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Quantum Mechanics *Homework 2* *4/25/2017*

1. For a system of two particles with the angular momentum $j = 1$, respectively, work out the couplings of the total angular momenta explictly by finding out the coupling states and the corresponding Clebsch-Gordan coefficients starting from applying the total lowing operator $\hat{J}_-$ on the highest state $|2,2\rangle = |1,1;1,1\rangle$.

2. If two electrons carry the orbital angular momentum $2\hbar$ and $\hbar$, respectively, and in the state $|l_1 l_2; lm\rangle = |2,1;2,0\rangle$. If the measurement of L_{1z} is made in this state, What values may be found and with what probabilities?

3. If a hydrogen atom in at D-state with $j = 3/2, m_j = -1/2$, what is the probability of finding its electron with the spin pointing upward?

4. Consider two nonidentical spin $s = 1/2$ particles with Hamiltonian

$$\hat{\mathbf{H}} = \frac{\epsilon_o}{\hbar^2}(\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2)^2 + \frac{\epsilon_o}{\hbar^2}(\hat{S}_{1z} + \hat{S}_{2z})^2,$$

where ϵ_o is a constant having the dimensions of energy. Find the energy levels and their degeneracies.

5. Consider a quantum system with just three independent states. The Hamiltonian, in matrix form, is

$$H = V_o \begin{pmatrix} 2 & -\epsilon & 0 \\ \epsilon & 1 & 0 \\ 0 & 0 & 3+\epsilon \end{pmatrix},$$

where V_o is a constant and ϵ is some small number ($\epsilon \ll 1$).

(a) Write down the unpeturbated and peturbated Hamiltonian.

(b) Find the 2nd order corrected energies and 1st order corrected wave functions for H by peturbation theory.

(c) Solve for the exact eigenvalues of H. Expand each of them as a power series in ϵ, up to second order.

或
$$E(\lambda)=\varepsilon_0+\varepsilon_1\lambda+\varepsilon_2\lambda^2+\cdots+\varepsilon_n\lambda^n+\cdots \tag{9.8}$$

假設狀態 $|\varphi(\lambda)\rangle$ 亦可以 λ 之多次式展開（非泰勒級數）表示為

$$|\varphi(\lambda)\rangle=|0\rangle+\lambda|1\rangle+\lambda^2|2\rangle+\cdots+\lambda^n|n\rangle+\cdots \tag{9.9}$$

（上式為微擾理論中之唯一假設）其中 $\varepsilon_1,\varepsilon_2,\cdots,\varepsilon_n$，及 $|0\rangle,|1\rangle,\cdots,|n\rangle$ 即為我們所要解出的結果。將式(9.8)、(9.9)代入(9.7)得

$$(\hat{H}_0+\lambda\hat{V})(|0\rangle+\lambda|1\rangle+\lambda^2|2\rangle+\cdots)$$
$$=(\varepsilon_0+\varepsilon_1\lambda+\varepsilon_2\lambda^2+\ldots)(|0\rangle+\lambda|1\rangle+\lambda^2|2\rangle+\cdots) \tag{9.10}$$

比較等號兩邊 λ 各次方之係數，可得

λ^0 之係數
$$\hat{H}_0|0\rangle=\varepsilon_0|0\rangle \tag{9.11}$$

λ^1 之係數
$$\hat{H}_0|1\rangle+\hat{V}|0\rangle=\varepsilon_0|1\rangle+\varepsilon_1|0\rangle \tag{9.12}$$

或
$$(\hat{H}_0-\varepsilon_0)|1\rangle+(\hat{V}-\varepsilon_1)|0\rangle=0 \tag{9.13}$$

λ^2 之係數
$$\hat{H}_0|2\rangle+\hat{V}|1\rangle=\varepsilon_0|2\rangle+\varepsilon_1|1\rangle+\varepsilon_2|0\rangle \tag{9.14}$$

或
$$(\hat{H}_0-\varepsilon_0)|2\rangle+(\hat{V}-\varepsilon_1)|1\rangle-\varepsilon_2|0\rangle=0 \tag{9.15}$$

