Perturbation theory: time independent case

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In every physical theory, we are confronted with the need to obtain approximate solutions to the equations, because exact solutions are usually be found only for the simplest models of the physical situations. Nevertheless, the approximations are often useful since they may serve as a key starting point for understanding the physics lying in the complicated equations of the actual system. The perturbation method are examples of such an approach. Here we discuss the perturbation theory with the time-independent Hamiltonian. There are two types of methods, (i) the non-degenerate system where the eigenstates of the unperturbed system are not degenerate, (ii) the degenerate system where the eigenstates of the unperturbed system is degenerate.

There are two methods: **Rayleigh-Schrödinger** (RS) method and **Brillouin-Wigner** (BW) method. The BW perturbation theory is less widely used than the (RS) version. At first order in the perturbation, the two theories are equivalent. However, BW perturbation theory extends more easily to higher orders, and avoids the need for separate treatment of nondegenerate and degenerate levels.

1 Perturbation theory: non-degenerate case (Rayleigh-Schrödinger method)

We consider the Hamiltonian of the system

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}_1 ,$$

where $\hat{H}_0$ is an unperturbed Hamiltonian and $\hat{H}_1$ is the perturbation. The parameter λ is assumed to be real and is very small.

Fig. Energy eigenstates for the unperturbed Hamiltonian $\hat{H}_0$ (non-degenerate case).

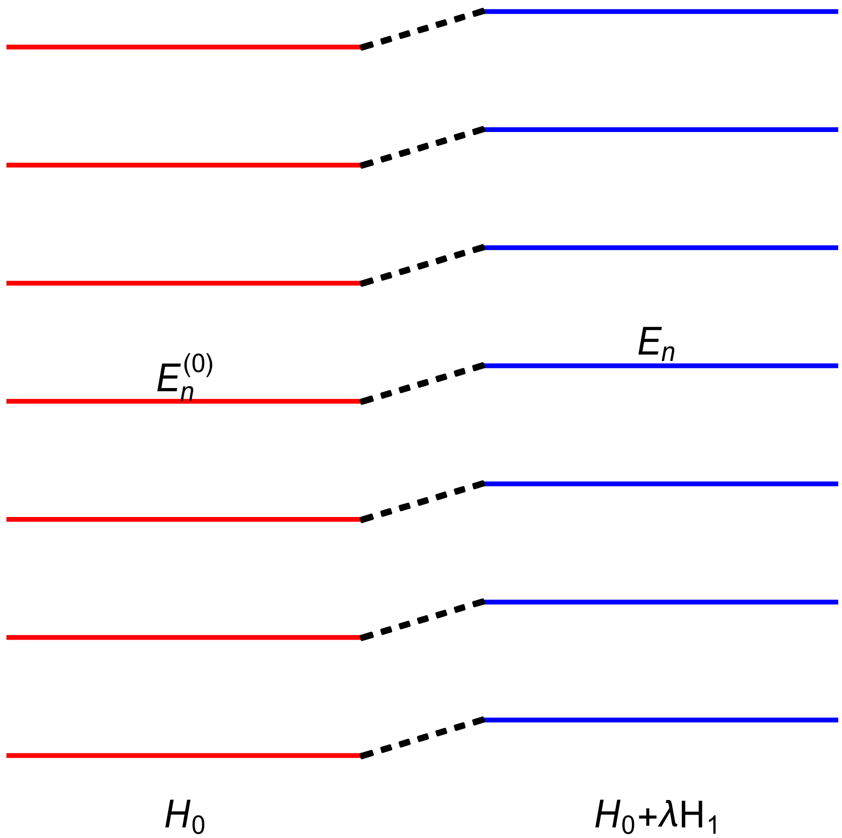

Fig. Shift of the energy levels when the perturbed Hamiltonian ($\lambda\hat{H}_1$) is added to the system.

Here we discuss an approximate solution of the $\hat{H}(\lambda)$ eigenvalue equation (non-degenerate case). We start with the eigenvalue problem

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle,$$

where $|\psi_n\rangle$ is the eigenket of $\hat{H}$ with the energy eigenvalue E_n. $|\psi_n\rangle$ is a non-degenerate state. We assume that

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ...$$

and

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + ...$$

where

$$\hat{H}_0\left|\psi_n^{(0)}\right\rangle = E_n^{(0)}\left|\psi_n^{(0)}\right\rangle.$$

The energy eigenvalue $E_n^{(0)}$ is different for different states (the non-degenerate case). Then we get

$$(\hat{H}_0 + \lambda\hat{H}_1)(\left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle + \lambda^2\left|\psi_n^{(2)}\right\rangle + ...)$$

$$= (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ...)(\left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle + \lambda^2\left|\psi_n^{(2)}\right\rangle + ...).$$

For the 0-th order terms in λ,

$$(\hat{H}_0 - E_n^{(0)})\left|\psi_n^{(0)}\right\rangle = 0, \qquad \text{or} \qquad \hat{H}_0\left|\psi_n^{(0)}\right\rangle = E_n^{(0)}\left|\psi_n^{(0)}\right\rangle.$$

For the 1st-order terms in λ,

$$(\hat{H}_0 - E_n^{(0)})\left|\psi_n^{(1)}\right\rangle + (\hat{H}_1 - E_n^{(1)})\left|\psi_n^{(0)}\right\rangle = 0. \qquad (1)$$

For the 2nd-order terms in λ,

$$(\hat{H}_0 - E_n^{(0)})\left|\psi_n^{(2)}\right\rangle + (\hat{H}_1 - E_n^{(1)})\left|\psi_n^{(1)}\right\rangle - E_n^{(2)}\left|\psi_n^{(0)}\right\rangle = 0. \qquad (2)$$

For the 3rd-order terms in λ,

$$(\hat{H}_0 - E_n^{(0)})\left|\psi_n^{(3)}\right\rangle + (\hat{H}_1 - E_n^{(1)})\left|\psi_n^{(2)}\right\rangle - E_n^{(2)}\left|\psi_n^{(1)}\right\rangle - E_n^{(3)}\left|\psi_n^{(0)}\right\rangle = 0. \qquad (3)$$

For the 4-th order terms in λ,

$$\begin{aligned}&(\hat{H}_0 - E_n^{(0)})\left|\psi_n^{(4)}\right\rangle + (\hat{H}_1 - E_n^{(1)})\left|\psi_n^{(3)}\right\rangle - E_n^{(2)}\left|\psi_n^{(2)}\right\rangle - E_n^{(3)}\left|\psi_n^{(1)}\right\rangle \\ &- E_n^{(4)}\left|\psi_n^{(0)}\right\rangle = 0\end{aligned} \qquad (4)$$

((**Mathematica**))

Perturbation theory : nondegenerate case

```
Clear["Global`*"]; eq1 = (H0 + λ H1) (Sum[λ^q ψn[q], {q, 0, 10}]) - (Sum[λ^q En[q], {q, 0, 10}]) ((Sum[λ^q ψn[q], {q, 0, 10}]));

eq2 = Table[{n, Coefficient[eq1, λ, n]}, {n, 0, 4}] // FullSimplify;
eq2 // TableForm
```

```
0    (H0 - En[0]) ψn[0]
1    (H1 - En[1]) ψn[0] + (H0 - En[0]) ψn[1]
2    -En[2] ψn[0] + (H1 - En[1]) ψn[1] + (H0 - En[0]) ψn[2]
3    -En[3] ψn[0] - En[2] ψn[1] + (H1 - En[1]) ψn[2] + (H0 - En[0]) ψn[3]
4    -En[4] ψn[0] - En[3] ψn[1] - En[2] ψn[2] + (H1 - En[1]) ψn[3] + (H0 - En[0]) ψn[4]
```

2 The first-order energy shift

The eigenket $\left|\psi_n^{(0)}\right\rangle$ forms the complete set. We start with Eq.(1) and take the inner product with $\left\langle\psi_n^{(0)}\right|$

$$\left\langle\psi_n^{(0)}\right|(\hat{H}_0 - E_n^{(0)})\left|\psi_n^{(1)}\right\rangle + \left\langle\psi_n^{(0)}\right|(\hat{H}_1 - E_n^{(1)})\left|\psi_n^{(0)}\right\rangle = 0,$$

or

$$E_n^{(1)} = \left\langle\psi_n^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle.$$

((**Note**)) This expression can be obtained directly using the Feynman-Hellmann theorem.

$$\frac{\partial E_n}{\partial\lambda} = \langle\psi_n(\lambda)|\frac{\partial\hat{H}}{\partial\lambda}|\psi_n(\lambda)\rangle.$$

The first-order correction of Eq.(1) with $\left\langle\psi_k^{(0)}\right|$ for $k \neq n$.

$$\left\langle\psi_k^{(0)}\right|\hat{H}_0 - E_n^{(0)}\left|\psi_n^{(1)}\right\rangle + \left\langle\psi_k^{(0)}\right|\hat{H}_1 - E_n^{(1)}\left|\psi_n^{(0)}\right\rangle = 0.$$

Since

$$\left\langle\psi_k^{(0)}\middle|\psi_n^{(0)}\right\rangle = 0 \qquad \text{for } k \neq n.$$

the above equation can be rewritten as

$$(E_k^{(0)} - E_n^{(0)})\langle\psi_k^{(0)}|\psi_n^{(1)}\rangle + \langle\psi_k^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle = 0,$$

or

$$\langle\psi_k^{(0)}|\psi_n^{(1)}\rangle = \frac{\langle\psi_k^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}. \qquad (k \neq n)$$

since $E_n^{(0)} \neq E_k^{(0)}$. If we use the basis states $|\psi_k^{(0)}\rangle$ to express $|\psi_n^{(1)}\rangle$ as

$$|\psi_n^{(1)}\rangle = \sum_k |\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\psi_n^{(1)}\rangle, \qquad \text{(closure relation)}$$

or

$$\begin{aligned}|\psi_n^{(1)}\rangle &= |\psi_n^{(0)}\rangle\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle + \sum_{k\neq n}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\psi_n^{(1)}\rangle \\ &= |\psi_n^{(0)}\rangle\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle + |\varphi_n^{(1)}\rangle\end{aligned}.$$

where

$$|\varphi_n^{(1)}\rangle = \sum_{k\neq n}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\psi_n^{(1)}\rangle.$$

((**Normalization-I**))

Here we need to show that

$$\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle = 0.$$

If so, we get

$$|\psi_n^{(1)}\rangle = |\varphi_n^{(1)}\rangle.$$

and

$$\langle\psi_n^{(0)}|\varphi_n^{(1)}\rangle = 0$$

This can be proved from the condition of normalization as follows.

$$1 = \langle\psi_n|\psi_n\rangle = \langle\psi_n^{(0)}|\psi_n^{(0)}\rangle + \lambda(\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle + \langle\psi_n^{(1)}|\psi_n^{(0)}\rangle) + ...$$

$$+\lambda^2(\langle\psi_n^{(2)}|\psi_n^{(0)}\rangle+\langle\psi_n^{(1)}|\psi_n^{(1)}\rangle+\langle\psi_n^{(0)}|\psi_n^{(2)}\rangle)+...$$

Since $\langle\psi_n^{(0)}|\psi_n^{(0)}\rangle=1$, through the first order in λ, we must have

$$\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle+\langle\psi_n^{(1)}|\psi_n^{(0)}\rangle=0,$$

or

$$\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle+\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle^*=2\,\mathrm{Re}[\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle]=0.$$

Then we have

$$\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle=ia \quad (a\text{: real}), \qquad \text{i.e. (purely imaginary)}$$

This means that

$$|\psi_n^{(1)}\rangle=ia|\psi_n^{(0)}\rangle+|\varphi_n^{(1)}\rangle.$$

Then we have

$$\begin{aligned}|\psi_n\rangle&=|\psi_n^{(0)}\rangle+\lambda(ia|\psi_n^{(0)}\rangle+|\varphi_n^{(1)}\rangle)+....\\&=(1+ia\lambda)|\psi_n^{(0)}\rangle+\lambda|\varphi_n^{(1)}\rangle+....\\&=e^{ia\lambda}|\psi_n^{(0)}\rangle+\lambda|\varphi_n^{(1)}\rangle+....\end{aligned}$$

where we use

$$e^{ia\lambda}=1+ia\lambda+...\cong 1+ia\lambda \qquad \text{for } |a\lambda|<<1.$$

For convenience, we assume that $a = 0$:

$$\langle\psi_n^{(0)}|\varphi_n^{(1)}\rangle=ia=0$$

Then we have

$$|\psi_n^{(1)}\rangle=|\varphi_n^{(1)}\rangle=\sum_{k\neq n}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\psi_n^{(1)}\rangle,$$

So we have

$$\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle = 0$$

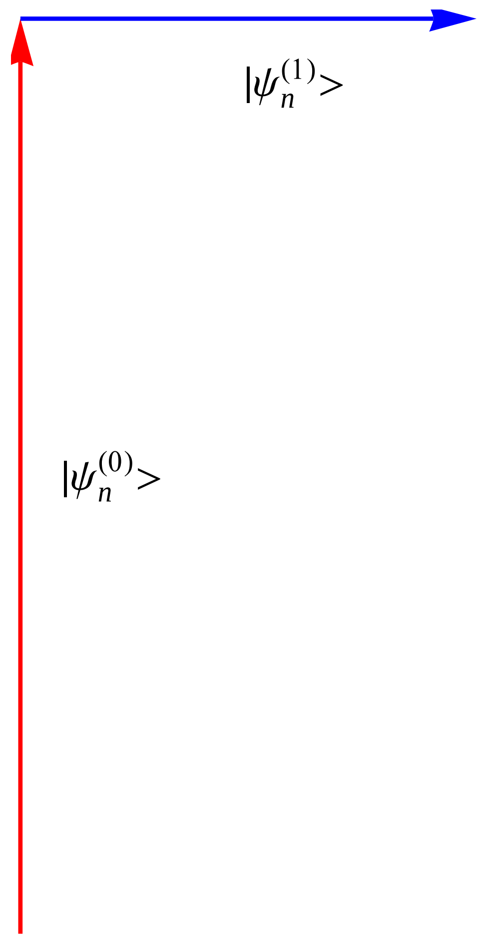

Fig. $\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle = 0$., where $|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda |\psi_n^{(1)}\rangle + \lambda^2 |\psi_n^{(2)}\rangle + ...$

Then we have

$$|\psi_n^{(1)}\rangle = |\varphi_n^{(1)}\rangle = \sum_{k \neq n} |\psi_k^{(0)}\rangle \langle \psi_k^{(0)} | \psi_n^{(1)}\rangle = \sum_{k \neq n} |\psi_k^{(0)}\rangle \frac{\langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}}$$

In summary

$$E_n = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle$$

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda \sum_{k \neq n} |\psi_k^{(0)}\rangle \frac{\langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}}$$

((**Note**))

As will be discussed later, we use the concept of the renormalization wave function such that $\langle\psi_n^{(0)}|\psi_n\rangle = 1$, instead of $\langle\psi_n|\psi_n\rangle = 1$. To the first order of λ, the same condition $\langle\psi_n^{(0)}|\psi_n\rangle = 1$ can be derived from the condition for the renormalization wave function $\langle\psi_n^{(0)}|\psi_n\rangle = 1$.

3. The second-order energy shift

We start with

$$(\hat{H}_0 - E_n^{(0)})|\psi_n^{(2)}\rangle + (\hat{H}_1 - E_n^{(1)})|\psi_n^{(1)}\rangle - E_n^{(2)}|\psi_n^{(0)}\rangle = 0 \qquad (2)$$

We take the inner product of Eq.(2) with the bra $\langle\psi_n^{(0)}|$

$$\langle\psi_n^{(0)}|\hat{H}_0 - E_n^{(0)}|\psi_n^{(2)}\rangle + \langle\psi_n^{(0)}|\hat{H}_1 - E_n^{(1)}|\psi_n^{(1)}\rangle - E_n^{(2)} = 0$$

Since $\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle = 0$, we have

$$\begin{aligned}
E_n^{(2)} &= \langle\psi_n^{(0)}|\hat{H}_1|\psi_n^{(1)}\rangle \\
&= \langle\psi_n^{(0)}|\hat{H}_1 \sum_{k\neq n}|\psi_k^{(0)}\rangle \frac{\langle\psi_k^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} \\
&= \sum_{k\neq n}\frac{\langle\psi_n^{(0)}|\hat{H}_1|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} \\
&= \sum_{k\neq n}\frac{\left|\langle\psi_n^{(0)}|\hat{H}_1|\psi_k^{(0)}\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}}
\end{aligned}$$

In summary

$$E_n^{(2)} = \sum_{k\neq n}\frac{\left|\langle\psi_n^{(0)}|\hat{H}_1|\psi_k^{(0)}\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}} = \sum_{k\neq n}\frac{\langle\psi_n^{(0)}|\hat{H}_1|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}$$

4. Wave-function renormalization

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + \lambda^3|\psi_n^{(3)}\rangle + ...$$

Here we need to specify how the states $|\psi_n^{(0)}\rangle$ and $|\psi_n\rangle$ overlap. Since $|\psi_n\rangle$ is considered not to be very different from $|\psi_n^{(0)}\rangle$, we have

$$\langle\psi_n^{(0)}|\psi_n\rangle \approx 1 .$$

It is convenient to depart from the usual normalization condition that

$$\langle\psi_n|\psi_n\rangle = 1.$$

Rather we set

$$\langle\psi_n^{(0)}|\psi_n\rangle = 1$$ (this is the definition we use here)

even for $\lambda \neq 0$. Then we get

$$\langle\psi_n^{(0)}|\psi_n\rangle = \langle\psi_n^{(0)}|\psi_n^{(0)}\rangle + \lambda\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle + \lambda^2\langle\psi_n^{(0)}|\psi_n^{(2)}\rangle + \lambda^3\langle\psi_n^{(0)}|\psi_n^{(3)}\rangle + ... ,$$

with

$$\langle\psi_n^{(0)}|\psi_n^{(0)}\rangle = 1 , \qquad \langle\psi_n^{(0)}|\psi_n^{(1)}\rangle = 0 , \qquad \langle\psi_n^{(0)}|\psi_n^{(2)}\rangle = 0 ,....$$

In other words, $|\psi_n^{(k)}\rangle$ (k = 1, 2, 3, 4, ...) is orthogonal to $|\psi_n^{(0)}\rangle$

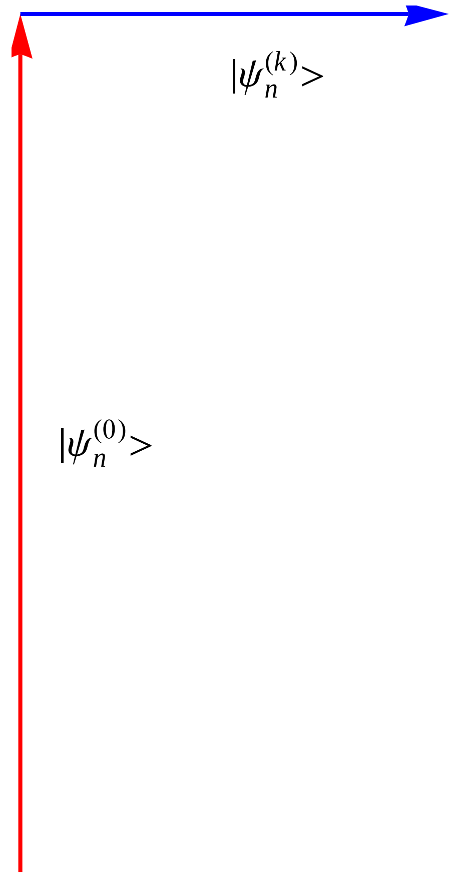

Fig. $\langle \psi_n{}^{(0)} | \psi_n{}^{(k)} \rangle = 0$ where k = 1, 2, 3, ….

In such conditions, we have

$$\begin{aligned}
\langle \psi_n | \psi_n \rangle &= (\langle \psi_n{}^{(0)} | + \lambda \langle \psi_n{}^{(1)} | + \lambda^2 \langle \psi_n{}^{(2)} | + \lambda^3 \langle \psi_n{}^{(3)} | + ...) \\
&\quad \times (| \psi_n{}^{(0)} \rangle + \lambda | \psi_n{}^{(1)} \rangle + \lambda^2 | \psi_n{}^{(2)} \rangle + \lambda^3 | \psi_n{}^{(3)} \rangle + ...) \\
&= \langle \psi_n{}^{(0)} | \psi_n{}^{(0)} \rangle + \lambda [\langle \psi_n{}^{(0)} | \psi_n{}^{(1)} \rangle + \langle \psi_n{}^{(0)} | \psi_n{}^{(1)} \rangle^*] \\
&\quad + \lambda^2 [\langle \psi_n{}^{(0)} | \psi_n{}^{(2)} \rangle + \langle \psi_n{}^{(2)} | \psi_n{}^{(0)} \rangle^* + \langle \psi_n{}^{(1)} | \psi_n{}^{(1)} \rangle] + ... \\
&= 1 + \lambda^2 \langle \psi_n{}^{(1)} | \psi_n{}^{(1)} \rangle + O(\lambda^2) \\
&= 1 + \lambda^2 \sum_{k \neq n} \frac{\left| \langle \psi_k{}^{(0)} | \hat{H}_1 | \psi_n{}^{(0)} \rangle \right|^2}{(E_n{}^{(0)} - E_k{}^{(0)})^2} + O(\lambda^2)
\end{aligned}$$

since

$$\left|\psi_n^{(1)}\right\rangle = \sum_{k\neq n}\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\middle|\psi_n^{(1)}\right\rangle = \sum_{k\neq n}\left|\psi_k^{(0)}\right\rangle\frac{\left\langle\psi_k^{(0)}\middle|\hat{H}_1\middle|\psi_n^{(0)}\right\rangle}{E_n^{(0)}-E_k^{(0)}}$$

In other words, $\left|\psi_n\right\rangle$ is, to the first order, normalized to 1, with the first correction occurring in the second order.

