdot\boldsymbol{r_0}}{r^2}\right)^{\frac{1}{2}}$$

$$|r-r_0|=r\sqrt{1-2\frac{\vec{r}\cdot\vec{r}_0}{r^2}}\approx r\left(1-\frac{\vec{r}\cdot\vec{r}_0}{r^2}\right)=\vec{r}-\hat{r}\cdot\vec{r}_0$$

令$\vec{k}=k\hat{r}$,$e^{ik(\vec{r}-\vec{r}_0)}=e^{ikr-ik\hat{r}\cdot\vec{r}_0}=e^{ikr}e^{-i\vec{k}\cdot\vec{r}_0}$

因此有：$\frac{e^{ik|\vec{r}-\vec{r}_0|}}{|\vec{r}-\vec{r}_0|}\approx\frac{e^{ikr}\cdot e^{-i\vec{k}\cdot\vec{r}_0}}{r}$，入射波$\psi_0(\vec{r})=Ae^{ikz}$

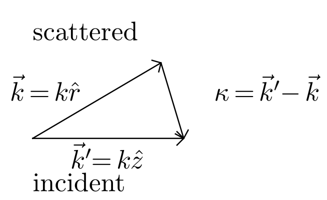
$$\begin{aligned}\psi(r)&=Ae^{ikz}-\frac{m}{2\pi\hbar^2}\int\frac{e^{ikr}}{r}e^{-i\vec{k}\cdot\vec{r}_0}V(r_0)\,\psi(\vec{r}_0)\,\mathrm{d}^3r_0\\&=Ae^{ikz}-\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int e^{-i\vec{k}\cdot\vec{r}_0}V(r_0)\,\psi(r_0)\,\mathrm{d}^3r_0\end{aligned}$$

而对照$\psi=A\left[e^{ikz}+\frac{e^{ikr}}{r}f(\theta)\right]$

$$f(\theta)=-\frac{m}{2\pi\hbar^2A}\int e^{-i\vec{k}\cdot\vec{r}_0}V(r_0)\,\psi(r_0)\,\mathrm{d}^3r_0$$

玻恩近似： $\psi(\vec{r}_0)\approx\psi_0(\vec{r}_0)=Ae^{ikz_0}=Ae^{i\vec{k}\cdot\vec{r}_0}$，其中$\vec{k}=k\hat{z}$(沿着$z$轴)

$$\Rightarrow f(\theta)=-\frac{m}{2\pi\hbar^2}\int e^{i(\vec{k}'-\vec{k})\cdot\vec{r}_0}V(r_0)\,\mathrm{d}^3r$$



low-energy(long-wave) Scattering

$e^{i(\vec{k}'-\vec{k})\cdot\vec{r}_0}\approx e^0=1,\ \lambda\gg2\pi r_0\Leftrightarrow r_0\ll1$

$$f(\theta)=-\frac{m}{2\pi\hbar^2}\int V(\vec{r})\,\mathrm{d}^3r$$

球对称情形下$V(r)=V(r,\theta,\varphi)$

定义$\vec{\kappa}=\vec{k}'-\vec{k}$, 表示$\vec{k}'$与$k$之间存在的动量传递。

$$(\vec{k}'-\vec{k})\cdot r_0=\kappa r_0\cos\theta$$

$$f(\theta)=-\frac{m}{2\pi\hbar^2}\int r_0^2\mathrm{d}r_0\int_0^{\pi}\mathrm{d}\theta_0\sin\theta_0 e^{i\kappa r_0\cos\theta_0}\int_0^{2\pi}\mathrm{d}\phi_0 V(r)$$

$$f(\theta)=-\frac{2m}{\hbar^2\kappa}\int_0^{\infty}rV(r)\sin(\kappa r)\,\mathrm{d}r$$

其中$\kappa=2k\sin\frac{\theta}{2}$.

例. 11.5 汤川散射

$$V(r)=\beta\frac{e^{-\mu r}}{r}$$

$$\Rightarrow f(\theta)=-\frac{2mq_1q_2}{4\pi\varepsilon_0\hbar^2\kappa^2}=-\frac{2mq_1q_2}{4\pi\varepsilon_0\hbar^2\left(2\sqrt{\frac{2mE}{\hbar^2}}\sin\frac{\theta}{2}\right)^2}=-\frac{q_1q_2}{16\pi\varepsilon_0 E\sin^2\left(\frac{\theta}{2}\right)}$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}=|f(\theta)|^2=\left(\frac{q_1q_2}{16\pi\varepsilon_0 E\sin^2\left(\frac{\theta}{2}\right)}\right)^2$$

11.4.3 Born Series

$$\psi(r)=\psi_0(r)+\int g(r-r_0)V(\vec{r}_0)\psi(\vec{r}_0)\,\mathrm{d}^3r_0\qquad g(r)\equiv-\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}$$

$$\Rightarrow\psi=\psi_0+\int gV\psi\,(\text{代入上式的}\psi)$$

$$\psi=\psi_0+\int gV\psi_0+\iint gVgV\psi_0+\iiint gVgVgV\psi_0+\cdots[11.101]$$

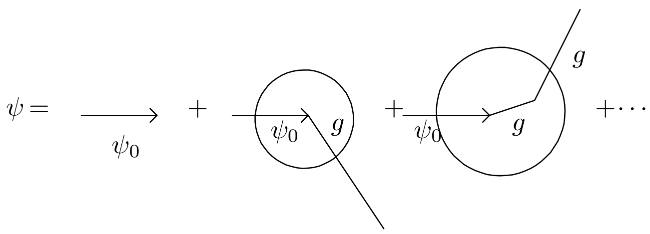


图. 玻恩级数的图形分析

每一项被积函数中只有入射波函数ψ_0,零阶波函数不受势的影响，一阶波函数与势相互作用一次，沿新方向传播，二阶作用两次...

本文档主要参考卢海舟老师2023秋季学期量子力学二的板书内容以及格里菲斯《 Introduction To Quantum Mechanics》 中相关章节的内容， 由李乐安和孙全超整理并编写。 如有错误， 请发送您的观点到邮箱12110811@mail.sustech.edu.cn， 经核实更正后我们将会更新并为您提供最新的文档版本。