若要求固有向量 $|\varphi(\lambda)\rangle$ 具有歸一化條件

$$\langle\varphi(\lambda)|\varphi(\lambda)\rangle=1 \tag{9.16}$$

則在零級或對 λ^0 之係數而言

$$\boxed{\langle 0|0\rangle = 1} \tag{9.17}$$

對一級或 λ^1 之係數而言

$$\begin{aligned}\langle \varphi(\lambda)|\varphi(\lambda)\rangle &= 1\\ &= (\langle 0| + \lambda\langle 1|)(|0\rangle + \lambda|1\rangle) + \lambda^2 \text{ 以上之高次項（記作 } O(\lambda^2)\text{）}\\ &= \langle 0|0\rangle + \lambda(\langle 1|0\rangle + \langle 0|1\rangle) + O(\lambda^2)\end{aligned} \tag{9.18}$$

故

$$\langle 1|0\rangle + \langle 0|1\rangle = 0 \tag{9.19}$$

若

$$\langle 0|1\rangle = \text{實數} = \langle 1|0\rangle \tag{9.20}$$

由式(9.19)與(9.20)，所以

$$\boxed{\langle 1|0\rangle = 0 = \langle 0|1\rangle} \tag{9.21}$$

同理，對二級或 λ^2 之係數而言

$$\begin{aligned}\langle \varphi(\lambda)|\varphi(\lambda)\rangle &= 1\\ &= (\langle 0| + \lambda\langle 1| + \lambda^2\langle 2|)(|0\rangle + \lambda|1\rangle + \lambda^2|2\rangle) + O(\lambda^4)\\ &= \langle 0|0\rangle + \lambda(\langle 0|1\rangle + \langle 1|0\rangle) + \lambda^2(\langle 1|1\rangle + \langle 2|0\rangle + \langle 0|2\rangle) + O(\lambda^3)\end{aligned} \tag{9.22}$$

因要求

$$\langle 0|\varphi(\lambda)\rangle = \text{實數} = \langle 0|0\rangle + \lambda\langle 0|1\rangle + \lambda^2\langle 0|2\rangle \tag{9.23}$$

故

$$\langle 0|2\rangle = \text{實數} = \langle 2|0\rangle \tag{9.24}$$

由式(9.21)和(9.22)知

$$\langle 1|1\rangle + \langle 2|0\rangle + \langle 0|2\rangle = 0 \tag{9.25}$$

再由式(9.24)，所以

$$\langle 1|1\rangle = -2\langle 0|2\rangle \quad \text{或} \quad \boxed{\langle 0|2\rangle = \langle 2|0\rangle = -\frac{1}{2}\langle 1|1\rangle} \tag{9.26}$$

9.2 對無退化狀態的微擾

若 $\hat{H}_0$ 的固有值 E_n^0 不含退化狀態，則所對應的固有狀態僅有唯一的 $|\varphi_n\rangle$，即

$$\hat{H}_0|\varphi_n\rangle = E_n^0|\varphi_n\rangle \tag{9.27}$$

因在 $\lambda \to 0$ 時

$$\begin{aligned}\hat{H}(\lambda)|\varphi(\lambda)\rangle &= \hat{H}_0|\varphi(\lambda=0)\rangle = \hat{H}_0|0\rangle \\ &= E(\lambda)|\varphi(\lambda)\rangle = E_n^0|\varphi(\lambda=0)\rangle = E_n^0|0\rangle\end{aligned} \tag{9.28}$$

與零級方程式(9.11)比較，得

$$\varepsilon_0 = E_n^0 \quad , \quad |0\rangle = |\varphi_n\rangle \tag{9.29}$$

我們將於底下，推導並求得 $E(\lambda)$ 之一級與二級修正項，即 ε_1 與 ε_2，以及 $|\varphi(\lambda)\rangle$ 之一級修正項，即狀態 $|1\rangle$。

(一) **一級修正**（求得能量解 ε_1 與狀態 $|1\rangle$ 之形式）

(1) 將式(9.13)投影在 $|\varphi_n\rangle$ 上，得

$$\langle\varphi_n|\hat{H}_0 - \varepsilon_0|1\rangle + \langle\varphi_n|\hat{V} - \varepsilon_1|0\rangle = 0 \tag{9.30}$$

$$E_n^0\langle\varphi_n|1\rangle - \varepsilon_0\langle\varphi_n|1\rangle + \langle\varphi_n|\hat{V}|0\rangle - \varepsilon_1\langle\varphi_n|0\rangle = 0 \tag{9.31}$$