Here we define $\left|\psi_n\right\rangle_N$ which satisfies the usual normalization.

$$\left|\psi_n\right\rangle_N = \sqrt{Z_n}\left|\psi_n\right\rangle$$

Z_n is called as the wave function normalization constant.

$$_N\left\langle\psi_n\middle|\psi_n\right\rangle_N = 1 = Z_n\left\langle\psi_n\middle|\psi_n\right\rangle$$

or

$$Z_n = \frac{1}{\left\langle\psi_n\middle|\psi_n\right\rangle} = 1-\lambda^2\sum_{k\neq n}\frac{\left|\left\langle\psi_k^{(0)}\middle|\hat{H}_1\middle|\psi_n^{(0)}\right\rangle\right|^2}{(E_n^{(0)}-E_k^{(0)})^2}+O(\lambda^2)$$

Then we have

$$\left\langle\psi_n^{(0)}\middle|\psi_n\right\rangle_N = \sqrt{Z_n}\left\langle\psi_n^{(0)}\middle|\psi_n\right\rangle = \sqrt{Z_n}$$

P is the probability of observing $\left|\psi_n\right\rangle_N$ in the unperturbed state $\left|\psi_n^{(0)}\right\rangle$,

$$\left|\left\langle\psi_n^{(0)}\middle|\psi_n\right\rangle_N\right|^2 = Z_n = P = 1-\lambda^2\sum_{k\neq n}\frac{\left|\left\langle\psi_k^{(0)}\middle|\hat{H}_1\middle|\psi_n^{(0)}\right\rangle\right|^2}{(E_n^{(0)}-E_k^{(0)})^2}.$$

The second term is to be understood as the probability for leakage to state other than $\left|\psi_n^{(0)}\right\rangle$. Note that Z_n is less than 1.

Note that the energy E_n is given by

$$E_n = E_n^{(0)} + \lambda\left\langle\psi_n^{(0)}\middle|\hat{H}_1\middle|\psi_n^{(0)}\right\rangle + \lambda^2\sum_{k\neq n}\frac{\left|\left\langle\psi_k^{(0)}\middle|\hat{H}_1\middle|\psi_n^{(0)}\right\rangle\right|^2}{E_n^{(0)}-E_k^{(0)}}.$$

The derivative of E_n with respect to $E_n^{(0)}$ is given by

$$\frac{\partial E_n}{\partial E_n^{(0)}} = 1 - \lambda^2 \sum_{k\neq n} \frac{\left|\left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle\right|^2}{(E_n^{(0)} - E_k^{(0)})^2} = Z_n ,$$

where the matrix element of $\hat{H}_1$ is assumed to be independent of $E_n^{(0)}$.

5. Derivation of the expression of $\left|\psi_n^{(2)}\right\rangle$

Now we take the inner product of Eq.(2)

$$(\hat{H}_0 - E_n^{(0)})\left|\psi_n^{(2)}\right\rangle + (\hat{H}_1 - E_n^{(1)})\left|\psi_n^{(1)}\right\rangle - E_n^{(2)}\left|\psi_n^{(0)}\right\rangle = 0 , \qquad (2)$$

with the bra $\left\langle \psi_k^{(0)} \right|$ $\quad (k \neq n)$

$$\left\langle \psi_k^{(0)} \right| \hat{H}_0 - E_n^{(0)} \left| \psi_n^{(2)} \right\rangle + \left\langle \psi_k^{(0)} \right| \hat{H}_1 - E_n^{(1)} \left| \psi_n^{(1)} \right\rangle = 0 ,$$

or

$$(E_k^{(0)} - E_n^{(0)})\left\langle \psi_k^{(0)} \middle| \psi_n^{(2)} \right\rangle + \left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_n^{(1)} \right\rangle - E_n^{(1)} \left\langle \psi_k^{(0)} \middle| \psi_n^{(1)} \right\rangle = 0 ,$$

or

$$(E_k^{(0)} - E_n^{(0)})\left\langle \psi_k^{(0)} \middle| \psi_n^{(2)} \right\rangle + \sum_{l\neq n} \frac{\left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_l^{(0)} \right\rangle \left\langle \psi_l^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_l^{(0)}}$$
$$- E_n^{(1)} \sum_{l\neq n} \frac{\left\langle \psi_k^{(0)} \middle| \psi_l^{(0)} \right\rangle \left\langle \psi_l^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_l^{(0)}} = 0$$

or

$$(E_n^{(0)} - E_k^{(0)})\left\langle \psi_k^{(0)} \middle| \psi_n^{(2)} \right\rangle = \sum_{l\neq n} \frac{\left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_l^{(0)} \right\rangle \left\langle \psi_l^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{(E_n^{(0)} - E_l^{(0)})}$$
$$- E_n^{(1)} \sum_{l\neq n} \frac{\left\langle \psi_k^{(0)} \middle| \psi_l^{(0)} \right\rangle \left\langle \psi_l^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_l^{(0)}}$$

or

$$\left\langle \psi_k^{(0)} \middle| \psi_n^{(2)} \right\rangle = \sum_{l\neq n} \frac{\left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_l^{(0)} \right\rangle \left\langle \psi_l^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{(E_n^{(0)} - E_l^{(0)})(E_n^{(0)} - E_k^{(0)})} - E_n^{(1)} \frac{\left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{(E_n^{(0)} - E_k^{(0)})^2} .$$

Here we use the relations

$$\left|\psi_n^{(1)}\right\rangle = \sum_{l \neq n} \left|\psi_l^{(0)}\right\rangle \frac{\left\langle \psi_l^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_l^{(0)}},$$

Thus we have

$$\begin{aligned}
\left|\psi_n^{(2)}\right\rangle &= \sum_{k \neq n} \left|\psi_k^{(0)}\right\rangle \left\langle \psi_k^{(0)} \middle| \psi_n^{(2)} \right\rangle \\
&= \sum_{\substack{k \neq n \\ l \neq n}} \left|\psi_k^{(0)}\right\rangle \frac{\left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_l^{(0)} \right\rangle \left\langle \psi_l^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{(E_n^{(0)} - E_l^{(0)})(E_n^{(0)} - E_k^{(0)})} \\
&\quad - E_n^{(1)} \sum_{k \neq n} \left|\psi_k^{(0)}\right\rangle \frac{\left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{(E_n^{(0)} - E_k^{(0)})^2}] \\
&= \sum_{\substack{k \neq n \\ l \neq n}} \left|\psi_k^{(0)}\right\rangle \frac{\left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_l^{(0)} \right\rangle \left\langle \psi_l^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_l^{(0)})} \\
&\quad - \sum_{k \neq n} \left|\psi_k^{(0)}\right\rangle \frac{\left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle \left\langle \psi_n^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{(E_n^{(0)} - E_k^{(0)})^2}
\end{aligned}$$

or

$$\left|\psi_n^{(2)}\right\rangle = \sum_{k \neq n} \left|\psi_k^{(0)}\right\rangle [\sum_{l \neq n} \frac{\left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_l^{(0)} \right\rangle \left\langle \psi_l^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_l^{(0)})} - \frac{\left\langle \psi_k^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle \left\langle \psi_n^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle}{(E_n^{(0)} - E_k^{(0)})^2}].$$

6. Summary

Summarizing the above results, we may write the energy eigenvalue and eigenstates of the perturbed Hamiltonian to the second order in λ as

(a) Energy eigenvalue

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + O(\lambda^3),$$

with

$$E_n^{(1)} = \left\langle \psi_n^{(0)} \right| \hat{H}_1 \left| \psi_n^{(0)} \right\rangle,$$

$$E_n^{(2)} = \sum_{k\neq n} \frac{\left|\langle \psi_n^{(0)} | \hat{H}_1 | \psi_k^{(0)} \rangle\right|^2}{E_n^{(0)} - E_k^{(0)}}.$$

(b) Energy eigenstate

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + O(\lambda^3),$$

with

$$|\psi_n^{(1)}\rangle = \sum_{k\neq n} |\psi_k^{(0)}\rangle \frac{\langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}},$$

and

$$\begin{aligned}
|\psi_n^{(2)}\rangle &= \sum_{k\neq n} |\psi_k^{(0)}\rangle [\sum_{l\neq n} \frac{\langle \psi_k^{(0)} | \hat{H}_1 | \psi_l^{(0)} \rangle \langle \psi_l^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_l^{(0)})} \\
&\quad - \frac{\langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle \langle \psi_n^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{(E_n^{(0)} - E_k^{(0)})^2}] \\
&= \sum_{\substack{k\neq n \\ l\neq n}} |\psi_k^{(0)}\rangle \frac{\langle \psi_k^{(0)} | \hat{H}_1 | \psi_l^{(0)} \rangle \langle \psi_l^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_l^{(0)})} \\
&\quad - \sum_{k\neq n} \frac{\langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle \langle \psi_n^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{(E_n^{(0)} - E_k^{(0)})^2}]
\end{aligned}$$

We note that $|\psi_n\rangle$ is not normalized, so an extra calculation must be performed in order to obtain the normalization factor.

7. Formal theory of perturbation ((Sakurai)); nondegenerate case

This method is the same as the **Rayleigh-Schrödinger method**.

We start with the Schrödinger equation given by

$$(\hat{H}_0 + \lambda\hat{H}_1)|\psi_n\rangle = E_n|\psi_n\rangle,$$

where E_n is the energy eigenvalue. When the perturbation vanishes, we get

$$\hat{H}_0|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle.$$

We define

$$\Delta_n = E_n - E_n^{(0)}.$$

Then we get

$$(H_0 + \lambda \hat{H}_1)\left|\psi_n\right\rangle = (\Delta_n + E_n^{(0)})\left|\psi_n\right\rangle,$$

or

$$(E_n^{(0)} - \hat{H}_0)\left|\psi_n\right\rangle = (\lambda \hat{H}_1 - \Delta_n)\left|\psi_n\right\rangle, \qquad (1)$$

We introduce the projection operators, $\hat{M}$ and $\hat{P}$ such that

$$\hat{M} = \left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right|, \qquad \hat{P} = \hat{1} - \left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right| = \sum_{k\neq n}\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|.$$

We note that

$$[\hat{P}, \hat{H}_0] = 0, \qquad [\hat{M}, \hat{H}_0] = 0$$

$$\hat{M}^2 = \hat{M}, \qquad \hat{P}^2 = \hat{P}$$

$$\hat{P} + \hat{M} = \hat{1}, \qquad \hat{P}\hat{M} = (\hat{1} - \hat{M})\hat{M} = \hat{M} - \hat{M}^2 = 0$$

$$\hat{M}\left|\psi_n^{(0)}\right\rangle = \left|\psi_n^{(0)}\right\rangle, \qquad \hat{P}\left|\psi_n^{(0)}\right\rangle = 0$$

(a) Derivation of $\left|\psi_n\right\rangle$

Multiplying Eq.(1)

$$(\lambda \hat{H}_1 - \Delta_n)\left|\psi_n\right\rangle = (E_n^{(0)} - \hat{H}_0)\left|\psi_n\right\rangle, \qquad (1)$$

by $\hat{P}$ from the left side, we have

$$\hat{P}(\lambda \hat{H}_1 - \Delta_n)\left|\psi_n\right\rangle = \hat{P}(E_n^{(0)} - \hat{H}_0)\left|\psi_n\right\rangle = (E_n^{(0)} - \hat{H}_0)\hat{P}\left|\psi_n\right\rangle.$$

So we get

$$
\begin{aligned}
\hat{P}|\psi_n\rangle &= \frac{1}{E_n{}^{(0)} - H_0}\hat{P}(\lambda\hat{H}_1 - \Delta_n)|\psi_n\rangle \\
&= \frac{1}{E_n{}^{(0)} - H_0}\hat{P}^2(\lambda\hat{H}_1 - \Delta_n)|\psi_n\rangle \\
&= \hat{P}\frac{1}{E_n{}^{(0)} - H_0}\hat{P}(\lambda\hat{H}_1 - \Delta_n)|\psi_n\rangle \\
&= \hat{P}^2\frac{1}{E_n{}^{(0)} - H_0}(\lambda\hat{H}_1 - \Delta_n)|\psi_n\rangle \\
&= \hat{P}\frac{1}{E_n{}^{(0)} - H_0}(\lambda\hat{H}_1 - \Delta_n)|\psi_n\rangle \\
&= \frac{\hat{P}}{E_n{}^{(0)} - H_0}(\lambda\hat{H}_1 - \Delta_n)|\psi_n\rangle
\end{aligned}
.
$$

or simply,

$$
\hat{P}|\psi_n\rangle = \frac{\hat{P}}{E_n{}^{(0)} - H_0}(\lambda\hat{H}_1 - \Delta_n)|\psi_n\rangle
$$

A suitable final form is

$$
\begin{aligned}
|\psi_n\rangle &= (\hat{M} + \hat{P})|\psi_n\rangle \\
&= \hat{M}|\psi_n\rangle + \hat{P}|\psi_n\rangle \\
&= |\psi_n{}^{(0)}\rangle + \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0}(\lambda\hat{H}_1 - \Delta_n)|\psi_n\rangle \\
&= |\psi_n{}^{(0)}\rangle + \lambda|\psi_n{}^{(1)}\rangle + \lambda|\psi_n{}^{(2)}\rangle + ...
\end{aligned}
$$

where

$$
\begin{aligned}
\frac{1}{E_n{}^{(0)} - \hat{H}_0}\hat{P} &= \hat{P}\frac{1}{E_n{}^{(0)} - \hat{H}_0} \\
&= \hat{P}^2\frac{1}{E_n{}^{(0)} - \hat{H}_0} \quad , \\
&= \hat{P}\frac{1}{E_n{}^{(0)} - \hat{H}_0}\hat{P}
\end{aligned}
$$

because of $\hat{P}^2 = \hat{P}$, or simply

$$\frac{1}{E_n{}^{(0)} - \hat{H}_0}\hat{P} = \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0}.$$

Note that

$$\left\langle \psi_n{}^{(0)} \middle| \psi_n{}^{(k)} \right\rangle = 0$$

since

$$\hat{P}\left|\psi_n\right\rangle = \lambda\left|\psi_n{}^{(1)}\right\rangle + \lambda\left|\psi_n{}^{(2)}\right\rangle + .$$

(b) Derivation of Δ_n

On multiplying Eq.(1) by $\left\langle \psi_n{}^{(0)} \right|$,

$$\left\langle \psi_n{}^{(0)} \middle| (E_n{}^{(0)} - H_0) \middle| \psi_n \right\rangle = 0 = \left\langle \psi_n{}^{(0)} \middle| (\lambda\hat{H}_1 - \Delta_n) \middle| \psi_n \right\rangle,$$

or

$$\lambda\left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n \right\rangle = \Delta_n \left\langle \psi_n{}^{(0)} \middle| \psi_n \right\rangle = \Delta_n$$

or

$$\begin{aligned}\Delta_n &= \lambda\Delta_n{}^{(1)} + \lambda^2\Delta_n{}^{(2)} + \lambda^3\Delta_n{}^{(3)} + ...\\ &= \lambda\left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n \right\rangle \\ &= \lambda\left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n{}^{(0)} \right\rangle + \lambda^2\left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n{}^{(1)} \right\rangle + \lambda^3\left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n{}^{(2)} \right\rangle + ...\end{aligned}.$$

Here we have

$$\Delta_n{}^{(1)} = \left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n{}^{(0)} \right\rangle,$$

$$\Delta_n{}^{(2)} = \left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n{}^{(1)} \right\rangle,$$

$$\Delta_n{}^{(3)} = \left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n{}^{(2)} \right\rangle.$$

(c) The final results

The final form is given by

$$
\begin{aligned}
\left|\psi_n\right\rangle &= \left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle + \lambda^2\left|\psi_n^{(2)}\right\rangle + ...\\
&= \left|\psi_n^{(0)}\right\rangle + \frac{\hat{P}}{E_n^{(0)} - \hat{H}_0}[\lambda(\hat{H}_1 - \Delta_n^{(1)}) - \lambda^2\Delta_n^{(2)} - \lambda^3\Delta_n^{(3)} - ....]\\
&\times(\left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle + \lambda^2\left|\psi_n^{(2)}\right\rangle + ...)
\end{aligned}
$$

or

$$
\begin{aligned}
\left|\psi_n\right\rangle &= \left|\psi_n^{(0)}\right\rangle + \lambda\frac{\hat{P}}{E_n^{(0)} - \hat{H}_0}\hat{H}_1\left|\psi_n^{(0)}\right\rangle\\
&+ \lambda^2\frac{\hat{P}}{E_n^{(0)} - \hat{H}_0}(\hat{H}_1 - \Delta_n^{(1)})\left|\psi_n^{(1)}\right\rangle\\
&+ \lambda^3\frac{\hat{P}}{E_n^{(0)} - \hat{H}_0}(\hat{H}_1 - \Delta_n^{(1)})\left|\psi_n^{(2)}\right\rangle - \lambda^3\frac{\hat{P}}{E_n^{(0)} - \hat{H}_0}\Delta_n^{(2)}\left|\psi_n^{(1)}\right\rangle\\
&+ \lambda^4\frac{\hat{P}}{E_n^{(0)} - \hat{H}_0}(\hat{H}_1 - \Delta_n^{(1)})\left|\psi_n^{(3)}\right\rangle - \lambda^4\frac{\hat{P}}{E_n^{(0)} - \hat{H}_0}\Delta_n^{(3)}\left|\psi_n^{(1)}\right\rangle\\
&- \lambda^4\frac{\hat{P}}{E_n^{(0)} - \hat{H}_0}\Delta_n^{(2)}\left|\psi_n^{(2)}\right\rangle + ...
\end{aligned}
$$

where

$$
\hat{P}\left|\psi_n^{(0)}\right\rangle = 0.
$$

(i) Coefficient the powers of λ:

$$
\begin{aligned}
\left|\psi_n^{(1)}\right\rangle &= \frac{\hat{P}}{E_n^{(0)} - \hat{H}_0}\hat{H}_1\left|\psi_n^{(0)}\right\rangle\\
&= \frac{1}{E_n^{(0)} - \hat{H}_0}\hat{P}\hat{H}_1\left|\psi_n^{(0)}\right\rangle\\
&= \sum_k \frac{1}{E_n^{(0)} - \hat{H}_0}\hat{P}\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle\\
&= \sum_{k\neq n} \frac{1}{E_n^{(0)} - \hat{H}_0}\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle\\
&= \sum_{k\neq n} \frac{\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle}{E_n^{(0)} - E_k^{(0)}}
\end{aligned}
$$

and

$$\Delta_n{}^{(2)} = \left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n{}^{(1)} \right\rangle$$

$$= \left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} \hat{H}_1 \middle| \psi_n{}^{(0)} \right\rangle$$

$$= \left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \hat{P} \frac{1}{E_n{}^{(0)} - \hat{H}_0} \hat{H}_1 \middle| \psi_n{}^{(0)} \right\rangle$$

$$= \sum_k \left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \hat{P} \middle| \psi_k{}^{(0)} \right\rangle \left\langle \psi_k{}^{(0)} \middle| \frac{1}{E_n{}^{(0)} - \hat{H}_0} \hat{H}_1 \middle| \psi_n{}^{(0)} \right\rangle \cdot$$

$$= \sum_{k \neq n} \frac{\left\langle \psi_k{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n{}^{(0)} \right\rangle \left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \middle| \psi_k{}^{(0)} \right\rangle}{E_n{}^{(0)} - E_k{}^{(0)}}$$

$$= \sum_{k \neq n} \frac{\left| \left\langle \psi_k{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n{}^{(0)} \right\rangle \right|^2}{E_n{}^{(0)} - E_k{}^{(0)}}$$

(ii) Coefficient the powers of λ^2:

$$\left| \psi_n{}^{(2)} \right\rangle == \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} (\hat{H}_1 - \Delta_n{}^{(1)} \left| \psi_n{}^{(1)} \right\rangle$$

$$= \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} \hat{H}_1 \left| \psi_n{}^{(1)} \right\rangle - \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} \Delta_n{}^{(1)} \left| \psi_n{}^{(1)} \right\rangle$$

$$= \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} \hat{H}_1 \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} \hat{H}_1 \left| \psi_n{}^{(0)} \right\rangle$$

$$- \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} \Delta_n{}^{(1)} \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} \hat{H}_1 \left| \psi_n{}^{(0)} \right\rangle$$

$$= \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} \hat{H}_1 \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} \hat{H}_1 \left| \psi_n{}^{(0)} \right\rangle$$

$$- \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} \left\langle \psi_n{}^{(0)} \middle| \hat{H}_1 \middle| \psi_n{}^{(0)} \right\rangle \frac{\hat{P}}{E_n{}^{(0)} - \hat{H}_0} \hat{H}_1 \left| \psi_n{}^{(0)} \right\rangle$$

or

$$
\begin{aligned}
\left|\psi_n{}^{(2)}\right\rangle &= \sum_{k\neq n}\sum_{l\neq n}\left|\psi_k{}^{(0)}\right\rangle\left\langle\psi_k{}^{(0)}\right|\frac{1}{E_n{}^{(0)}-\hat{H}_0}\hat{H}_1\left|\psi_l{}^{(0)}\right\rangle\left\langle\psi_l{}^{(0)}\right|\frac{1}{E_n{}^{(0)}-\hat{H}_0}\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle \\
&\quad -\sum_{k\neq n}\left|\psi_k{}^{(0)}\right\rangle\left\langle\psi_k{}^{(0)}\right|\frac{\hat{P}}{E_n{}^{(0)}-\hat{H}_0}\left\langle\psi_n{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle\frac{\hat{P}}{E_n{}^{(0)}-\hat{H}_0}\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle \\
&= \sum_{k\neq n}\sum_{l\neq n}\left|\psi_k{}^{(0)}\right\rangle\frac{\left\langle\psi_k{}^{(0)}\right|\hat{H}_1\left|\psi_l{}^{(0)}\right\rangle\left\langle\psi_l{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle}{(E_n{}^{(0)}-E_k{}^{(0)})(E_n{}^{(0)}-E_l{}^{(0)})} \\
&\quad -\sum_{k\neq n}\left|\psi_k{}^{(0)}\right\rangle\frac{\left\langle\psi_k{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle\left\langle\psi_n{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle}{(E_n{}^{(0)}-E_k{}^{(0)})^2}
\end{aligned}
$$

$$
\begin{aligned}
\Delta_n{}^{(3)} &= \left\langle\psi_n{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(2)}\right\rangle \\
&= \left\langle\psi_n{}^{(0)}\right|\hat{H}_1[\sum_{k\neq n}\sum_{l\neq n}\left|\psi_k{}^{(0)}\right\rangle\frac{\left\langle\psi_k{}^{(0)}\right|\hat{H}_1\left|\psi_l{}^{(0)}\right\rangle\left\langle\psi_l{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle}{(E_n{}^{(0)}-E_k{}^{(0)})(E_n{}^{(0)}-E_l{}^{(0)})} \\
&\quad -\sum_{k\neq n}\left|\psi_k{}^{(0)}\right\rangle\frac{\left\langle\psi_n{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle\left\langle\psi_k{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle}{(E_n{}^{(0)}-E_k{}^{(0)})^2}] \\
&= \sum_{k\neq n}\sum_{l\neq n}\frac{\left\langle\psi_n{}^{(0)}\right|\hat{H}_1\left|\psi_k{}^{(0)}\right\rangle\left\langle\psi_k{}^{(0)}\right|\hat{H}_1\left|\psi_l{}^{(0)}\right\rangle\left\langle\psi_l{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle}{(E_n{}^{(0)}-E_k{}^{(0)})(E_n{}^{(0)}-E_l{}^{(0)})} \\
&\quad -\sum_{k\neq n}\frac{\left\langle\psi_n{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle\left\langle\psi_n{}^{(0)}\right|\hat{H}_1\left|\psi_k{}^{(0)}\right\rangle\left\langle\psi_k{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle}{(E_n{}^{(0)}-E_k{}^{(0)})^2}]
\end{aligned}
$$

In this approach,

$$
\left\langle\psi_n^{(0)}\middle|\psi_n^{(k)}\right\rangle = 0 \qquad (k = 1, 2, 3, \ldots).
$$

Then we have

$$
\begin{aligned}
\left\langle\psi_n\middle|\psi_n\right\rangle &= \left\langle\psi_n{}^{(0)}\middle|\psi_n{}^{(0)}\right\rangle + \lambda[\left\langle\psi_n{}^{(0)}\middle|\psi_n{}^{(1)}\right\rangle + \left\langle\psi_n{}^{(0)}\middle|\psi_n{}^{(1)}\right\rangle^*] \\
&\quad + \lambda^2[\left\langle\psi_n{}^{(0)}\middle|\psi_n{}^{(2)}\right\rangle + \left\langle\psi_n{}^{(2)}\middle|\psi_n{}^{(0)}\right\rangle^* + \left\langle\psi_n{}^{(1)}\middle|\psi_n{}^{(1)}\right\rangle] + \ldots \\
&= 1 + \lambda^2\left\langle\psi_n{}^{(1)}\middle|\psi_n{}^{(1)}\right\rangle + O(\lambda^2) \\
&= 1 + \lambda^2\sum_{k\neq n}\frac{\left|\left\langle\psi_k{}^{(0)}\right|\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle\right|^2}{(E_n{}^{(0)}-E_k{}^{(0)})^2} + O(\lambda^2)
\end{aligned}
$$

The wave function normalization factor is

$$Z_n = \frac{1}{\langle \psi_n | \psi_n \rangle} = 1 - \lambda^2 \sum_{k \neq n} \frac{\left| \langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle \right|^2}{(E_n^{(0)} - E_k^{(0)})^2} + O(\lambda^2)$$

8. Example, Hamiltonian with 2x2 matix.

We consider a two-dimensional problem. In a given orthonormal basis the Hamiltonian is represented by the matrix

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} + \begin{pmatrix} 0 & \varepsilon \\ \varepsilon & 0 \end{pmatrix},$$

under the basis of $\{|1\rangle$ and $|2\rangle\}$, where ε is negligibly small. First we find the exact eigenvalues of $\hat{H}$

$$\begin{vmatrix} 1-\lambda & \varepsilon \\ \varepsilon & 2-\lambda \end{vmatrix} = 0,$$

or

$$\lambda = \frac{3 \pm \sqrt{1+4\varepsilon^2}}{2}.$$

This can be expanded in a binomial series:

$$\lambda = 2 + \varepsilon^2, \text{ or } \lambda = 1 - \varepsilon^2.$$

Next we use the second order perturbation to determine the eigenvalues.

$$E_1 = E_1^{(0)} + \langle 1 | \hat{H} | 1 \rangle + \frac{\left| \langle 2 | \hat{H} | 1 \rangle \right|^2}{E_1^{(0)} - E_2^{(0)}} = 1 + 0 + \frac{\varepsilon^2}{1-2} = 1 - \varepsilon^2,$$

$$E_2 = E_2^{(0)} + \langle 2 | \hat{H} | 2 \rangle + \frac{\left| \langle 1 | \hat{H} | 2 \rangle \right|^2}{E_2^{(0)} - E_1^{(0)}} = 2 + 0 + \frac{\varepsilon^2}{2-1} = 2 + \varepsilon^2$$

Then the second order corrections are the same as the result of the series expansion.

---

9. Simple harmonics

We consider the system whose Hamiltonian consists of the un-perturbed Hamiltonian of the simple harmonics, given by

$$\hat{H}_0 = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega_0{}^2\hat{x}^2 \,,$$

and the perturbing Hamiltonian given by

$$\hat{H}_1 = \frac{1}{2}\varepsilon m\omega_0{}^2\hat{x}^2 = \frac{\varepsilon}{4}\hbar\omega_0(\hat{a} + \hat{a}^+)^2 \,.$$

We note that

$$\hat{H}_0|n\rangle = E_n{}^{(0)}|n\rangle \,,$$

with

$$E_n{}^{(0)} = (n + \frac{1}{2})\hbar\omega_0$$

$$\hat{H}_1|n\rangle = \frac{1}{4}\varepsilon\hbar\omega_0[\sqrt{n(n-1)}|n-2\rangle + (2n+1)|n\rangle + \sqrt{(n+1)(n+2)}|n+2\rangle]$$

$$\langle n+2|\hat{H}_1|n\rangle = \frac{1}{4}\varepsilon\hbar\omega_0\sqrt{(n+1)(n+2)}$$

$$\langle n|\hat{H}_1|n\rangle = \frac{1}{2}\varepsilon\hbar\omega_0(n + \frac{1}{2})$$

$$\langle n-2|\hat{H}_1|n\rangle = \frac{1}{4}\varepsilon\hbar\omega_0\sqrt{n(n-1)}$$

Then

$$E_n = E_n{}^{(0)} + \langle n|\hat{H}_1|n\rangle + \sum_{k\neq n}\frac{\left|\langle n|\hat{H}_1|k\rangle\right|^2}{E_n{}^{(0)} - E_k{}^{(0)}} + \ldots$$

or

$$E_n = E_n{}^{(0)} + \langle n|\hat{H}_1|n\rangle + \frac{\left|\langle n|\hat{H}_1|n-2\rangle\right|^2}{E_n{}^{(0)} - E_{n-2}{}^{(0)}} + \frac{\left|\langle n|\hat{H}_1|n+2\rangle\right|^2}{E_n{}^{(0)} - E_{n+2}{}^{(0)}}$$

or

$$E_n = E_n^{(0)} + \frac{1}{2}\varepsilon\hbar\omega_0(n+\frac{1}{2}) + \frac{\varepsilon^2\hbar\omega_0}{32}[n(n-1)-(n+1)(n+2)]$$

or

$$E_n = \hbar\omega_0(n+\frac{1}{2})(1+\frac{1}{2}\varepsilon - \frac{1}{8}\varepsilon^2 + ...)$$

((**Note**))

$$\hat{\pi}|n\rangle = (-1)^n|n\rangle$$

Since

$\hat{\pi}\hat{x}\hat{\pi} = -\hat{x}$: odd parity

$\hat{\pi}\hat{x}^2\hat{\pi} = \hat{\pi}\hat{x}\hat{\pi}\hat{\pi}\hat{x}\hat{\pi} = \hat{x}^2$: even parity

Here

$$\hat{\pi}^2 = 1, \qquad \hat{\pi}^+ = \hat{\pi}$$

$\langle n|\hat{x}^2|m\rangle \neq 0$ for both *n* and *m* being odd and for both *n* and *m* being even.

When *n* is fixed, *m* should be $m = n$ and $m = n \pm 2$.

((**Note**)) **Exact solution**

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega_0^{\ 2}(1+\varepsilon)\hat{x}^2$$

Then we have

$$E_n = \hbar\omega_0\sqrt{1+\varepsilon}(n+\frac{1}{2}) = E_n^{(0)}\sqrt{1+\varepsilon}$$
$$= E_n^{(0)}(1+\frac{1}{2}\varepsilon - \frac{1}{8}\varepsilon^2 + \frac{1}{16}\varepsilon^3 - \frac{5}{128}\varepsilon^4 + \frac{7}{256}\varepsilon^5 + ...)$$

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10. Anharmonic oscillator

We calculate the eigenstates of the anharmonic oscillator whose Hamiltonian consists of the unperturbed Hamiltonian given by

$$\hat{H}_0 = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega_0{}^2\hat{x}^2 ,$$

and the perturbed Hamiltonian

$$\hat{H}_1 = K\hat{x}^4 = \frac{K}{4\beta^4}(\hat{a}+\hat{a}^+)^4 . \qquad \text{(anharmonic term)}$$

The unperturbed system:

$$\hat{H}_0|n\rangle = E_n{}^{(0)}|n\rangle ,$$

with

$$E_n{}^{(0)} = (n+\frac{1}{2})\hbar\omega_0 ,$$

$$\begin{aligned}\hat{H}_1|n\rangle = \frac{K}{4\beta^4}[&\sqrt{n(n-1)(n-2)(n-3}|n-4\rangle + 2(2n-1)\sqrt{n(n-1)}|n-2\rangle \\ &+3(1+2n+2n^2)|n\rangle + (6+4n)\sqrt{(n+2)(n+1)}|n+2\rangle \\ &+\sqrt{(n+4)(n+3)(n+2)(n+1)}|n+4\rangle]\end{aligned} ,$$

$$E_n = E_n{}^{(0)} + \langle n|\hat{H}_1|n\rangle + \sum_{k\neq n}\frac{|\langle n|\hat{H}_1|k\rangle|^2}{E_n{}^{(0)} - E_k{}^{(0)}}$$

or

$$\begin{aligned}E_n &= E_n{}^{(0)} + \langle n|\hat{H}_1|n\rangle + \sum_{k\neq n}\frac{|\langle k|\hat{H}_1|n\rangle|^2}{\hbar\omega_0(n-k)} \\ &= E_n{}^{(0)} + \langle n|\hat{H}_1|n\rangle \\ &+ \frac{1}{\hbar\omega_0}\left[\frac{|\langle n-4|\hat{H}_1|n\rangle|^2}{[n-(n-4)]} + \frac{|\langle n-2|\hat{H}_1|n\rangle|^2}{[n-(n-2)]} + \frac{|\langle n+2|\hat{H}_1|n\rangle|^2}{[n-(n+2)]} + \frac{|\langle n+4|\hat{H}_1|n\rangle|^2}{[n-(n+4)]}\right] \\ &= E_n{}^{(0)} + \langle n|\hat{H}_1|n\rangle \\ &+ \frac{1}{\hbar\omega_0}\left[\frac{|\langle n-4|\hat{H}_1|n\rangle|^2}{4} + \frac{|\langle n-2|\hat{H}_1|n\rangle|^2}{2} - \frac{|\langle n+2|\hat{H}_1|n\rangle|^2}{2} - \frac{|\langle n+4|\hat{H}_1|n\rangle|^2}{4}\right]\end{aligned}$$

where

$$\langle n|\hat{H}_1|n\rangle = \frac{K}{4\beta^4}(6n^2+6n+3),$$

$$\left|\langle n-4|\hat{H}_1|n\rangle\right|^2 = (\frac{K}{4\beta^4})^2 n(n-1)(n-2)(n-3),$$

$$\left|\langle n-2|\hat{H}_1|n\rangle\right|^2 = (\frac{K}{4\beta^4})^2[4(2n-1)^2 n(n-1)],$$

$$\left|\langle n+2|\hat{H}_1|n\rangle\right|^2 = (\frac{K}{4\beta^4})^2(6+4n)^2(n+2)(n+1),$$

$$\left|\langle n-4|\hat{H}_1|n\rangle\right|^2 = (\frac{K}{4\beta^4})^2(n+1)(n+2)(n+3)(n+4).$$

((**Note**))
Formula: matrix element of the simple harmonics for the perturbation calculation

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}.$$

The annihilation and creation operators

$$\hat{a} = \frac{\beta}{\sqrt{2}}(\hat{x} + i\frac{\hat{p}}{m\omega_0}),$$

$$\hat{a}^+ = \frac{\beta}{\sqrt{2}}(\hat{x} - i\frac{\hat{p}}{m\omega_0}),$$

$$[\hat{a}, \hat{a}^+] = 1,$$

$$\hat{N} = \hat{a}^+\hat{a},$$

$$\hat{H} = \hbar\omega_0(\hat{N} + \frac{1}{2}),$$

$$\hat{a}\,|\,n> = \sqrt{n}\,|\,n-1>,$$

$$\hat{a}^+\,|\,n> = \sqrt{n+1}\,|\,n+1>,$$

$$\hat{N}\,|\,n>=n\,|\,n>,$$

$$|\,n>=\frac{1}{\sqrt{n!}}(\hat{a}^{+})^{n}\,|\,0>,$$

$$[\hat{N},\hat{a}]=-\hat{a},$$

$$[\hat{N},\hat{a}^{+}]=\hat{a}^{+}.$$

The parity operator:

$$\hat{\pi}\,|\,n>=(-1)^{n}\,|\,n>,$$

$$\hat{x}=\frac{1}{\sqrt{2}\beta}(\hat{a}^{+}+\hat{a}),$$

$$\hat{p}=\frac{m\omega_{0}}{i}(\frac{\hat{a}-\hat{a}^{+}}{\sqrt{2}\beta}),$$

$$\hat{x}\left|n\right\rangle=\frac{1}{\sqrt{2}\beta}(\sqrt{n}\left|n-1\right\rangle+\sqrt{n+1}\left|n+1\right\rangle),$$

$$\hat{x}^{2}\left|n\right\rangle=\frac{1}{2\beta^{2}}(\sqrt{n(n-1)}\left|n-2\right\rangle+(2n+1)\left|n\right\rangle+\sqrt{(n+1)(n+2)}\left|n+2\right\rangle),$$

$$\hat{x}^{3}\left|n\right\rangle=\frac{1}{2\sqrt{2}\beta^{3}}(\sqrt{n(n-1)(n-2)}\left|n-3\right\rangle+3n^{3/2}\left|n-1\right\rangle+3(n+1)^{3/2}\left|n+1\right\rangle$$
$$+\sqrt{(n+1)(n+2)(n+3)}\left|n+3\right\rangle$$

$$\hat{x}^{4}\left|n\right\rangle=\frac{1}{4\beta^{4}}(\sqrt{n(n-1)(n-2)(n-3)}\left|n-4\right\rangle+2\sqrt{(n-1)n}(2n-1)\left|n-2\right\rangle$$
$$+3(2n^{2}+2n+1)\left|n\right\rangle+(6+4n)\sqrt{(n+1)(n+2)}\left|n+2\right\rangle$$
$$+\sqrt{(n+1)(n+2)(n+3)(n+4)}\left|n+4\right\rangle$$

$$\hat{x}^5|n\rangle = \frac{1}{4\sqrt{2}\beta^5}(\sqrt{n(n-1)(n-2)(n-3)(n-4)}|n-5\rangle$$
$$+5(n-1)\sqrt{(n-2)(n-1)n}|n-3\rangle + 5(2n^2+1)\sqrt{n}|n-1\rangle$$
$$+5(2n^2+4n+3)\sqrt{n+1}|n+1\rangle + 5(n+2)\sqrt{(n+1)(n+2)(n+3)}|n+3\rangle$$
$$+\sqrt{(n+1)(n+2)(n+3)(n+4)(n+5)}|n+5\rangle$$

11. Projection operator as a formulation of the perturbation theory

We consider the Schrödinger equation given by

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle .$$

with

$$\hat{H} = \hat{H}_0 + \hat{H}_1 .$$

Note that

$$\hat{H}_0|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle .$$

Now we assume that

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + |\Phi\rangle$$

and

$$\langle\psi_n^{(0)}|\Phi\rangle = 0 .$$

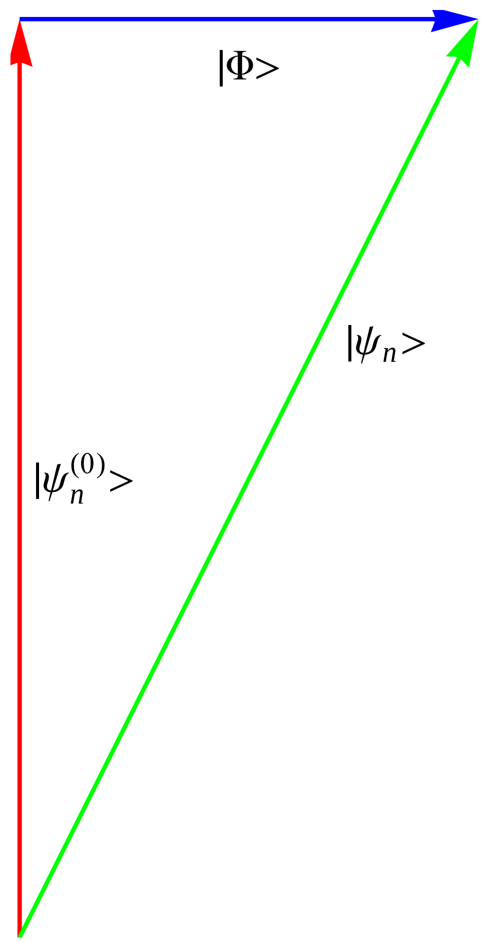

Fig. Schematic diagram. $\left|\psi_n\right\rangle = \left|\psi_n^{(0)}\right\rangle + \left|\Phi\right\rangle$ with $\left\langle\psi_n^{(0)}\middle|\Phi\right\rangle = 0$.