由式(9.29)及(9.31)，得

$$\varepsilon_1 = \langle\varphi_n|\hat{V}|0\rangle = \langle\varphi_n|\hat{V}|\varphi_n\rangle \tag{9.32}$$

所以，能量修正為

$$E_n(\lambda) = \varepsilon_0 + \lambda\varepsilon_1 + O(\lambda^2) = E_n^0 + \lambda\langle\varphi_n|\hat{V}|\varphi_n\rangle + O(\lambda^2) \tag{9.33}$$

或

$$\boxed{E_n = E_n^{(0)} + H'_{nn}} \qquad \textbf{（一級修正）} \tag{9.34}$$

此處

$$H'_{nn} = \langle\varphi_n|\hat{H}'|\varphi_n\rangle = \langle\varphi_n|\lambda\hat{V}|\varphi_n\rangle \tag{9.35}$$

故對於不含退化狀態的能量 E_n^0 之一級修正，就只是在計算微擾項 $\hat{H}'$ 在不受干擾前之狀態 $|\varphi_n\rangle$ 上之平均值而已。

(2) 將式(9.13)投影在除了 $|\varphi_n\rangle$ 以外的所有 $|\varphi_p^i\rangle$ 上（i 表退化指標）得

$$\langle \varphi_p^i|(\hat{H}_0-\varepsilon_0)|1\rangle+\langle \varphi_p^i|(\hat{V}-\varepsilon_1)|\varphi_n\rangle=0 \qquad (\text{其中 } p\neq n\ )$$

$$(E_p^0-E_n^0)\langle \varphi_p^i|1\rangle+\langle \varphi_p^i|\hat{V}|\varphi_n\rangle-\varepsilon_1\langle \varphi_p^i|\varphi_n\rangle=0 \tag{9.36}$$

由式(9.5)正交關係，故

$$\langle \varphi_p^i|1\rangle=\frac{1}{E_n^0-E_p^0}\langle \varphi_p^i|\hat{V}|\varphi_n\rangle \tag{9.37}$$

另一方面，由

$$\langle \varphi_n|1\rangle=\langle 0|1\rangle=0 \tag{9.38}$$

及完全集關係式(9.5)知：

$$|1\rangle=\sum_p\sum_i|\varphi_p^i\rangle\langle \varphi_p^i|1\rangle=|\varphi_n\rangle\underbrace{\langle \varphi_n|1\rangle}_{0}+\sum_{p\neq n}\sum_i|\varphi_p^i\rangle\langle \varphi_p^i|1\rangle$$

$$=\sum_{p\neq n}\sum_i\frac{\langle \varphi_p^i|\hat{V}|\varphi_n\rangle}{E_n^0-E_p^0}|\varphi_p^i\rangle \tag{9.39}$$

所以，波函數 $|\varphi_n(\lambda)\rangle$ 為

$$|\varphi_n(\lambda)\rangle=|0\rangle+\lambda|1\rangle+O(\lambda^2)$$

$$=|\varphi_n\rangle+\lambda\sum_{p\neq n}\sum_i\frac{\langle \varphi_p^i|\hat{V}|\varphi_n\rangle}{E_n^0-E_p^0}|\varphi_p^i\rangle+O(\lambda^2) \tag{9.40}$$

或

$$\varphi_n=\varphi_n^{(0)}+\sum_{p\neq n}\frac{\hat{H}'_{pn}}{E_n^{(0)}-E_p^{(0)}}\varphi_p^{i(0)} \qquad (\textbf{一級修正}) \tag{9.41}$$

此處 $$H'_{pn}=\langle \varphi_p|\hat{H}'|\varphi_n\rangle \quad \text{或} \quad \langle \varphi_p^i|H'|\varphi_n\rangle \tag{9.42}$$

所以，**如果**第二項中之分子值愈大，即 $\hat{H}'$ 在 $|\varphi_p\rangle$ 與 $|\varphi_n\rangle$ 之間造成的作用愈強，或者分母值愈小，即 E_p^0 **與** E_n^0 **之間的能**