From the normalization condition of $\left\langle\psi_n\middle|\psi_n\right\rangle = 1$, we get

$$\begin{aligned}\left\langle\psi_n\middle|\psi_n\right\rangle &= (\left\langle\psi_n^{(0)}\right| + \left\langle\Phi\right|)(\left|\psi_n^{(0)}\right\rangle + \left|\Phi\right\rangle) \\ &= \left\langle\psi_n^{(0)}\middle|\psi_n^{(0)}\right\rangle + \left\langle\psi_n^{(0)}\middle|\Phi\right\rangle + \left\langle\Phi\middle|\psi_n^{(0)}\right\rangle + \left\langle\Phi\middle|\Phi\right\rangle \\ &= 1 + \left\langle\Phi\middle|\Phi\right\rangle \approx 1\end{aligned}$$

Here we define the projection operator given by

$$\hat{M} = \left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right|$$

where

$$\hat{M}\left|\psi_n^{(0)}\right\rangle = \left|\psi_n^{(0)}\right\rangle$$

(i) $\hat{M}$ is the Hermitian operator.

$$\hat{M}^+ = (\left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right|)^+ = \left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right| = \hat{M}$$

$$\hat{M}\left|\psi_n^{(0)}\right\rangle = \left|\psi_n^{(0)}\right\rangle$$

or

$$\left\langle\psi_n^{(0)}\right|\hat{M}^+ = \left\langle\psi_n^{(0)}\right|$$

or

$$\left\langle\psi_n^{(0)}\right|\hat{M} = \left\langle\psi_n^{(0)}\right|$$

(ii) $\hat{M}^2 = \hat{M}$

$$\hat{M}^2\left|\psi_n^{(0)}\right\rangle = \hat{M}\hat{M}\left|\psi_n^{(0)}\right\rangle = \hat{M}\left|\psi_n^{(0)}\right\rangle = \left|\psi_n^{(0)}\right\rangle$$

(iii) The projection operator $\hat{P}$

$$\hat{P} = \hat{1} - \hat{M},$$

which is the complementary projection operator.

$$\hat{M}\hat{P} = \hat{M}(\hat{1} - \hat{M}) = 0.$$

We note that

$$\hat{P}\left|\psi_n^{(0)}\right\rangle = 0$$

$$\hat{P}\left|\Phi\right\rangle = \left|\Phi\right\rangle$$

((**Proof**))

$$\hat{P}\left|\psi_n^{(0)}\right\rangle = (\hat{1} - \left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right|)\left|\left|\psi_n^{(0)}\right\rangle\right\rangle = 0$$

$$\hat{P}\left|\Phi\right\rangle = (\hat{1} - \left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right|)\left|\Phi\right\rangle = \left|\Phi\right\rangle$$

(iv) The commutation relation

$$[\hat{M}, \hat{H}_0] = 0 .$$

since

$$M\hat{H}_0 - \hat{H}_0\hat{M} = \left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right|\hat{H}_0 - \hat{H}_0\left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right|$$
$$= E_n^{(0)}\left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right| - E_n^{(0)}\left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right| = 0$$

(v) The commutation relation

$$[\hat{P}, \hat{H}_0] = 0$$

since

$$\hat{P}\hat{H}_0 - \hat{H}_0\hat{P} = (\hat{1} - \hat{M})\hat{H}_0 - \hat{H}_0(\hat{1} - \hat{M}) = -[\hat{M}, \hat{H}_0] = 0$$

---

12. Brillouin-Wigner series
(see J.M. Ziman, Element of Advanced Quantum Mechanics)

We start with the Schrödinger equation given by

$$\hat{H}\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle$$

with

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

Note that E_n is the energy eigenket of $\hat{H}$. Then we get

$$(\hat{H}_0 + \hat{H}_1)\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle$$

or

$$(\hat{H}_0 + \hat{H}_1)(\left|\psi_n^{(0)}\right\rangle + \left|\Phi\right\rangle) = E_n(\left|\psi_n^{(0)}\right\rangle + \left|\Phi\right\rangle)$$

or

$$E_n\left|\psi_n^{(0)}\right\rangle + E_n\left|\Phi\right\rangle = (\hat{H}_0 + \hat{H}_1)\left|\psi_n^{(0)}\right\rangle + (\hat{H}_0 + \hat{H}_1)\left|\Phi\right\rangle)$$

$$= E_n^{(0)}\left|\psi_n^{(0)}\right\rangle + \hat{H}_0\left|\Phi\right\rangle + \hat{H}_1\left|\psi_n^{(0)}\right\rangle + \hat{H}_1\left|\Phi\right\rangle$$

$$= E_n^{(0)}\left|\psi_n^{(0)}\right\rangle + \hat{H}_0\left|\Phi\right\rangle + \hat{H}_1\left|\psi_n\right\rangle$$

Finally we have

$$(E_n - \hat{H}_0)\left|\Phi\right\rangle = \hat{H}_1\left|\psi_n\right\rangle - (E_n - E_n^{(0)})\left|\psi_n^{(0)}\right\rangle$$

Projecting on both sides with $\hat{P}$

$$\hat{P}(E_n - \hat{H}_0)\left|\Phi\right\rangle = \hat{P}\hat{H}_1\left|\psi_n\right\rangle - (E_n - E_n^{(0)})\hat{P}\left|\psi_n^{(0)}\right\rangle$$

Noting that $\hat{P}\left|\psi_n^{(0)}\right\rangle = 0$ and $\hat{P}\left|\Phi\right\rangle = \left|\Phi\right\rangle$, and $[\hat{P}, \hat{H}_0] = 0$, we get

$$(E_n - \hat{H}_0)\hat{P}\left|\Phi\right\rangle = \hat{P}\hat{H}_1\left|\psi_n\right\rangle$$

or

$$(E_n - \hat{H}_0)\left|\Phi\right\rangle = \hat{P}\hat{H}_1\left|\psi_n\right\rangle$$

or

$$\left|\Phi\right\rangle = (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1\left|\psi_n\right\rangle$$

Thus we get the final form

$$\left|\psi_n\right\rangle = \left|\psi_n^{(0)}\right\rangle + (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1\left|\psi_n\right\rangle$$

We solve this by iteration method,

$$\begin{aligned}
\left|\psi_n\right\rangle &= \left|\psi_n^{(0)}\right\rangle + (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1(\left|\psi_n^{(0)}\right\rangle + (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1\left|\psi_n\right\rangle) \\
&= \left|\psi_n^{(0)}\right\rangle + (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1\left|\psi_n^{(0)}\right\rangle \\
&\quad + (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1\left|\psi_n^{(0)}\right\rangle + \\
&\quad + (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1\left|\psi_n^{(0)}\right\rangle + \\
&\quad + (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1\left|\psi_n^{(0)}\right\rangle + \ldots
\end{aligned}$$

where

$$[\hat{H}_0, \hat{P}] = 0 .$$

This equation can be rewritten by a geometric series

$$\begin{aligned}
\left|\psi_n\right\rangle &= \left|\psi_n{}^{(0)}\right\rangle + (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1\left|\psi_n{}^{(0)}\right\rangle + [(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1]^2\left|\psi_n{}^{(0)}\right\rangle \\
&\quad + [(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1]^3\left|\psi_n{}^{(0)}\right\rangle + \ldots + [(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1]^n\left|\psi_n{}^{(0)}\right\rangle + \ldots \\
&= \sum_{k=0}^{\infty}[(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1]^k\left|\psi_n{}^{(0)}\right\rangle \\
&= [\hat{1} - (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1]^{-1}\left|\psi_n{}^{(0)}\right\rangle
\end{aligned}$$

Note that

$$\begin{aligned}
[\hat{1} - (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1]^{-1} &= [(E_n - \hat{H}_0)^{-1}(E_n - \hat{H}_0) - (E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1]^{-1} \\
&= [(E_n - \hat{H}_0)^{-1}(E_n - \hat{H}_0 - \hat{P}\hat{H}_1)]^{-1} \\
&= (E_n - \hat{H}_0 - \hat{P}\hat{H}_1)^{-1}(E_n - \hat{H}_0)
\end{aligned}$$

and

$$\begin{aligned}
(E_n - \hat{H}_0 - \hat{P}\hat{H}_1)^{-1}(E_n - \hat{H}_0)\left|\psi_n{}^{(0)}\right\rangle &= (E_n - E_n{}^{(0)} - \hat{P}\hat{H}_1)^{-1}(E_n - E_n{}^{(0)})\left|\psi_n{}^{(0)}\right\rangle \\
&= \frac{E_n - E_n{}^{(0)}}{E_n - \hat{H}_0 - \hat{P}\hat{H}_1}\left|\psi_n{}^{(0)}\right\rangle
\end{aligned}$$

Thus we have

$$\left|\psi_n\right\rangle = \frac{E_n - E_n{}^{(0)}}{E_n - E_n{}^{(0)} - \hat{P}\hat{H}_1}\left|\psi_n{}^{(0)}\right\rangle$$

The formula is very similar to the Rayleigh-Schrödinger series of conventional perturbation theory, except that the perturbed energy of E_n.

13. Energy shift

What is the energy shift due to the perturbation? To this end, we start with

$$(E_n - \hat{H}_0)\left|\psi_n\right\rangle = \hat{H}_1\left|\psi_n\right\rangle$$

Projecting on both sides with $\hat{M}$

$$\hat{M}(E_n - \hat{H}_0)|\psi_n\rangle = \hat{M}\hat{H}_1|\psi_n\rangle$$

or

$$(E_n - \hat{H}_0)\hat{M}|\psi_n\rangle = \hat{M}\hat{H}_1|\psi_n\rangle,$$

or

$$(E_n - \hat{H}_0)\left|\psi_n^{(0)}\right\rangle = \hat{M}\hat{H}_1|\psi_n\rangle,$$

where we use the commutation relation,

$$[\hat{M}, \hat{H}_0] = 0.$$

Multiplying on both sides with $\left\langle\psi_n^{(0)}\right|$

$$\left\langle\psi_n^{(0)}\right|(E_n - \hat{H}_0)\left|\psi_n^{(0)}\right\rangle = \left\langle\psi_n^{(0)}\right|\hat{M}\hat{H}_1|\psi_n\rangle$$

Then the energy shift is obtained as

$$E_n - E_n^{(0)} = \left\langle\psi_n^{(0)}\right|\hat{M}\hat{H}_1|\psi_n\rangle = \left\langle\psi_n^{(0)}\right|\hat{H}_1|\psi_n\rangle$$

Through the iteration method, we have

$$\begin{aligned} E_n - E_n^{(0)} &= \left\langle\psi_n^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle + \left\langle\psi_n^{(0)}\right|\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1\left|\psi_n^{(0)}\right\rangle \\ &\quad + \left\langle\psi_n^{(0)}\right|\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1\left|\psi_n^{(0)}\right\rangle + \\ &\quad + \left\langle\psi_n^{(0)}\right|\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1(E_n - \hat{H}_0)^{-1}\hat{P}\hat{H}_1\left|\psi_n^{(0)}\right\rangle + \end{aligned}$$

(i) The first-order energy shift:

$$E_n^{(1)} = \left\langle\psi_n^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle.$$

(ii) The second-order energy shift:

$$E_n^{(2)} = \langle \psi_n^{(0)} | \hat{H}_1 (E_n - \hat{H}_0)^{-1} \hat{P} \hat{H}_1 | \psi_n^{(0)} \rangle$$

$$= \sum_{k \neq n} \langle \psi_n^{(0)} | \hat{H}_1 (E_n - \hat{H}_0)^{-1} \hat{P} | \psi_k^{(0)} \rangle \langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle$$

$$+ \langle \psi_n^{(0)} | \hat{H}_1 (E_n - \hat{H}_0)^{-1} \hat{P} | \psi_n^{(0)} \rangle \langle \psi_n^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle$$

$$= \sum_{k \neq n} \langle \psi_n^{(0)} | \hat{H}_1 (E_n - \hat{H}_0)^{-1} \hat{P} | \psi_k^{(0)} \rangle \langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle$$

$$= \sum_{k \neq n} \frac{\left| \langle \psi_n^{(0)} | \hat{H}_1 | \psi_k^{(0)} \rangle \right|^2}{E_n - E_k^{(0)}}$$

since $\hat{P} | \psi_n^{(0)} \rangle = 0$. When $E_n \rightarrow E_n^{(0)}$, we get a "Rayleigh-Schrödinger series of conventional perturbation theory." Then the final form of the second order of the energy shift is given by

$$E_n^{(2)} = \sum_{k \neq n} \frac{\left| \langle \psi_n^{(0)} | \hat{H}_1 | \psi_k^{(0)} \rangle \right|^2}{E_n^{(0)} - E_k^{(0)}} .$$

or

$$E_n^{(2)} = \sum_{k \neq n} \frac{\langle \psi_n^{(0)} | \hat{H}_1 | \psi_k^{(0)} \rangle \langle \psi_k^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}}$$

where $E_n \rightarrow E_n^{(0)}$.

(iii) The third order of the energy shift:

$$E_n^{(3)} = \langle \psi_n^{(0)} | \hat{H}_1 (E_n - \hat{H}_0)^{-1} \hat{P} \hat{H}_1 (E_n - \hat{H}_0)^{-1} \hat{P} \hat{H}_1 | \psi_n^{(0)} \rangle$$

$$= \sum_{k \neq n. l \neq n} \langle \psi_n^{(0)} | \hat{H}_1 (E_n - \hat{H}_0)^{-1} \hat{P} | \psi_k^{(0)} \rangle \langle \psi_k^{(0)} | \hat{H}_1 (E_n - \hat{H}_0)^{-1} \hat{P} | \psi_l^{(0)} \rangle \langle \psi_l^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle$$

$$= \sum_{k \neq n. l \neq n} \frac{\langle \psi_n^{(0)} | \hat{H}_1 | \psi_k^{(0)} \rangle \langle \psi_k^{(0)} | \hat{H}_1 | \psi_l^{(0)} \rangle \langle \psi_l^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{(E_n - E_k^{(0)})(E_n - E_l^{(0)})}$$

or

$$E_n^{(3)} \approx \sum_{k \neq n. l \neq n} \frac{\langle \psi_n^{(0)} | \hat{H}_1 | \psi_k^{(0)} \rangle \langle \psi_k^{(0)} | \hat{H}_1 | \psi_l^{(0)} \rangle \langle \psi_l^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_l^{(0)})}$$

where $E_n \rightarrow E_n^{(0)}$.

(iv) The fourth-order of the energy shift:

$$E_n^{(4)} \approx \sum_{\substack{k\neq n.l\neq n\\ m\neq n}} \frac{\langle\psi_n^{(0)}|\hat{H}_1|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{H}_1|\psi_l^{(0)}\rangle\langle\psi_l^{(0)}|\hat{H}_1|\psi_m^{(0)}\rangle\langle\psi_m^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{(E_n^{(0)}-E_k^{(0)})(E_n^{(0)}-E_l^{(0)})(E_n^{(0)}-E_m^{(0)})}$$

where $E_n \to E_n^{(0)}$.

14. The form of $|\Phi\rangle$

Next we discuss the from of $|\Phi\rangle$.

(i) The first order of wave function:

$$\begin{aligned}|\psi_n^{(1)}\rangle &= (E_n-\hat{H}_0)^{-1}\hat{P}\hat{H}_1|\psi_n^{(0)}\rangle\\ &= \sum_{k\neq n}(E_n-\hat{H}_0)^{-1}\hat{P}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle\\ &= \sum_{k\neq n}\frac{|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{(E_n-E_k^{(0)})}\end{aligned}$$

or

$$|\psi_n^{(1)}\rangle \approx \sum_{k\neq n}\frac{|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{(E_n^{(0)}-E_k^{(0)})}$$

where $E_n \to E_n^{(0)}$.

(ii) The second order of the wave function:

$$\begin{aligned}|\psi_n^{(2)}\rangle &= (E_n-\hat{H}_0)^{-1}\hat{P}\hat{H}_1(E_n-\hat{H}_0)^{-1}\hat{P}\hat{H}_1|\psi_n^{(0)}\rangle\\ &= \sum_{k\neq n,l\neq n}(E_n-\hat{H}_0)^{-1}\hat{P}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{H}_1(E_n-\hat{H}_0)^{-1}\hat{P}|\psi_l^{(0)}\rangle\langle\psi_l^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle\\ &= \sum_{k\neq n,l\neq n}\frac{|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{H}_1|\psi_l^{(0)}\rangle\langle\psi_l^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{(E_n^{(0)}-E_k^{(0)})(E_n^{(0)}-E_l^{(0)})}\end{aligned}$$

or

$$|\psi_n^{(2)}\rangle = \sum_{k\neq n,l\neq n}\frac{|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{H}_1|\psi_l^{(0)}\rangle\langle\psi_l^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{(E_n^{(0)}-E_k^{(0)})(E_n^{(0)}-E_l^{(0)})}$$

where $E_n \to E_n^{(0)}$.

(iii) The third order of the wave function:

$$\left|\psi_n^{(3)}\right\rangle \approx \sum_{\substack{k\neq n, l\neq n \\ m\neq n}} \frac{\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\hat{H}_1\left|\psi_l^{(0)}\right\rangle\left\langle\psi_l^{(0)}\right|\hat{H}_1\left|\psi_m^{(0)}\right\rangle\left\langle\psi_m^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle}{(E_n^{(0)}-E_k^{(0)})(E_n^{(0)}-E_l^{(0)})(E_n^{(0)}-E_m^{(0)})}.$$

(iv) The fourth order of the wave function:

$$\left|\psi_n^{(4)}\right\rangle \approx \sum_{\substack{k\neq n, l\neq n \\ m\neq n}} \frac{\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\hat{H}_1\left|\psi_l^{(0)}\right\rangle\left\langle\psi_l^{(0)}\right|\hat{H}_1\left|\psi_m^{(0)}\right\rangle\left\langle\psi_m^{(0)}\right|\hat{H}_1\left|\psi_p^{(0)}\right\rangle\left\langle\psi_p^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle}{(E_n^{(0)}-E_k^{(0)})(E_n^{(0)}-E_l^{(0)})(E_n^{(0)}-E_m^{(0)})(E_n^{(0)}-E_p^{(0)})}.$$

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15. Degenerate case (simple case)

Here is the procedure of calculation for the perturbation with degeneracy. We have now *g*-degenerate states with

$$\hat{H}_0\left|\varphi_{n,\mu}^{(0)}\right\rangle = E_n^{(0)}\left|\varphi_{n,\mu}^{(0)}\right\rangle$$

with

$$\left|\varphi_{n,\mu}^{(0)}\right\rangle \qquad (\mu = 1, 2, 3, ..., g)$$

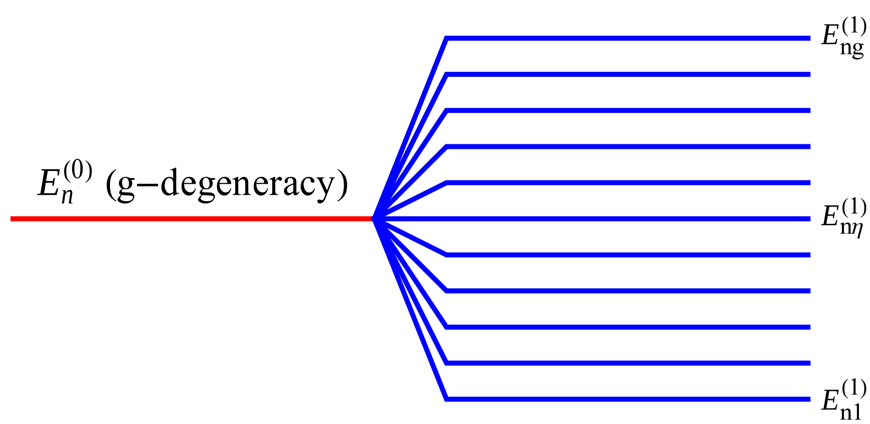


Fig. Energy level with the *g*-degeneracy for the unperturbed system. Under the perturbation, the energy level splits into various energy levels.

The new Hamiltonian *H* is given by

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \qquad (\hat{H}_1 \text{ is the perturbation}).$$

In order to get the energy eigenvalue of $\hat{H}$ we need to calculate $\hat{H}_1\left|\varphi_{n,\mu}{}^{(0)}\right\rangle$.

(i) The simplest case

$$\hat{H}_1\left|\varphi_{n,\mu}{}^{(0)}\right\rangle = \varepsilon_\mu\left|\varphi_{n,\mu}{}^{(0)}\right\rangle$$

where ε_μ are different for different μ. The perturbed energy is given by $E_n{}^{(0)} + \varepsilon_\mu$. since

$$(\hat{H}_0 + \hat{H}_1)\left|\varphi_{n,\mu}{}^{(0)}\right\rangle = (E_n{}^{(0)} + \varepsilon_\mu)\left|\varphi_{n,\mu}{}^{(0)}\right\rangle$$

(ii) The simple case.

Suppose that we get

$$\hat{H}_1\left|\varphi_{n,1}{}^{(0)}\right\rangle = A_{11}\left|\varphi_{n,1}{}^{(0)}\right\rangle + A_{12}\left|\varphi_{n,2}{}^{(0)}\right\rangle$$

$$\hat{H}_1\left|\varphi_{n,2}{}^{(0)}\right\rangle = A_{21}\left|\varphi_{n,1}{}^{(0)}\right\rangle + A_{22}\left|\varphi_{n,2}{}^{(0)}\right\rangle$$

$$\hat{H}_1\left|\varphi_{n,\mu}{}^{(0)}\right\rangle = \varepsilon_\mu\left|\varphi_{n,\mu}{}^{(0)}\right\rangle \qquad \text{with } \mu = 3,4,\ldots, g.$$

In this case, we already know that $\left|\varphi_{n,\mu}{}^{(0)}\right\rangle$ with $\mu = 3,4,\ldots, g$ is the eigenket of $\hat{H}$ with the energy eigenvalue $E_n{}^{(0)} + \varepsilon_\mu$. Here we consider the case where

$$\hat{H}_1\left|\varphi_{n,1}{}^{(0)}\right\rangle = A_{11}\left|\varphi_{n,1}{}^{(0)}\right\rangle + A_{12}\left|\varphi_{n,2}{}^{(0)}\right\rangle$$

$$\hat{H}_1\left|\varphi_{n,2}{}^{(0)}\right\rangle = A_{21}\left|\varphi_{n,1}{}^{(0)}\right\rangle + A_{22}\left|\varphi_{n,2}{}^{(0)}\right\rangle$$

We introduce the matrix notation;

$$\hat{H}_1 = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

we get

$$\hat{H}_1\left|\psi_{n,1}{}^{(0)}\right\rangle = \varepsilon_1\left|\psi_{n,1}{}^{(0)}\right\rangle, \qquad \hat{H}_1\left|\psi_{n,2}{}^{(0)}\right\rangle = \varepsilon_2\left|\psi_{n,1}{}^{(0)}\right\rangle$$

Using the Unitary matrix

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}$$

we have

$$\left|\psi_{n,1}{}^{(0)}\right\rangle = \hat{U}\left|\varphi_{n,1}{}^{(0)}\right\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix}$$

$$\left|\psi_{n,2}{}^{(0)}\right\rangle = \hat{U}\left|\varphi_{n,2}{}^{(0)}\right\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix}$$

(i) For $\lambda = \varepsilon_1$,

$$\hat{H}_1\left|\psi_{n,1}{}^{(0)}\right\rangle = \varepsilon_1\left|\psi_{n,1}{}^{(0)}\right\rangle,$$

or

$$\hat{H}_1\hat{U}\left|\varphi_{n,1}{}^{(0)}\right\rangle = \varepsilon_1\hat{U}\left|\varphi_{n,1}{}^{(0)}\right\rangle\left|\varphi_{n,1}{}^{(0)}\right\rangle$$

or

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = \varepsilon_1\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix}$$ (eigenvalue problem)

(ii) For $\lambda = \varepsilon_2$,

$$\hat{H}_1\left|\psi_{n,2}{}^{(0)}\right\rangle = \varepsilon_2\left|\psi_{n,2}{}^{(0)}\right\rangle,$$

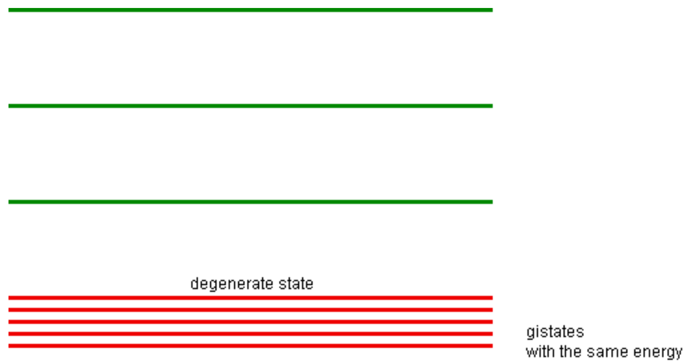
or

$$\hat{H}_1\hat{U}\left|\varphi_{n,2}{}^{(0)}\right\rangle = \varepsilon_1\hat{U}\left|\varphi_{n,2}{}^{(0)}\right\rangle$$

or

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\begin{pmatrix} U_{21} \\ U_{22} \end{pmatrix} = \varepsilon_2\begin{pmatrix} U_{21} \\ U_{22} \end{pmatrix}$$ (eigenvalue problem)

16. Degenerate case (general case):



In the absence of the perturbation, we assume that there are *g*-states with the independent eigenstates given by

$$\left|\varphi_{n,\mu}{}^{(0)}\right\rangle \qquad (\mu = 1, 2, 3, ..., g)$$

What happens to these eigenvalues and eigenstates when the perturbation $\hat{H}_1$ is applied to the system?

$$(\hat{H}_0 + \lambda\hat{H}_1)(\left|\psi_n{}^{(0)}\right\rangle + \lambda\left|\psi_n{}^{(1)}\right\rangle + \lambda^2\left|\psi_n{}^{(2)}\right\rangle + ...)$$
$$= (E_n{}^{(0)} + \lambda E_n{}^{(1)} + \lambda^2 E_n{}^{(2)} + ...)(\left|\psi_n{}^{(0)}\right\rangle + \lambda\left|\psi_n{}^{(1)}\right\rangle + \lambda^2\left|\psi_n{}^{(2)}\right\rangle + ...)$$

For the 0-th order terms in λ,

$$(\hat{H}_0 - E_n{}^{(0)})\left|\psi_n{}^{(0)}\right\rangle = 0\,, \qquad (1)$$

For the 1st-order terms in λ,

$$(\hat{H}_0 - E_n{}^{(0)})\left|\psi_n{}^{(1)}\right\rangle + (\hat{H}_1 - E_n{}^{(1)})\left|\psi_n{}^{(0)}\right\rangle = 0\,, \qquad (2)$$

For the 2nd-order terms in λ,

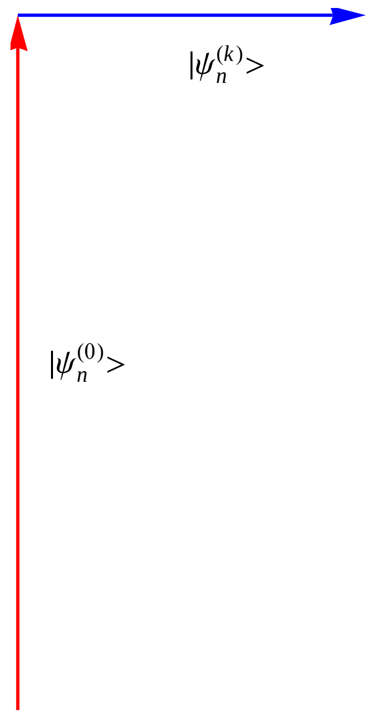
$$(\hat{H}_0 - E_n{}^{(0)})\left|\psi_n{}^{(2)}\right\rangle + (\hat{H}_1 - E_n{}^{(1)})\left|\psi_n{}^{(1)}\right\rangle - E_n{}^{(2)}\left|\psi_n{}^{(0)}\right\rangle = 0\,, \qquad (3)$$

For the 3rd-order terms in λ,

$$(\hat{H}_0 - E_n{}^{(0)})\left|\psi_n{}^{(3)}\right\rangle + (\hat{H}_1 - E_n{}^{(1)})\left|\psi_n{}^{(2)}\right\rangle - E_n{}^{(2)}\left|\psi_n{}^{(1)}\right\rangle - E_n{}^{(3)}\left|\psi_n{}^{(0)}\right\rangle = 0$$

where we assume that

$$\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle = 0 , \qquad \langle \psi_n^{(0)} | \psi_n^{(2)} \rangle = 0 , \ldots\ldots$$



17. Degenerate case: the first order

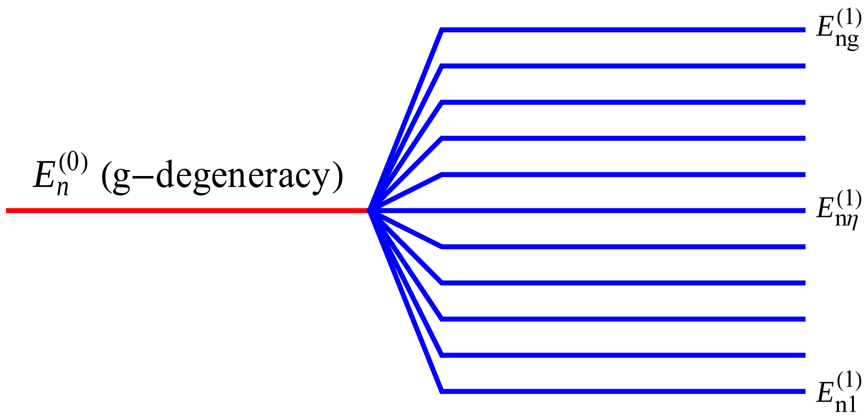
We have now g-degenerate states with

$$|\psi_n^{(0)}\rangle = |\varphi_{n,\mu}^{(0)}\rangle , \qquad (\mu = 1, 2, 3, \ldots., g)$$

where

$$\hat{H}_0 |\varphi_{n,\mu}^{(0)}\rangle = E_n^{(0)} |\varphi_{n,\mu}^{(0)}\rangle .$$

$|\varphi_{n,\mu}^{(0)}\rangle$ is different state for different μ.



For the 1st-order terms in λ,

$$(\hat{H}_0 - E_n^{(0)})\left|\psi_n^{(1)}\right\rangle + (\hat{H}_1 - E_n^{(1)})\left|\psi_n^{(0)}\right\rangle = 0\,. \qquad (1)$$

By taking an inner product of $\left\langle \varphi_{n,\mu}^{(0)}\right|$ and Eq.(1), we get

$$\left\langle \varphi_{n,\mu}^{(0)}\right|(\hat{H}_0 - E_n^{(0)})\left|\psi_n^{(1)}\right\rangle + \left\langle \varphi_{n,\mu}^{(0)}\right|(\hat{H}_1 - E_n^{(1)})\left|\psi_n^{(0)}\right\rangle = 0\,,$$

or

$$\left\langle \varphi_{n,\mu}^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle = E_n^{(1)}\left\langle \varphi_{n,\mu}^{(0)}\middle|\psi_n^{(0)}\right\rangle.$$

Using the closure relation, we have

$$\sum_{\nu=1}^{g}\left\langle \varphi_{n,\mu}^{(0)}\right|\hat{H}_1\left|\varphi_{n,\nu}^{(0)}\right\rangle\left\langle \varphi_{n,\nu}^{(0)}\middle|\psi_n^{(0)}\right\rangle = E_n^{(1)}\left\langle \varphi_{n,\mu}^{(0)}\middle|\psi_n^{(0)}\right\rangle.$$

We need to calculate the matrix elements;

$$\left\langle \varphi_{n,\mu}^{(0)}\right|\hat{H}_1\left|\varphi_{n,\nu}^{(0)}\right\rangle.$$

Then we solve the eigenvalue problem

$$\sum_{\nu=1}^{g}[\left\langle \varphi_{n,\mu}^{(0)}\right|\hat{H}_1\left|\varphi_{n,\nu}^{(0)}\right\rangle - E_n^{(1)}\delta_{\mu\nu}]\left\langle \varphi_{n,\nu}^{(0)}\middle|\psi_n^{(0)}\right\rangle = 0\,,$$

where μ = 1, 2, ..., g, and ν = 1, 2, ..., g

or

$$\begin{pmatrix} H_{11}-E_n^{(1)} & H_{12} & H_{13} & . & . & . & H_{1g} \\ H_{21} & H_{22}-E_n^{(1)} & H_{23} & . & . & . & H_{2g} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ H_{g1} & H_{g2} & H_{g3} & . & . & . & H_{gg}-E_n^{(1)} \end{pmatrix} \begin{pmatrix} \langle \varphi_{n,1}^{(0)} | \psi_n^{(0)} \rangle \\ \langle \varphi_{n,2}^{(0)} | \psi_n^{(0)} \rangle \\ . \\ . \\ . \\ . \\ \langle \varphi_{n,g}^{(0)} | \psi_n^{(0)} \rangle \end{pmatrix} = 0$$

for the eigenvalue $E_n^{(1)}$. The Unitary transformation:

$$\left| \psi_{n,\mu}^{(0)} \right\rangle = \hat{U} \left| \varphi_{n,\mu}^{(0)} \right\rangle = \begin{pmatrix} U_{1\mu} \\ U_{2\mu} \\ . \\ . \\ U_{n\mu} \end{pmatrix}$$

where the Unitary operator is given by

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} & . & . & U_{1g} \\ U_{21} & U_{22} & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ U_{g1} & U_{g2} & . & . & U_{gg} \end{pmatrix}$$

and the matrix form of the bases are given by

$$\left| \varphi_{n,1}^{(0)} \right\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ . \\ . \\ . \\ 0 \end{pmatrix}, \quad \left| \varphi_{n,2}^{(0)} \right\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ . \\ . \\ . \\ 0 \end{pmatrix}, \quad \ldots\ldots\ldots\ldots\ldots\ldots, \quad \left| \varphi_{n,g}^{(0)} \right\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ . \\ . \\ . \\ 1 \end{pmatrix}$$

Then we have the resultant energy as

$$E_n^{(0)} + E_{n,\mu}^{(1)} \qquad (\mu = 1, 2, 3, ..., g).$$

$$\left|\psi_{n,\mu}^{(0)}\right\rangle = \begin{pmatrix} U_{1\mu} \\ U_{2\mu} \\ . \\ . \\ . \\ . \\ . \\ U_{g\mu} \end{pmatrix}.$$

((Note)) **Projection operator**

$$\hat{M} = \sum_{\mu=1}^{g} \left|\varphi_{n,\mu}^{(0)}\right\rangle\left\langle\varphi_{n,\mu}^{(0)}\right| = \sum_{\mu=1}^{g} \left|\mu\right\rangle\left\langle\mu\right|$$

$$\hat{M}\left|\psi_n^{(0)}\right\rangle = \sum_{\mu=1}^{g} \left|\varphi_{n,\mu}^{(0)}\right\rangle\left\langle\varphi_{n,\mu}^{(0)}\middle|\psi_n^{(0)}\right\rangle$$

$$\begin{aligned}\left\langle\varphi_{n,\nu}^{(0)}\middle|\hat{M}\middle|\psi_n^{(0)}\right\rangle &= \sum_{\mu=1}^{g} \left\langle\varphi_{n,\nu}^{(0)}\middle|\varphi_{n,\mu}^{(0)}\right\rangle\left\langle\varphi_{n,\mu}^{(0)}\middle|\psi_n^{(0)}\right\rangle \\ &= \sum_{\mu=1}^{g} \delta_{\mu,\nu}\left\langle\varphi_{n,\mu}^{(0)}\middle|\psi_n^{(0)}\right\rangle \\ &= \left\langle\varphi_{n,\nu}^{(0)}\middle|\psi_n^{(0)}\right\rangle\end{aligned}$$

or

$$\left\langle\varphi_{n,\mu}^{(0)}\middle|\hat{M}\middle|\psi_n^{(0)}\right\rangle = \left\langle\varphi_{n,\mu}^{(0)}\middle|\psi_n^{(0)}\right\rangle$$

So $\hat{M}$ plays a role of the closure relation under the basis of $\{\left|\varphi_{n,\mu}^{(0)}\right\rangle\}$.

18. Degenerate case: second-order correction

Now we consider the second-order correction

$$(\hat{H}_0 - E_n^{(0)})\left|\psi_n^{(2)}\right\rangle + (\hat{H}_1 - E_n^{(1)})\left|\psi_n^{(1)}\right\rangle - E_n^{(2)}\left|\psi_n^{(0)}\right\rangle = 0$$

$$\left\langle \varphi_{n,\mu}{}^{(0)} \right| \times$$

$$\left\langle \varphi_{n,\mu}{}^{(0)} \right| (\hat{H}_0 - E_n{}^{(0)}) \left| \psi_n{}^{(2)} \right\rangle + \left\langle \varphi_{n,\mu}{}^{(0)} \right| (\hat{H}_1 - E_n{}^{(1)}) \left| \psi_n{}^{(1)} \right\rangle - E_n{}^{(2)} \left\langle \varphi_{n,\mu}{}^{(0)} \middle| \psi_n{}^{(0)} \right\rangle = 0$$

or

$$\left\langle \varphi_{n,\mu}{}^{(0)} \right| (\hat{H}_1 - E_n{}^{(1)}) \left| \psi_n{}^{(1)} \right\rangle - E_n{}^{(2)} \left\langle \varphi_{n,\mu}{}^{(0)} \middle| \psi_n{}^{(0)} \right\rangle = 0$$

or

$$\left\langle \varphi_{n,\mu}{}^{(0)} \right| \hat{H}_1 \left| \psi_n{}^{(1)} \right\rangle - E_n{}^{(1)} \left\langle \varphi_{n,\mu}{}^{(0)} \middle| \psi_n{}^{(1)} \right\rangle - E_n{}^{(2)} \left\langle \varphi_{n,\mu}{}^{(0)} \middle| \psi_n{}^{(0)} \right\rangle = 0 \qquad (1)$$

Here we use

$$\left| \psi_n{}^{(1)} \right\rangle = \sum_{k \neq n} \frac{\left| \psi_k{}^{(0)} \right\rangle \left\langle \psi_k{}^{(0)} \right| \hat{H}_1 \left| \psi_n{}^{(0)} \right\rangle}{E_n{}^{(0)} - E_k{}^{(0)}}$$

which is obtained from the perturbation theory for the non-degenerate case, where

$$E_n{}^{(0)} \neq E_k{}^{(0)}$$

We note that

$$\left\langle \psi_k{}^{(0)} \right| \hat{H}_1 \left| \psi_n{}^{(0)} \right\rangle = \sum_{\nu=1}^{g} \left\langle \psi_k{}^{(0)} \right| \hat{H}_1 \left| \varphi_{n,\nu}{}^{(0)} \right\rangle \left\langle \varphi_{n,\nu}{}^{(0)} \middle| \psi_n{}^{(0)} \right\rangle$$

and

$$\left\langle \varphi_{n,\nu}{}^{(0)} \middle| \psi_n{}^{(1)} \right\rangle = 0$$

From Eq.(1), we get

$$\left\langle \varphi_{n,\mu}{}^{(0)} \right| \hat{H}_1 \left| \psi_n{}^{(1)} \right\rangle = E_n{}^{(2)} \left\langle \varphi_{n,\mu}{}^{(0)} \middle| \psi_n{}^{(0)} \right\rangle$$

or

$$\sum_{\nu=1}^{g} \sum_{k \neq n} \frac{\left\langle \varphi_{n,\mu}{}^{(0)} \right| \hat{H}_1 \left| \psi_k{}^{(0)} \right\rangle \left\langle \psi_k{}^{(0)} \right| \hat{H}_1 \left| \varphi_{n,\nu}{}^{(0)} \right\rangle \left\langle \varphi_{n,\nu}{}^{(0)} \middle| \psi_n{}^{(0)} \right\rangle}{E_n{}^{(0)} - E_k{}^{(0)}} = E_n{}^{(2)} \left\langle \varphi_{n,\mu}{}^{(0)} \middle| \psi_n{}^{(0)} \right\rangle$$

We define the following operator

$$\hat{\Lambda} = \sum_{k \neq n} \frac{\hat{H}_1 \left|\psi_k^{(0)}\right\rangle \left\langle \psi_k^{(0)}\right| \hat{H}_1}{E_n^{(0)} - E_k^{(0)}}$$

Then we have

$$\sum_{\nu=1}^{g} \left\langle \varphi_{n,\mu}^{(0)} \right| \hat{\Lambda} \left| \varphi_{n,\nu}^{(0)} \right\rangle \left\langle \varphi_{n,\nu}^{(0)} \middle| \psi_n^{(0)} \right\rangle = E_n^{(2)} \left\langle \varphi_{n,\mu}^{(0)} \middle| \psi_n^{(0)} \right\rangle$$

$$\left|\psi^{(0)}\right\rangle = \sum_{\mu} a_\mu \left|\varphi_{n,\mu}^{(0)}\right\rangle$$

When we use $\left|\varphi_{n,\mu}^{(0)}\right\rangle = |\mu\rangle$ for convenience, the above form can be rewritten as

$$\sum_{\nu=1}^{g} \langle \mu | \hat{\Lambda} | \nu \rangle \left\langle \nu \middle| \psi_n^{(0)} \right\rangle = E_n^{(2)} \left\langle \mu \middle| \psi_n^{(0)} \right\rangle$$

19. Perturbation theory for the degenerate case (Sakurai)

The projection operator is defined as

$$\hat{M} = \sum_{\mu=1}^{g} \left|\varphi_{n,\mu}^{(0)}\right\rangle \left\langle \varphi_{n,\mu}^{(0)}\right| = \sum_{\mu=1}^{g} |\mu\rangle\langle\mu|$$

$$\hat{P} = \hat{1} - \hat{M}$$

$$[\hat{M}, \hat{H}_0] = 0, \qquad [\hat{P}, \hat{H}_0] = 0$$

((Note)) **Property of the projection operator** $\hat{M}$

We consider a arbitrary $\left|\psi^0\right\rangle$ which is given by the form

$$\left|\psi^{(0)}\right\rangle = \sum_{\mu} a_\mu \left|\varphi_{n,\mu}^{(0)}\right\rangle = \sum_{\mu} a_\mu |\mu\rangle$$

with $a_\mu = \left\langle \varphi_{n,\mu}^{(0)} \middle| \psi^{(0)} \right\rangle$. In this case $\left|\psi^{(0)}\right\rangle$ can be rewritten as

$$\begin{aligned}\left|\psi^{(0)}\right\rangle &= \sum_{\mu}\left\langle \varphi_{n,\mu}{}^{(0)} \middle| \psi^{(0)}\right\rangle \left|\varphi_{n,\mu}{}^{(0)}\right\rangle \\ &= \sum_{\mu}\left|\varphi_{n,\mu}{}^{(0)}\right\rangle\left\langle \varphi_{n,\mu}{}^{(0)} \middle| \psi^{(0)}\right\rangle \\ &= \hat{M}\left|\psi^{(0)}\right\rangle\end{aligned}$$

or

$$\hat{M}\left|\psi^{(0)}\right\rangle = \left|\psi^{(0)}\right\rangle$$

The eigenvalue problem

$$(\hat{H}_0 + \lambda\hat{V})\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle$$

or

$$0 = (E_n - \hat{H}_0 - \lambda\hat{V})\left|\psi_n\right\rangle$$

The state vector can be expressed by

$$\begin{aligned}\left|\psi_n\right\rangle &= (\hat{P} + \hat{M})\left|\psi_n\right\rangle \\ &= \hat{M}\left|\psi_n\right\rangle + \hat{P}\left|\psi_n\right\rangle\end{aligned}$$

Using this form of $\left|\psi_n\right\rangle$, we have

$$0 = (E_n - \hat{H}_0 - \lambda\hat{V})(\hat{M}\left|\psi_n\right\rangle + \hat{P}\left|\psi_n\right\rangle)$$

or

$$0 = (E_n - \hat{H}_0 - \lambda\hat{V})\hat{M}\left|\psi_n\right\rangle + (E_n - \hat{H}_0 - \lambda\hat{V})\hat{P}\left|\psi_n\right\rangle \qquad (1)$$

(a)

Multiplying Eq.(1) by $\hat{M}$ from the left

$$0 = \hat{M}(E_n - \hat{H}_0 - \lambda\hat{V})\hat{M}\left|\psi_n\right\rangle + \hat{M}(E_n - \hat{H}_0 - \lambda\hat{V})\hat{P}\left|\psi_n\right\rangle$$

Noting that

$$\hat{M}(E_n - \hat{H}_0) = (E_n - \hat{H}_0)\hat{M}, \qquad \hat{P}\hat{M} = 0, \qquad \hat{M}^2 = \hat{M}$$

we have

$$0 = (E_n - \hat{H}_0 - \lambda\hat{M}\hat{V})\hat{M}|\psi_n\rangle - \lambda\hat{M}\hat{V}\hat{P}|\psi_n\rangle$$

or

$$0 = (E_n - \hat{H}_0 - \lambda\hat{M}\hat{V}\hat{M})\hat{M}|\psi_n\rangle - \lambda\hat{M}\hat{V}\hat{P}\hat{P}|\psi_n\rangle \qquad (2)$$

since

$$\hat{M}^2 = \hat{M} \text{ and } \hat{P}^2 = \hat{P}$$

(b)

Multiplying Eq.(1) by $\hat{P}$ from the left

$$0 = \hat{P}(E_n - \hat{H}_0 - \lambda\hat{V})\hat{M}|\psi_n\rangle + \hat{P}(E_n - \hat{H}_0 - \lambda\hat{V})\hat{P}|\psi_n\rangle$$

or

$$0 = -\lambda\hat{P}\hat{V}\hat{M}|\psi_n\rangle + (E_n - \hat{H}_0 - \lambda\hat{P}\hat{V})\hat{P}|\psi_n\rangle$$

or

$$0 = -\lambda\hat{P}\hat{V}\hat{M}|\psi_n\rangle + (E_n - \hat{H}_0 - \lambda\hat{P}\hat{V}\hat{P})\hat{P}|\psi_n\rangle \qquad (3)$$

since

$$\hat{P}^2 = \hat{P}$$

(a) Expression for $\hat{P}|\psi_n\rangle$

From Eq.(3), we have

$$\hat{P}|\psi_n\rangle = \frac{\lambda}{(E_n - \hat{H}_0 - \lambda\hat{P}\hat{V}\hat{P})}\hat{P}\hat{V}\hat{M}|\psi_n\rangle \qquad (4)$$

We assume that

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + \ldots$$

where

$$\hat{M}\left|\psi_n^{(0)}\right\rangle = \left|\psi_n^{(0)}\right\rangle, \qquad \hat{P}\left|\psi_n^{(0)}\right\rangle = 0$$

Then we have

$$\begin{aligned}\hat{P}\left|\psi_n\right\rangle &= \hat{P}\left|\psi_n{}^{(0)}\right\rangle + \lambda\hat{P}\left|\psi_n{}^{(1)}\right\rangle + \lambda^2\hat{P}\left|\psi_n{}^{(2)}\right\rangle + ... \\ &= \lambda\hat{P}\left|\psi_n{}^{(1)}\right\rangle + \lambda^2\hat{P}\left|\psi_n{}^{(2)}\right\rangle + ...\end{aligned}$$

or

$$\lambda\hat{P}\left|\psi_n{}^{(1)}\right\rangle + \lambda^2\hat{P}\left|\psi_n{}^{(2)}\right\rangle + ... = \frac{\lambda}{(E_n - \hat{H}_0 - \lambda\hat{P}\hat{V}\hat{P})}\hat{P}\hat{V}\hat{M}\left|\psi_n\right\rangle$$

Here we note that

$$\hat{M}\left|\psi_n\right\rangle = \left|\psi_n{}^{(0)}\right\rangle$$

and

$$\begin{aligned}\frac{1}{E_n - \hat{H}_0 - \lambda P\hat{V}\hat{P}} &= \frac{1}{E_n - \hat{H}_0} + \frac{1}{E_n - \hat{H}_0}\lambda\hat{P}\hat{V}\hat{P}\frac{1}{E_n - \hat{H}_0 - \lambda P\hat{V}\hat{P}} \\ &= \frac{1}{E_n - \hat{H}_0} + \frac{1}{E_n - \hat{H}_0}\lambda\hat{P}\hat{V}\hat{P}\frac{1}{E_n - \hat{H}_0} \\ &\quad + \frac{1}{E_n - \hat{H}_0}\lambda\hat{P}\hat{V}\hat{P}\frac{1}{E_n - \hat{H}_0}\lambda\hat{P}\hat{V}\hat{P}\frac{1}{E_n - \hat{H}_0} + ..\end{aligned}$$

(The formula necessary for the derivation will be shown later.) Using the approximation

$$E_n - E_n{}^{(0)} = \lambda\Delta_n{}^{(1)} + \lambda^2\Delta_n{}^{(2)} + ...$$

Thus we get

$$\lambda\hat{P}\left|\psi_n^{(1)}\right\rangle + \lambda^2\hat{P}\left|\psi_n^{(2)}\right\rangle + ... = \frac{1}{(E_n - \hat{H}_0 - \lambda\hat{P}\hat{V}\hat{P})}\lambda\hat{P}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle$$

$$= \frac{1}{(E_n^{(0)} + \Delta_n - \hat{H}_0 - \lambda\hat{P}\hat{V}\hat{P})}\lambda\hat{P}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle$$

$$= \frac{1}{(E_n^{(0)} - \hat{H}_0 - \lambda\hat{P}\hat{V}\hat{P} + \lambda\Delta_n^{(1)} + ...)}\lambda\hat{P}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle$$

$$= \frac{1}{E_n^{(0)} - \hat{H}_0}\lambda\hat{P}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle + \frac{1}{E_n^{(0)} - \hat{H}_0}\lambda(\hat{P}\hat{V}\hat{P} - \Delta_n^{(1)})\frac{1}{E_n^{(0)} - \hat{H}_0}\lambda\hat{P}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle + ...$$

((Note))

$$\frac{1}{(E_n^{(0)} - \hat{H}_0 - \lambda\hat{P}\hat{V}\hat{P} + \lambda\Delta_n^{(1)} + ...)} = \frac{1}{E_n^{(0)} - \hat{H}_0} + \frac{1}{E_n^{(0)} - \hat{H}_0}(\lambda\hat{P}\hat{V}\hat{P} - \lambda\Delta_n^{(1)} - \lambda^2\Delta_n^{(2)} - ...) \times \frac{1}{(E_n^{(0)} - \hat{H}_0 - \lambda\hat{P}\hat{V}\hat{P} + \lambda\Delta_n^{(1)} + ...)}$$

$$= \frac{1}{E_n^{(0)} - \hat{H}_0} + \frac{1}{E_n^{(0)} - \hat{H}_0}\lambda(\hat{P}\hat{V}\hat{P} - \Delta_n^{(1)} - \lambda\Delta_n^{(2)} - ...) \times \frac{1}{E_n^{(0)} - \hat{H}_0} + \frac{1}{E_n^{(0)} - \hat{H}_0}\lambda^2(\hat{P}\hat{V}\hat{P} - \Delta_n^{(1)} - \lambda\Delta_n^{(2)} - ...) \times \frac{1}{E_n^{(0)} - \hat{H}_0}(\hat{P}\hat{V}\hat{P} - \Delta_n^{(1)} - \lambda\Delta_n^{(2)} - ...)\frac{1}{E_n^{(0)} - \hat{H}_0}$$

To the order of λ,

$$\hat{P}\left|\psi_n^{(1)}\right\rangle = \hat{P}^2\left|\psi_n^{(1)}\right\rangle = \hat{P}\frac{1}{E_n^{(0)} - \hat{H}_0}\hat{P}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle$$

noting that

$$\hat{P}^2 = \hat{P}.$$

For simplicity we use the notation

$$\hat{P}\left|\psi_n^{(1)}\right\rangle = \sum_{k\neq n}\hat{P}\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\frac{1}{E_n^{(0)}-\hat{H}_0}\hat{P}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle$$
$$= \sum_{k\neq n}\frac{\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\hat{P}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle}{E_n^{(0)}-E_k^{(0)}}$$
$$= \sum_{k\neq n}\frac{\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\hat{V}\left|\psi_n^{(0)}\right\rangle}{E_n^{(0)}-E_k^{(0)}}$$

where

$$\hat{M}\left|\psi_n^{(0)}\right\rangle = \left|\psi_n^{(0)}\right\rangle, \qquad \hat{P}\left|\psi_k^{(0)}\right\rangle = \left|\psi_k^{(0)}\right\rangle \qquad (k\neq n)$$

Note that $\left|\psi_n^{(0)}\right\rangle$ should be determined from the eigenvalue problem (which will be discussed later). We also have

$$\hat{P}\left|\psi_n^{(2)}\right\rangle = \hat{P}^2\left|\psi_n^{(2)}\right\rangle$$
$$= \sum_{k\neq n}\hat{P}\left|\psi_k^{(0)}\right\rangle\frac{1}{E_n-\hat{H}_0}(\hat{P}\hat{V}\hat{P}-\Delta_n^{(1)})\frac{1}{E_n-\hat{H}_0}\hat{P}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle$$
$$= \sum_{k,l\neq n}\frac{\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\hat{P}\hat{V}\hat{P}-\Delta_n^{(1)}\left|\psi_l^{(0)}\right\rangle\left\langle\psi_l^{(0)}\right|\hat{P}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle}{(E_n^{(0)}-E_k^{(0)})(E_n^{(0)}-E_l^{(0)})}$$
$$= \sum_{k,l\neq n}\frac{\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\hat{V}\left|\psi_l^{(0)}\right\rangle\left\langle\psi_l^{(0)}\right|\hat{V}\left|\psi_n^{(0)}\right\rangle}{(E_n^{(0)}-E_k^{(0)})(E_n^{(0)}-E_l^{(0)})}$$
$$-\Delta_n^{(1)}\sum_{k\neq n}\frac{\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\hat{V}\left|\psi_n^{(0)}\right\rangle}{(E_n^{(0)}-E_k^{(0)})^2}$$

Note that $\Delta_n^{(1)}$ and $\left|\psi_n^{(0)}\right\rangle$ can be determined from the energy eigenvalue problem.

(b) Energy eigenvalue problems

Determination of the form of the eigenket $\left|\psi_n^{(0)}\right\rangle$ and associated energy eigenvalues

By substituting Eq.(4) into Eq.(2)

$$\hat{P}\left|\psi_n\right\rangle = \frac{\lambda}{(E_n-\hat{H}_0-\lambda\hat{P}\hat{V}\hat{P})}\hat{P}\hat{V}\hat{M}\left|\psi_n\right\rangle \qquad (4)$$

$$0=(E_n-\hat{H}_0-\lambda\hat{M}\hat{V}\hat{M})\hat{M}\left|\psi_n\right\rangle-\lambda\hat{M}\hat{V}\hat{P}\hat{P}\left|\psi_n\right\rangle \tag{2}$$

we get

$$\begin{aligned}0&=(E_n-\hat{H}_0-\lambda\hat{M}\hat{V}\hat{M})\hat{M}\left|\psi_n\right\rangle-\lambda\hat{M}\hat{V}\hat{P}\frac{\lambda}{(E_n-\hat{H}_0-\lambda\hat{P}\hat{V}\hat{P})}\hat{P}\hat{V}\hat{M}\left|\psi_n\right\rangle\\&=[E_n-E_n^{(0)}-\lambda\hat{M}\hat{V}\hat{M}-\lambda^2\hat{M}\hat{V}\hat{P}\frac{1}{(E_n-\hat{H}_0-\lambda P\hat{V}\hat{P})}\hat{P}\hat{V}\hat{M}]\hat{M}\left|\psi_n\right\rangle\\&=[E_n-E_n^{(0)}-\lambda\hat{M}\hat{V}\hat{M}-\lambda^2\hat{M}\hat{V}\hat{P}\frac{1}{(E_n-\hat{H}_0-\lambda P\hat{V}\hat{P})}\hat{P}\hat{V}\hat{M}]\left|\psi_n^{(0)}\right\rangle\end{aligned} \tag{3}$$

since

$$\hat{H}_0\hat{M}\left|\psi_n\right\rangle=\hat{H}_0\left|\psi_n^{(0)}\right\rangle=E_n^{(0)}\left|\psi_n^{(0)}\right\rangle=E_n^{(0)}\hat{M}\left|\psi_n\right\rangle$$

$$\hat{M}\left|\psi_n\right\rangle=\left|\psi_n^{(0)}\right\rangle$$

We assume that

$$E_n-E_n^{(0)}=\lambda\Delta_n^{(1)}+\lambda^2\Delta_n^{(2)}+...$$

Then

$$\begin{aligned}&[\lambda\Delta_n^{(1)}+\lambda^2\Delta_n^{(2)}+\lambda^3\Delta_n^{(3)}-\lambda\hat{M}\hat{V}\hat{M}\\&-\lambda^2\hat{M}\hat{V}\hat{P}\frac{1}{(E_n^{(0)}-\hat{H}_0-\lambda P\hat{V}\hat{P}+\lambda\Delta_n^{(1)})}\hat{P}\hat{V}\hat{M}]\hat{M}\left|\psi_n\right\rangle\end{aligned}$$

Using the formula

$$\frac{1}{E_n-\hat{H}_0-\lambda P\hat{V}\hat{P}+\lambda\Delta_n^{(1)}}\approx\frac{1}{E_n-\hat{H}_0}+\frac{\lambda}{E_n-\hat{H}_0}(P\hat{V}\hat{P}-\Delta_n^{(1)})\frac{1}{E_n-\hat{H}_0}+...$$

we have

$$\begin{aligned}&[\lambda(\Delta_n^{(1)}-\hat{M}\hat{V}\hat{M})+\lambda^2(\Delta_n^{(2)}-\hat{M}\hat{V}\hat{P}\frac{1}{E_n^{(0)}-\hat{H}_0}\hat{P}\hat{V}\hat{M})\\&+\lambda^3(\Delta_n^{(3)}-\hat{M}\hat{V}\hat{P}\frac{1}{E_n^{(0)}-\hat{H}_0}(P\hat{V}\hat{P}-\Delta_n^{(1)})\frac{1}{E_n^{(0)}-\hat{H}_0}\hat{P}\hat{V}\hat{M}]\hat{M}\left|\psi_n\right\rangle=0\end{aligned}$$

or

$$[\lambda(\Delta_n^{(1)} - \hat{M}\hat{V}\hat{M}) + \lambda^2(\Delta_n^{(2)} - \hat{M}\hat{V}\hat{P}\frac{1}{E_n^{(0)} - \hat{H}_0}\hat{P}\hat{V}\hat{M})$$
$$+ \lambda^3(\Delta_n^{(3)} - \hat{M}\hat{V}\hat{P}\frac{1}{E_n^{(0)} - \hat{H}_0}(P\hat{V}\hat{P} - \Delta_n^{(1)})\frac{1}{E_n^{(0)} - \hat{H}_0}\hat{P}\hat{V}\hat{M}]\left|\psi_n^{(0)}\right\rangle = 0 \qquad (5)$$

since $\hat{M}\left|\psi_n\right\rangle = \left|\psi_n^{(0)}\right\rangle$

(i) The order of λ in Eq.(5)

We get

$$(-\Delta_n^{(1)} + \hat{M}\hat{V}\hat{M})\left|\psi_n^{(0)}\right\rangle = 0$$

from Eq.(5). Multiplying the above equation by $\left\langle\mu\right| = \left\langle\varphi_{n,\mu}^{(0)}\right|$ from the left

$$\left\langle\mu\right| - \Delta_n^{(1)} + \hat{M}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle = 0$$

or

$$-\Delta_n^{(1)}\left\langle\mu\middle|\psi_n^{(0)}\right\rangle + \left\langle\mu\right|\hat{M}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle = 0$$

or

$$-\Delta_n^{(1)}\left\langle\mu\middle|\psi_n^{(0)}\right\rangle + \left\langle\mu\right|\hat{V}\left|\psi_n^{(0)}\right\rangle = 0$$

or

$$-\sum_\nu \Delta_n^{(1)}\delta_{\mu,\nu}\left\langle\nu\middle|\psi_n^{(0)}\right\rangle + \lambda\sum_\nu \left\langle\mu\right|\hat{V}\left|\nu\right\rangle\left\langle\nu\middle|\psi_n^{(0)}\right\rangle = 0$$

where

$$\left\langle\mu\right|\hat{M}\hat{V}\hat{M}\left|\psi_n^{(0)}\right\rangle = \left\langle\mu\right|\hat{V}\left|\psi_n^{(0)}\right\rangle$$

This can be expressed using the matrix as

$$\begin{pmatrix} V_{11}-\Delta_n^{(1)} & V_{12} & . & . & . & . & V_{1g} \\ V_{21} & V_{22}-\Delta_n^{(1)} & . & . & . & . & V_{2g} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ V_{g1} & V_{g2} & . & . & . & . & V_{gg}-\Delta_n^{(1)} \end{pmatrix} \begin{pmatrix} \langle 1|\psi_n{}^{(0)}\rangle \\ \langle 2|\psi_n{}^{(0)}\rangle \\ . \\ \langle \nu|\psi_n{}^{(0)}\rangle \\ . \\ . \\ \langle g|\psi_n{}^{(0)}\rangle \end{pmatrix} = 0$$

as $\lambda\hat{V} \to \hat{V}$, where

$$V_{\mu\nu} = \langle \varphi_{n,\mu}^{(0)}|\hat{V}|\varphi_{n,\nu}^{(0)}\rangle = \langle \mu|\hat{V}|\nu\rangle$$

The solution of the determinant = 0 yields the g-energy eigenvalue $\Delta_n^{(1)}$ and the corresponding eigenket $|\psi_n{}^{(0)}\rangle$.

When

$$V_{\mu\nu} = \langle \mu|\hat{V}|\nu\rangle = 0 \qquad \text{for } \mu \neq \nu$$

and

$$V_{11} = V_{22} = V_{33} = ... = V_{gg}$$

The degeneracy in the energy levels is not removed in the first order perturbation. So we need to go to the calculations with the high order.

(ii) The order of λ^2 in Eq.(5)

From Eq.(5), We get

$$(-\Delta_n{}^{(2)} + \hat{M}\hat{V}\hat{P}\frac{1}{E_n{}^{(0)} - \hat{H}_0}\hat{P}\hat{V}\hat{M})|\psi_n{}^{(0)}\rangle = 0$$

Multiplying the above equation by $\langle \mu|$ from the left

$$\langle \mu| - \Delta_n{}^{(2)} + \hat{M}\hat{V}\hat{P}\frac{1}{E_n{}^{(0)} - \hat{H}_0}\hat{P}\hat{V}\hat{M}|\psi_n{}^{(0)}\rangle = 0$$

or

$$-\Delta_n^{(2)}\langle\mu|\psi_n^{(0)}\rangle + \langle\mu|\hat{M}\hat{V}\hat{P}\frac{1}{E_n^{(0)}-\hat{H}_0}\hat{P}\hat{V}\hat{M}|\psi_n^{(0)}\rangle = 0$$

or

$$-\Delta_n^{(2)}\langle\mu|\psi_n^{(0)}\rangle + \sum_{k,\nu}\langle\mu|\hat{V}\hat{P}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\frac{1}{E_n^{(0)}-\hat{H}_0}\hat{P}\hat{V}|\nu\rangle\langle\nu|\psi_n^{(0)}\rangle = 0$$

$$\sum_{\nu}[-\Delta_n^{(2)}\delta_{\mu,\nu} + \sum_{k\neq n}\frac{\langle\mu|\hat{V}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{V}|\nu\rangle}{E_n^{(0)}-E_k^{(0)}}]\langle\nu|\psi_n^{(0)}\rangle = 0$$

For simplicity we introduce the matrix element

$$\Lambda_{\mu\nu} = \langle\mu|\hat{\Lambda}|\nu\rangle = \sum_{k\neq n}\frac{\langle\mu|\hat{V}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{V}|\nu\rangle}{E_n^{(0)}-E_k^{(0)}}$$

with a new operator defined by

$$\hat{\Lambda} = \sum_{k\neq n}\frac{\hat{V}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{V}}{E_n^{(0)}-E_k^{(0)}}$$

The eigenvalue problem:

$$\begin{pmatrix} \Lambda_{11}-\Delta_n^{(2)} & \Lambda_{12} & . & . & . & . & \Lambda_{1g} \\ \Lambda_{21} & \Lambda_{22}-\Delta_n^{(2)} & . & . & . & . & \Lambda_{2g} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ \Lambda_{g1} & \Lambda_{g2} & . & . & . & . & \Lambda_{gg}-\Lambda_n^{(2)} \end{pmatrix}\begin{pmatrix} \langle 1|\psi_n^{(0)}\rangle \\ \langle 2|\psi_n^{(0)}\rangle \\ . \\ \langle\nu|\psi_n^{(0)}\rangle \\ . \\ . \\ \langle g|\psi_n^{(0)}\rangle \end{pmatrix} = 0$$

where

$$\Lambda_{\mu\nu} = \langle\mu|\hat{\Lambda}|\nu\rangle$$

When

$$\Lambda_{\mu\nu} = 0 \qquad \text{for } \mu \neq \nu$$

and

$$\Lambda_{11} = \Lambda_{22} = \Lambda_{33} = ... = \Lambda_{gg}$$

The degeneracy in the energy levels is not removed in the second order perturbation.

(iii) The order of λ^3 in Eq.(5)

From Eq.(5), We get

$$\lambda^3(\Delta_n^{(3)} - \hat{M}\hat{V}\hat{P}\frac{1}{E_n^{(0)} - \hat{H}_0}(P\hat{V}\hat{P} - \Delta_n^{(1)})\frac{1}{E_n^{(0)} - \hat{H}_0}\hat{P}\hat{V}\hat{M}]\left|\psi_n^{(0)}\right\rangle$$

Here we assume that $\Delta_n^{(1)} = 0$. Multiplying the above equation by $\langle\mu|$ from the left, we have

$$\lambda^3\Delta_n^{(3)}\left\langle\mu\middle|\psi_n^{(0)}\right\rangle - \langle\mu|\hat{M}\hat{V}\hat{P}\frac{1}{E_n^{(0)} - \hat{H}_0}P\hat{V}\hat{P}\frac{1}{E_n^{(0)} - \hat{H}_0}\hat{P}\hat{V}\hat{M}]\left|\psi_n^{(0)}\right\rangle = 0$$

This can be rewritten as

$$\lambda^3\Delta_n^{(3)}\left\langle\mu\middle|\psi_n^{(0)}\right\rangle - \sum_{k,l}\langle\mu|\hat{M}\hat{V}\hat{P}\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\frac{1}{E_n^{(0)} - \hat{H}_0}P\hat{V}\hat{P}\left|\psi_l^{(0)}\right\rangle\left\langle\psi_l^{(0)}\right|\frac{1}{E_n^{(0)} - \hat{H}_0}\hat{P}\hat{V}\hat{M}]\left|\psi_n^{(0)}\right\rangle = 0$$

leading to the eigenvalue problem

$$\lambda^3\Delta_n^{(3)}\left\langle\mu\middle|\psi_n^{(0)}\right\rangle - \sum_{k\neq n, l\neq n}\frac{\left\langle\mu\middle|\hat{V}\middle|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\middle|\hat{V}\middle|\psi_l^{(0)}\right\rangle\left\langle\psi_l^{(0)}\middle|\hat{V}\middle|\psi_n^{(0)}\right\rangle}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_l^{(0)})} = 0 .$$

For simplicity we introduce the matrix element

$$\Gamma_{\mu\nu} = \langle\mu|\hat{\Gamma}|\nu\rangle = \sum_{k\neq n, l\neq n}\frac{\left\langle\mu\middle|\hat{V}\middle|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\middle|\hat{V}\middle|\psi_l^{(0)}\right\rangle\left\langle\psi_l^{(0)}\middle|\hat{V}\middle|\psi_n^{(0)}\right\rangle}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_l^{(0)})}$$

with a new operator defined by

$$\hat{\Gamma} = \sum_{k\neq n, l\neq n}\frac{\hat{V}\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\middle|\hat{V}\middle|\psi_l^{(0)}\right\rangle\left\langle\psi_l^{(0)}\right|\hat{V}}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_l^{(0)})}$$

The eigenvalue problem:

$$\begin{pmatrix} \Gamma_{11}-\Delta_n^{(3)} & \Gamma_{12} & . & . & . & . & \Gamma_{1g} \\ \Gamma_{21} & \Gamma_{22}-\Delta_n^{(3)} & . & . & . & . & \Gamma_{2g} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ \Gamma_{g1} & \Gamma_{g2} & . & . & . & . & \Gamma_{gg}-\Lambda_n^{(3)} \end{pmatrix} \begin{pmatrix} \langle 1|\psi_n{}^{(0)}\rangle \\ \langle 2|\psi_n{}^{(0)}\rangle \\ . \\ \langle \nu|\psi_n{}^{(0)}\rangle \\ . \\ . \\ \langle g|\psi_n{}^{(0)}\rangle \end{pmatrix} = 0$$

where

$$\Gamma_{\mu\nu} = \langle \mu|\hat{\Gamma}|\nu\rangle$$

((**Formula**))

$$\begin{aligned} (\hat{A}-\hat{B})^{-1} &= \hat{A}^{-1} + \hat{A}^{-1}\hat{B}(\hat{A}-\hat{B})^{-1} \\ &= \hat{A}^{-1} + \hat{A}^{-1}\hat{B}[\hat{A}^{-1} + \hat{A}^{-1}\hat{B}(\hat{A}-\hat{B})^{-1}] \\ &= \hat{A}^{-1} + \hat{A}^{-1}\hat{B}\hat{A}^{-1} + \hat{A}^{-1}\hat{B}\hat{A}^{-1}\hat{B}(\hat{A}-\hat{B})^{-1} \\ &= \hat{A}^{-1} + \hat{A}^{-1}\hat{B}\hat{A}^{-1} + \hat{A}^{-1}\hat{B}\hat{A}^{-1}\hat{B}\hat{A}^{-1} + .. \end{aligned}$$

$$\frac{1}{\hat{A}} - \frac{1}{\hat{B}} = \frac{1}{\hat{A}}(\hat{B}-\hat{A})\frac{1}{\hat{B}} = \frac{1}{\hat{B}}(\hat{B}-\hat{A})\frac{1}{\hat{A}}$$

20 Example-I

((Sakurai QM 5-10))
Consider a spinless particle in a 2D infinite square well:

a. What are the energy eigenvalues for the three lowest states? Is there any degeneracy?

$$V = \begin{cases} 0 & (0 \le x \le a, 0 \le y \le a) \\ \infty & otherwise \end{cases}$$

b. We now add a potential

$$V_1 = \lambda xy$$

Taking this as a weak perturbation, answer the following:

(i) Is the energy shift due to the perturbation linear or quadratic in λ for each of the three states?

(ii) Obtain expressions for the energy shifts of the three lowest states accurate to order λ. (You need not evaluate integrals that may appear.)

(iii) Draw an energy diagram with and without the perturbation for the three energy states. Make sure to specify which unperturbed state is connected to which perturbed state.

((**Solution**))

2D quantum box:

Schrödinger equation

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y)=E\psi(x,y)$$

where the wave function is given by

$$\psi(x,y)=X(x)Y(y) \qquad \text{(separation variable)}$$

We use the dispersion relation as

$$E=\frac{\hbar^2}{2m}(k_x{}^2+k_y{}^2)$$

Then we get

$$-\frac{\hbar^2}{2m}(X''Y+XY'')=\frac{\hbar^2}{2m}(k_x{}^2+k_y{}^2)XY$$

or

$$\frac{X''}{X}+\frac{Y''}{Y}=-(k_x{}^2+k_y{}^2)$$

We assume

$$X''=-k_x{}^2X$$

with the boundary conditions given by

$X=0$ at $x = 0$ and a.

Thus we have

$$X = A\sin(k_x a)$$

with

$$\sin(k_x a) = 0 \qquad \text{or} \qquad k_x a = n_x \pi \ \ (n_x = 1, 2, 3, \ldots..)$$

Similarly for Y, we have

$$Y'' = -k_y^{\,2} Y$$

with a boundary condition

$$Y = 0 \qquad \text{at } y = 0 \text{ and } y = a.$$

Thus we have

$$X = A\sin(k_y x)$$

with

$$\sin(k_y a) = 0 \qquad \text{or} \qquad k_y a = n_y \pi \ \ (n_y = 1, 2, 3, \ldots..)$$

So

$$E^{(0)}(n_x, n_y) = \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 (n_x^{\,2} + n_y^{\,2}) = E_a (n_x^{\,2} + n_y^{\,2})$$

$$\psi_{n_x, n_y}(x, y) = \frac{2}{a}\sin\left(\frac{n_x \pi}{a} x\right)\sin\left(\frac{n_y \pi}{a} y\right)$$

where n_x = 1, 2, 3, 4,….., and n_y = 1, 2, 3, 4,….

$$E_a = \frac{\hbar^2}{2m}(\frac{\pi}{a})^2$$

(i) Ground state ($n_x = 1$, $n_y = 1$)

$g_1 = 1$ (non-degeneracy)

$$E^{(0)}(n_x = 1, n_y = 1) = E^{(0)}(1,1) = 2E_a$$

(ii) First excited state ($n_x = 1$, $n_y = 2$, and $n_x = 2$, $n_y = 1$)

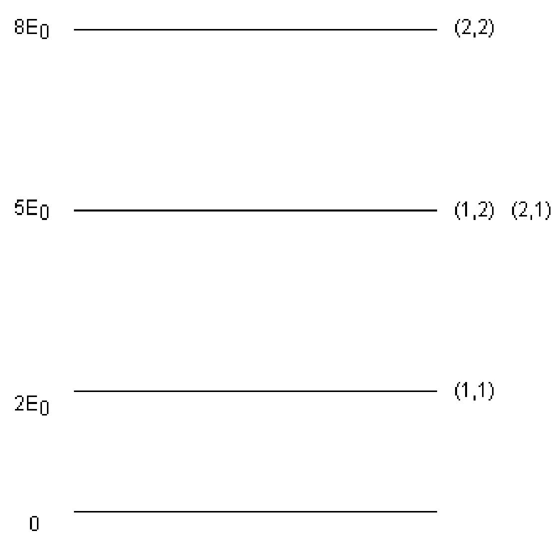
$g_2 = 2$ (doubly degeneracy)

$$E^{(0)}(n_x = 1, n_y = 2) = E^{(0)}(n_x = 2, n_y = 1) = 5E_a$$

(iii) Second excited state ($n_x = 2$, $n_y = 2$)

$g_3 = 1$ (non-degeneracy)

$$E^{(0)}(n_x = 2, n_y = 2) = E^{(0)}(2,2) = 8E_a$$



(b) The perturbation

$$\hat{V}_1 = \lambda \hat{x}\hat{y}$$

The matrix element

$$\langle n_x', n_y' | \hat{V}_1 | n_x, n_y \rangle = \lambda \left(\frac{2}{a}\right)^2 \int_0^a dx x \sin\left(\frac{n_x'\pi}{a} x\right) in\left(\frac{n_x \pi}{a} x\right) \int_0^a dy y \sin\left(\frac{n_y'\pi}{a} y\right) \sin\left(\frac{n_y \pi}{a} y\right)$$

We calculate the matrix element using Mathematica.

Ground state is non-degenerate

$$E_1 = E^{(0)}(1,1) + E^{(1)}(1,1) + E^{(2)}(1,1) + ... = 2E_a + \lambda\frac{a^2}{4} - 0.00558305\frac{\lambda^2}{E_a}a^4$$

with

$$E^{(0)}(1,1) = 2E_a$$

$$E^{(1)}(1,1) = \langle 1,1|\lambda\hat{V}_1|1,1\rangle = \lambda\frac{a^2}{4}$$

$$E^{(2)}(1,1) = \sum_{(n_x,n_y)\neq(1,1)}\frac{|\langle 1,1|\lambda\hat{V}_1|n_x,n_y\rangle|^2}{E^{(0)}(1,1)-E^{(0)}(n_x,n_y)}$$

$$= \frac{|\langle 1,1|\lambda\hat{V}_1|1,2\rangle|^2}{E^{(0)}(1,1)-E^{(0)}(1,2)} + \frac{|\langle 1,1|\lambda\hat{V}_1|2,1\rangle|^2}{E^{(0)}(1,1)-E^{(0)}(2,1)} + \frac{|\langle 1,1|\lambda\hat{V}_1|2,2\rangle|^2}{E^{(0)}(1,1)-E^{(0)}(2,2)}$$

$$= -\frac{\lambda^2}{E_a}a^4\left(2\frac{\left(\frac{8}{9\pi^2}\right)^2}{3} + \frac{\left(\frac{256}{81\pi^4}\right)^2}{6}\right)$$

$$= -0.00558305\frac{\lambda^2}{E_a}a^4$$

where

$$\langle 1,1|\hat{V}_1|1,2\rangle = -\frac{8a^2}{9\pi^2}, \quad \langle 1,1|\hat{V}_1|2,1\rangle = -\frac{8a^2}{9\pi^2}, \quad \langle 1,1|\hat{V}_1|2,2\rangle = \frac{256a^2}{81\pi^4}$$

Second excited state is non-degenerate

$$E_2 = E^{(0)}(2,2) + E^{(1)}(2,2) + E^{(2)}(2,2) + ... = 8E_a + \lambda\frac{a^2}{4} + 0.005583\frac{\lambda^2 a^4}{E_0}$$

with

$$E^{(0)}(2,2) = 8E_a$$

$$E^{(1)}(2,2) = \langle 2,2|\hat{V}_1|2,2\rangle = \lambda\frac{a^2}{4}$$

$$E^{(2)}(2,2)=\sum_{(n_x,n_y)\neq(1,1)}\frac{\left|\langle 2,2|\lambda\hat{V}_1|n_x,n_y\rangle\right|^2}{E^{(0)}(2,2)-E^{(0)}(n_x,n_y)}$$

$$=\frac{\left|\langle 2,2|\lambda\hat{V}_1|1,1\rangle\right|^2}{E^{(0)}(2,2)-E^{(0)}(1,1)}+\frac{\left|\langle 2,2|\lambda\hat{V}_1|2,1\rangle\right|^2}{E^{(0)}(2,2)-E^{(0)}(2,1)}+\frac{\left|\langle 2,2|\lambda\hat{V}_1|1,2\rangle\right|^2}{E^{(0)}(2,2)-E^{(0)}(1,2)}$$

$$=\frac{\lambda^2a^4}{E_0}\left(\frac{\left(\frac{256}{81\pi^4}\right)^2}{6}+\frac{2\left(\frac{8}{9\pi^2}\right)^2}{3}\right)$$

$$=0.005583\frac{\lambda^2a^4}{E_0}$$

where

$$\langle 2,2|\hat{V}_1|1,1\rangle=\frac{256a^2}{81\pi^4},\quad \langle 2,2|\hat{V}_1|2,1\rangle=-\frac{8a^2}{9\pi^2},\quad \langle 2,2|\hat{V}_1|1,2\rangle=-\frac{8a^2}{9\pi^2}$$

First excited state (doubly degenerate)

$$E^{(0)}(n_x=1,n_y=2)=E^{(0)}(n_x=2,n_y=1)=5E_a$$

$$\langle 1,2|\hat{V}_1|1,2\rangle=\frac{a^2}{4},\qquad \langle 1,2|\hat{V}_1|2,1\rangle=\frac{256a^2}{81\pi^4},$$

$$\langle 2,1|\hat{V}_1|1,2\rangle=\frac{256a^2}{81\pi^4},\quad \langle 2,1|\hat{V}_1|2,1\rangle=\frac{a^2}{4}$$

Then we have

$$M=\begin{pmatrix}\frac{1}{4} & \frac{256}{81\pi^4}\\ \frac{256}{81\pi^4} & \frac{1}{4}\end{pmatrix}$$

in the unit of λa^2. We solve the eigenvalue problem using the Mathematica

Eigensystem[M]

$$\left\{\left\{\frac{1}{4}+\frac{256}{81\,\pi^4},\ \frac{1}{4}-\frac{256}{81\,\pi^4}\right\},\ \{\{1,\ 1\},\ \{-1,\ 1\}\}\right\}$$

Then

(i)

$$E_1^{(1)} = 5E_a + \lambda a^2(\frac{1}{4} + \frac{256}{81\pi^4}) = 5E_a + \lambda a^2 0.282446$$

$$|\psi_1^{(1)}\rangle = \frac{1}{\sqrt{2}}[|n_x = 1, n_y = 2\rangle + |n_x = 2, n_y = 1\rangle]$$

(ii)

$$E_1^{2} = 5E_a + \lambda a^2(\frac{1}{4} - \frac{256}{81\pi^4}) = 5E_a + \lambda a^2 0.217554$$

$$|\psi_1^{(2)}\rangle = \frac{1}{\sqrt{2}}[|n_x = 1, n_y = 2\rangle - |n_x = 2, n_y = 1\rangle]$$

((Mathematica))

Solution of Sakurai 5-10

```
G[n1_, m1_, n2_, m2_] :=
 Simplify[(2/a)^2 (∫_0^a y Sin[m1 π/a y] Sin[m2 π/a y] ⅆy) (∫_0^a x Sin[n1 π/a x] Sin[n2 π/a x] ⅆx) ,
  Element[{n1, n2, m1, m2}, Integers]]

s1 = Table[{n1, n2, m1, m2, G[n1, n2, m1, m2]}, {n1, 1, 3, 1}, {n2, 1, 3, 1},
   {m1, 1, 3, 1}, {m2, 1, 3, 1}];

Grid[s1[[1]], Frame → All]
```

{{1, 1, 1, 1, $\frac{a^2}{4}$}, {1, 1, 1, 2, $-\frac{8 a^2}{9 \pi^2}$}, {1, 1, 1, 3, 0}}	{{1, 1, 2, 1, $-\frac{8 a^2}{9 \pi^2}$}, {1, 1, 2, 2, $\frac{256 a^2}{81 \pi^4}$}, {1, 1, 2, 3, 0}}	{{1, 1, 3, 1, 0}, {1, 1, 3, 2, 0}, {1, 1, 3, 3, 0}}
{{1, 2, 1, 1, $-\frac{8 a^2}{9 \pi^2}$}, {1, 2, 1, 2, $\frac{a^2}{4}$}, {1, 2, 1, 3, $-\frac{24 a^2}{25 \pi^2}$}}	{{1, 2, 2, 1, $\frac{256 a^2}{81 \pi^4}$}, {1, 2, 2, 2, $-\frac{8 a^2}{9 \pi^2}$}, {1, 2, 2, 3, $\frac{256 a^2}{75 \pi^4}$}}	{{1, 2, 3, 1, 0}, {1, 2, 3, 2, 0}, {1, 2, 3, 3, 0}}
{{1, 3, 1, 1, 0}, {1, 3, 1, 2, $-\frac{24 a^2}{25 \pi^2}$}, {1, 3, 1, 3, $\frac{a^2}{4}$}}	{{1, 3, 2, 1, 0}, {1, 3, 2, 2, $\frac{256 a^2}{75 \pi^4}$}, {1, 3, 2, 3, $-\frac{8 a^2}{9 \pi^2}$}}	{{1, 3, 3, 1, 0}, {1, 3, 3, 2, 0}, {1, 3, 3, 3, 0}}

```
Grid[s1[[2]], Frame → All]
```

{{2, 1, 1, 1, $-\frac{8 a^2}{9 \pi^2}$}, {2, 1, 1, 2, $\frac{256 a^2}{81 \pi^4}$}, {2, 1, 1, 3, 0}}	{{2, 1, 2, 1, $\frac{a^2}{4}$}, {2, 1, 2, 2, $-\frac{8 a^2}{9 \pi^2}$}, {2, 1, 2, 3, 0}}	{{2, 1, 3, 1, $-\frac{24 a^2}{25 \pi^2}$}, {2, 1, 3, 2, $\frac{256 a^2}{75 \pi^4}$}, {2, 1, 3, 3, 0}}
{{2, 2, 1, 1, $\frac{256 a^2}{81 \pi^4}$}, {2, 2, 1, 2, $-\frac{8 a^2}{9 \pi^2}$}, {2, 2, 1, 3, $\frac{256 a^2}{75 \pi^4}$}}	{{2, 2, 2, 1, $-\frac{8 a^2}{9 \pi^2}$}, {2, 2, 2, 2, $\frac{a^2}{4}$}, {2, 2, 2, 3, $-\frac{24 a^2}{25 \pi^2}$}}	{{2, 2, 3, 1, $\frac{256 a^2}{75 \pi^4}$}, {2, 2, 3, 2, $-\frac{24 a^2}{25 \pi^2}$}, {2, 2, 3, 3, $\frac{2304 a^2}{625 \pi^4}$}}
{{2, 3, 1, 1, 0}, {2, 3, 1, 2, $\frac{256 a^2}{75 \pi^4}$}, {2, 3, 1, 3, $-\frac{8 a^2}{9 \pi^2}$}}	{{2, 3, 2, 1, 0}, {2, 3, 2, 2, $-\frac{24 a^2}{25 \pi^2}$}, {2, 3, 2, 3, $\frac{a^2}{4}$}}	{{2, 3, 3, 1, 0}, {2, 3, 3, 2, $\frac{2304 a^2}{625 \pi^4}$}, {2, 3, 3, 3, $-\frac{24 a^2}{25 \pi^2}$}}

```
Grid[s1[[3]], Frame → All]
```

{{3, 1, 1, 1, 0}, {3, 1, 1, 2, 0}, {3, 1, 1, 3, 0}}	{{3, 1, 2, 1, $-\frac{24 a^2}{25 \pi^2}$}, {3, 1, 2, 2, $\frac{256 a^2}{75 \pi^4}$}, {3, 1, 2, 3, 0}}	{{3, 1, 3, 1, $\frac{a^2}{4}$}, {3, 1, 3, 2, $-\frac{8 a^2}{9 \pi^2}$}, {3, 1, 3, 3, 0}}
{{3, 2, 1, 1, 0}, {3, 2, 1, 2, 0}, {3, 2, 1, 3, 0}}	{{3, 2, 2, 1, $\frac{256 a^2}{75 \pi^4}$}, {3, 2, 2, 2, $-\frac{24 a^2}{25 \pi^2}$}, {3, 2, 2, 3, $\frac{2304 a^2}{625 \pi^4}$}}	{{3, 2, 3, 1, $-\frac{8 a^2}{9 \pi^2}$}, {3, 2, 3, 2, $\frac{a^2}{4}$}, {3, 2, 3, 3, $-\frac{24 a^2}{25 \pi^2}$}}
{{3, 3, 1, 1, 0}, {3, 3, 1, 2, 0}, {3, 3, 1, 3, 0}}	{{3, 3, 2, 1, 0}, {3, 3, 2, 2, $\frac{2304 a^2}{625 \pi^4}$}, {3, 3, 2, 3, $-\frac{24 a^2}{25 \pi^2}$}}	{{3, 3, 3, 1, 0}, {3, 3, 3, 2, $-\frac{24 a^2}{25 \pi^2}$}, {3, 3, 3, 3, $\frac{a^2}{4}$}}

21. Example-II

Consider the so-called spin Hamiltonian:

$$\hat{H} = \frac{a}{\hbar^2}\hat{S}_z^{\,2} + \frac{b}{\hbar^2}(\hat{S}_x^{\,2} - \hat{S}_y^{\,2}) = \hat{H}_0 + \hat{H}_1$$

for a system of spin $S = 1$, where $0 \le b << a$. Such a Hamiltonian obtains for a spin-1 ion located in a crystal with rhombic symmetry. Find the eigenvalues of this Hamiltonian using degenerate perturbation theory [Amit Goswami, Chapter 18, p.394 Problem((8))

Eigenvalue of $\hat{H}_0$

$$\hat{H}_0 = \frac{a}{\hbar^2}\hat{S}_z^{\,2}\left|1, m\right\rangle = am^2\left|1, m\right\rangle$$

$\left|1, m\right\rangle$ (m = 1, 0, -1) is the eigenket of $\hat{H}_0$:

$|1,\pm 1\rangle$ is the eigenket of $\hat{H}_0$ with energy *a* (degenerate)
$|1,0\rangle$ is the eigenket of $\hat{H}_0$ with energy 0 (nondegenerate)

Now we calculate $\hat{H}_1|1,m\rangle = \frac{b}{\hbar^2}(\hat{S}_x{}^2 - \hat{S}_y{}^2)|1,m\rangle$

$$S_x = \hbar\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \qquad S_y = \hbar\begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}, \; S_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

The Hamiltonian *H* is expressed by

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = \begin{pmatrix} a & 0 & b \\ 0 & 0 & 0 \\ b & 0 & a \end{pmatrix} = \begin{pmatrix} a & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & a \end{pmatrix} + \begin{pmatrix} 0 & 0 & b \\ 0 & 0 & 0 \\ b & 0 & 0 \end{pmatrix}$$

(1) Exact solution

We use the Mathematica to solve the eigenvalue problem.

Eigenvlaue $\varepsilon_1 = a + b$
Eigenket:

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|1,1\rangle + |1,-1\rangle)$$

Eigenvlaue $\varepsilon_2 = a - b$

Eigenket $|\psi_2\rangle = \frac{1}{\sqrt{2}}(|1,1\rangle - |1,-1\rangle)$

Eigenvalue $\varepsilon_3 = 0$
Eigenket $|\psi_3\rangle = |1,0\rangle$

((**Mathematica**))

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

H = {{a, 0, b}, {0, 0, 0}, {b, 0, a}};

eq1 = Eigensystem[H]
```

{{0, a - b, a + b}, {{0, 1, 0}, {-1, 0, 1}, {1, 0, 1}}}

```
ψ1 = Normalize[eq1[[2, 1]]]
```

{0, 1, 0}

```
ψ2 = Normalize[eq1[[2, 2]]]
```

$\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$

```
ψ3 = Normalize[eq1[[2, 3]]]
```

$\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$

```
{ψ1*.ψ2, ψ2*.ψ3, ψ3*.ψ1}
```

{0, 0, 0}

---

(2) Perturbation method

$$\hat{H}_1 = \begin{pmatrix} 0 & 0 & b \\ 0 & 0 & 0 \\ b & 0 & 0 \end{pmatrix}$$

$$\hat{H}_1 |1,1\rangle = b|1,-1\rangle$$

$$\hat{H}_1 |1,-1\rangle = b|1,1\rangle$$

Matrix of $\hat{H}_1$ of the basis of $|1,1\rangle$ and $|1,-1\rangle$ is

$$\hat{H}_{11} = \begin{pmatrix} 0 & b \\ b & 0 \end{pmatrix}$$

We use the Mathematica to solve the eigenvalue problem.

$\varepsilon_1' = b$ (or $\varepsilon_1 = a + b$)

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|1,1\rangle + |1,-1\rangle)$$

and

$\varepsilon_1' = -b$ (or $\varepsilon_2 = a - b$)

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|1,1\rangle - |1,-1\rangle)$$

((**Mathematica**))

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

H11 = (0 b
       b 0);

eq1 = Eigensystem[H11]

{{-b, b}, {{-1, 1}, {1, 1}}}

ψ1 = Normalize[eq1[[2, 1]]]

{-1/√2, 1/√2}

ψ2 = Normalize[eq1[[2, 2]]]

{1/√2, 1/√2}

{ψ1*. ψ2}

{0}
```

22. Example-III

This is a tricky problem because the degeneracy between the first and the second state is not removed in first order. See also Gottfried 1966, 397, Problem 1.) This problem is from Schiff 1968, 295, Problem 4. A system that has three unperturbed states can be represented by the pertrurbed Hamiltonian matrix

$$\begin{pmatrix} E_1 & 0 & a \\ 0 & E_1 & b \\ a^* & b^* & E_2 \end{pmatrix}$$

where E_2>E_1. The quantities a and b are to be regarded as perturbations that are of the same order and are small compared with E_2-E_1. Use the second-order nondegenerate perturbation theory to calculate the perturbed eigenvalues. (Is this procedure correct?) Then diagonalize the matrix to find the exact eigenvalues. Finally, use the second-order degenerate perturbation theory. Compare the three results obtained.

((**Exact solution**))

$$H = \begin{pmatrix} E_1 & 0 & a \\ 0 & E_1 & b \\ a^* & b^* & E_2 \end{pmatrix}$$

Det[H - λI] = 0

$$\lambda = E_1,$$

$$\lambda = \frac{E_1 + E_2}{2} \pm \frac{1}{2}\sqrt{(E_2 - E_1)^2 + 4(|a|^2 + |b|^2)}$$

$$= \frac{E_1 + E_2}{2} \pm \frac{1}{2}(E_2 - E_1)[1 + \frac{4(|a|^2 + |b|^2)}{(E_2 - E_1)^2}]^{1/2}$$

When $|a| << E_2 - E_1$, $|b| << E_2 - E_1$,

$$\lambda = \frac{E_1 + E_2}{2} \pm [\frac{E_2 - E_1}{2} + \frac{(|a|^2 + |b|^2)}{(E_2 - E_1)}]$$

or

$$\lambda = E_1 - \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

$$\lambda = E_2 + \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

((**Perturbation theory**))

$$H_0 = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_1 & 0 \\ 0 & 0 & E_2 \end{pmatrix}, \qquad H_1 = \begin{pmatrix} 0 & 0 & a \\ 0 & 0 & b \\ a^* & b^* & 0 \end{pmatrix}$$

$$\hat{H}_0 \left|\phi_\alpha\right\rangle = E_1 \left|\phi_\alpha\right\rangle \qquad \left|\phi_\alpha\right\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\hat{H}_0 \left|\phi_\beta\right\rangle = E_1 \left|\phi_\beta\right\rangle \qquad \left|\phi_\beta\right\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\hat{H}_0 \left|\phi_\gamma\right\rangle = E_2 \left|\phi_\gamma\right\rangle \qquad \left|\phi_\gamma\right\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\hat{H}_0 \left|\phi_\alpha\right\rangle = E_1 \left|\phi_\alpha\right\rangle \qquad \left|\phi_\alpha\right\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\hat{H}_0 \left|\phi_\beta\right\rangle = E_1 \left|\phi_\beta\right\rangle \qquad \left|\phi_\beta\right\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\hat{H}_0 \left|\phi_\gamma\right\rangle = E_2 \left|\phi_\gamma\right\rangle \qquad \left|\phi_\gamma\right\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$\left|\phi_\gamma\right\rangle$ is the eigenket of $\hat{H}_0$ with the energy E_2. Since this state is nondegenerate, we can apply the perturbation theory (non-degenerate case) to calculate the energy

The resulting energy is

$$E_\gamma = E_2 + \left\langle \phi_\gamma \left| \hat{H}_1 \right| \phi_\gamma \right\rangle + \frac{\left| \left\langle \phi_\alpha \left| \hat{H}_1 \right| \phi_\gamma \right\rangle \right|^2}{E_2 - E_1} + \frac{\left| \left\langle \phi_\beta \left| \hat{H}_1 \right| \phi_\gamma \right\rangle \right|^2}{E_2 - E_1} = E_2 + \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

$$\hat{H}_1|\phi_\alpha\rangle = a^*|\phi_\gamma\rangle$$

$$\hat{H}_1|\phi_\beta\rangle = b^*|\phi_\gamma\rangle$$

$$\hat{H}_1|\phi_\gamma\rangle = a|\phi_\alpha\rangle + b|\phi_\beta\rangle$$

$|\phi_\alpha\rangle$ and $|\phi_\beta\rangle$ are degenerate.

This is the degenerate case.

((**Second order**))
The matrix element of $\hat{H}_1$ in the basis of $|\phi_\alpha\rangle$ and $|\phi_\beta\rangle$ is equal to zero. So we need to calculate the second order

$$\sum_{\nu=1}^{g} \langle \varphi_{n,\mu}{}^{(0)}|\hat{\Lambda}|\varphi_{n,\nu}{}^{(0)}\rangle\langle\varphi_{n,\nu}{}^{(0)}|\psi_n{}^{(0)}\rangle = E_n{}^{(2)}\langle\varphi_{n,\mu}{}^{(0)}|\psi_n{}^{(0)}\rangle$$

$$\hat{\Lambda} = \sum_{k\neq n} \frac{\hat{H}_1|\psi_k{}^{(0)}\rangle\langle\psi_k{}^{(0)}|\hat{H}_1}{E_n{}^{(0)} - E_k{}^{(0)}} = \frac{\hat{H}_1|\phi_\gamma\rangle\langle\phi_\gamma|\hat{H}_1}{E_1 - E_2}$$

The matrix element

$$\Lambda = \begin{pmatrix} \dfrac{\langle\phi_\alpha|\hat{H}_1|\phi_\gamma\rangle\langle\phi_\gamma|\hat{H}_1|\phi_\alpha\rangle}{E_1 - E_2} & \dfrac{\langle\phi_\alpha|\hat{H}_1|\phi_\gamma\rangle\langle\phi_\gamma|\hat{H}_1|\phi_\beta\rangle}{E_1 - E_2} \\ \dfrac{\langle\phi_\beta|\hat{H}_1|\phi_\gamma\rangle\langle\phi_\gamma|\hat{H}_1|\phi_\alpha\rangle}{E_1 - E_2} & \dfrac{\langle\phi_\beta|\hat{H}_1|\phi_\gamma\rangle\langle\phi_\gamma|\hat{H}_1|\phi_\alpha\rangle}{E_1 - E_2} \end{pmatrix} = \begin{pmatrix} \dfrac{|a|^2}{E_1 - E_2} & \dfrac{ab^*}{E_1 - E_2} \\ \dfrac{a^* b}{E_1 - E_2} & \dfrac{|b|^2}{E_1 - E_2} \end{pmatrix}$$

Det[Λ-λI] = 0.

$$\begin{vmatrix} \dfrac{|a|^2}{E_1 - E_2} - \lambda & \dfrac{ab^*}{E_1 - E_2} \\ \dfrac{a^* b}{E_1 - E_2} & \dfrac{|b|^2}{E_1 - E_2} - \lambda \end{vmatrix} = 0$$

$$(\frac{|a|^2}{E_2 - E_1} + \lambda)(\frac{|b|^2}{E_2 - E_1} + \lambda) - \frac{|a|^2|b|^2}{(E_1 - E_2)^2} = 0$$

or

$$\lambda[\lambda + \frac{|a|^2 + |b|^2}{E_2 - E_1}] = 0$$

Then we have

$$\lambda = 0 \text{ and } \lambda = -\frac{|a|^2 + |b|^2}{E_2 - E_1}$$

The final result is

$$\widetilde{E}_a = E_1$$

$$\widetilde{E}_\beta = E_1 - \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

$$\widetilde{E}_\gamma = E_2 + \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

---

23. Typical problems (II)

23.1. A simple harmonic oscillator (in one dimension) is subjected to a perturbation $\lambda H_1 = bX$ ($b = -eE$). (a) Calculate the energy shift of the ground state to lowest nonvanishing order. (b) Solve this problem exactly and compare with your result obtained in (a).

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}$$

$$\hat{H}_0 = \hbar\omega_0(\hat{n} + \frac{1}{2})$$

$$\hat{a}\,|n> = \sqrt{n}\,|n-1>$$

$$\hat{a}^+\,|n> = \sqrt{n+1}\,|n+1>$$

$$\hat{x} = \frac{1}{\sqrt{2}\beta}(\hat{a}^+ + \hat{a})$$

$$\hat{H}_1|n\rangle = \frac{1}{\sqrt{2}\beta}(-eE)(\hat{a}^+ + \hat{a})|n\rangle = \frac{-eE}{\sqrt{2}\beta}(\sqrt{n}|n-1\rangle + \sqrt{n+1}|n+1\rangle)$$

$$\begin{aligned}
E_n &= E_n^{(0)} + \langle n|\hat{H}_1|n\rangle + \frac{\left|\langle n+1|\hat{H}_1|n\rangle\right|^2}{E_n^{(0)} - E_{n+1}^{(0)}} + \frac{\left|\langle n-1|\hat{H}_1|n\rangle\right|^2}{E_n^{(0)} - E_{n-1}^{(0)}} \\
&= \hbar\omega_0(n+\frac{1}{2}) + \frac{e^2E^2}{2\beta^2\hbar\omega_0}n - \frac{e^2E^2}{2\beta^2\hbar\omega_0}(n+1) \\
&= \hbar\omega_0(n+\frac{1}{2}) - \frac{e^2E^2}{2\beta^2\hbar\omega_0} \\
&= \hbar\omega_0(n+\frac{1}{2}) - \frac{e^2E^2}{2m\omega_0^2}
\end{aligned}$$

((**Another solution**))

$$\begin{aligned}
\hat{H} &= \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega_0^2\hat{x}^2 - eE\hat{x} \\
&= \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega_0^2(\hat{x}^2 - \frac{2eE}{m\omega_0^2}\hat{x} + \frac{e^2E^2}{m^2\omega_0^4} - \frac{e^2E^2}{m^2\omega_0^4}) \\
&= \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega_0^2(\hat{x} - \frac{eE}{m\omega_0^2})^2 - \frac{e^2E^2}{2m\ \omega_0^2}
\end{aligned}$$

The eigenvalue of $\hat{H}$ is given by

$$E_n = \hbar\omega_0(n+\frac{1}{2}) - \frac{e^2E^2}{2m\omega_0^2}$$

See more detail in the Chapter of simple harmonics.

((**Classical theory**))
The potential energy

$$V(x) = \frac{1}{2}m\omega_0^2x^2 - eEx$$

$V(x)$ has a local minimum (= $-e^2E^2/2m\omega_0^2$) at a position x_0 at which

$$\frac{dV(x)}{dx} = 0 \qquad \text{at} \qquad x = x_0 = \frac{eE}{m\omega_0^2}$$

Thus the classical and quantum results are the same.

23.2 Given the matrix for H_0 and for the perturbation H_1 in the orthonormal basis $|\phi_1>$, $|\phi_2>$, and $|\phi_3>$, determine the energy eigenvalues correct to second order in the perturbation.

$$H_0 = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{pmatrix}, \qquad H_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

((Exact solution))
Eigenvalue problem

$$H = H_0 + H_1 = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 4 \end{pmatrix}$$

Eigensystem[H]:
Eigenvalues:
λ = 0.829914, 2.68889, and 4.48119.

((Perturbation theory))

$$\hat{H}_0|\phi_1\rangle = 2|\phi_1\rangle$$

$$\hat{H}_0|\phi_2\rangle = 2|\phi_2\rangle$$

$$\hat{H}_0|\phi_3\rangle = 4|\phi_3\rangle$$

$$\hat{H}_1|\phi_1\rangle = |\phi_2\rangle$$

$$\hat{H}_1|\phi_2\rangle = |\phi_1\rangle + |\phi_3\rangle$$

$$\hat{H}_1|\phi_3\rangle = |\phi_2\rangle$$

$|\phi_1\rangle$ and $|\phi_2\rangle$ are degenerate states: $E_1^{(0)} = 2$, $E_2^{(0)} = 2$
$|\phi_3\rangle$ is a nondegenerate state: $E_3^{(0)} = 4$

(1) Non-degenerate case (for the energy $E_3^{(0)} = 4$)

First order

$$E_3^{(1)} = \langle \phi_3 | \hat{H}_1 | \phi_3 \rangle = 0$$

Second order

$$E_3^{(2)} = \frac{|\langle \phi_1 | \hat{H}_1 | \phi_3 \rangle|^2}{E_3^{(0)} - E_1^{(1)}} + \frac{|\langle \phi_2 | \hat{H}_1 | \phi_3 \rangle|^2}{E_3^{(0)} - E_2^{(0)}} = \frac{0}{4-2} + \frac{1}{4-2} = \frac{1}{2}$$

Then we have

$$E_3 = E_3^{(0)} + E_3^{(1)} + E_3^{(2)} = 4 + 0.5 = 4.5 \text{ (exact sol. 4.48).}$$

(2) Degenerate case (for the energy $E_1^{(0)} = 2$, $E_2^{(0)} = 2$)

First order

The matrix only from the basis $\{|\phi_1\rangle$ and $|\phi_2\rangle\}$

$$\tilde{H}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Det[H_1-λI]= λ^2 - 1 = 0. or $\lambda = \pm 1$.

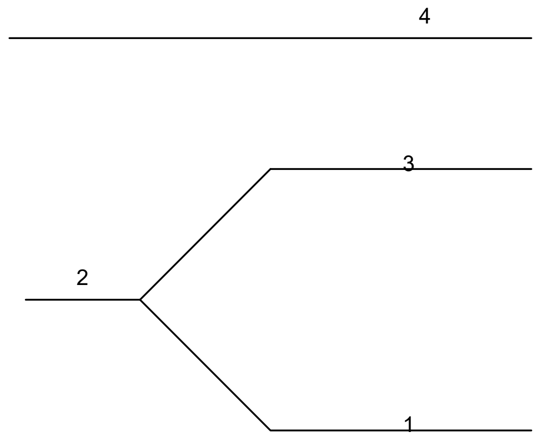
The upper state: $E_+ = 2 + 1 = 3$,

$$|\phi_+\rangle = \frac{1}{\sqrt{2}}(|\phi_1\rangle + |\phi_2\rangle): \hat{H}_1|\phi_+\rangle = |\phi_+\rangle$$

The lower state: $E_+ = 2 - 1 = 1$,

$$|\phi_-\rangle = \frac{1}{\sqrt{2}}(|\phi_1\rangle - |\phi_2\rangle): \hat{H}_1|\phi_-\rangle = -|\phi_-\rangle$$

$$\langle \phi_3 | \hat{H}_1 | \phi_2 \rangle = 1, \ \langle \phi_3 | \hat{H}_1 | \phi_+ \rangle = \frac{1}{\sqrt{2}}, \ \langle \phi_3 | \hat{H}_1 | \phi_- \rangle = -\frac{1}{\sqrt{2}}$$



The state $\left|\phi_{+}\right\rangle$ and $\left|\phi_{-}\right\rangle$ are now non-degenerate

Second order (non-degenerate case)

$$E_{-}^{(2)}=\frac{\left|\left\langle\phi_{+}\right|\hat{H}_{1}\left|\phi_{-}\right\rangle\right|^{2}}{E_{-}-E_{+}}+\frac{\left|\left\langle\phi_{3}\right|\hat{H}_{1}\left|\phi_{-}\right\rangle\right|^{2}}{E_{-}-E_{3}}=\frac{\left|\left\langle\phi_{3}\right|\hat{H}_{1}\left|\phi_{-}\right\rangle\right|^{2}}{1-4}=-\frac{1}{6}$$

Then

E_{-} = 1-1/6 = 5/6 = 0.83 (exact sol. 0.8299)

$$E_{+}^{(2)}=\frac{\left|\left\langle\phi_{-}\right|\hat{H}_{1}\left|\phi_{+}\right\rangle\right|^{2}}{E_{+}-E_{-}}+\frac{\left|\left\langle\phi_{3}\right|\hat{H}_{1}\left|\phi_{+}\right\rangle\right|^{2}}{E_{+}-E_{3}}=\frac{(1/2)}{3-4}=-\frac{1}{2}$$

Then

E_{+} = 3-1/2 = 5/2 = 2.5 (exact sol. 2.689)

23.3 Discuss how the threefold-degenerate energy of the two dimensional harmonic oscillator separate due to the perturbation $\hat{H}_1 = a\hat{x}\hat{y}$ (*a* is constant).

$$\hat{H}_0\left|n_x, n_y\right\rangle = E(n_x, n_y)\left|n_x, n_y\right\rangle$$

The state is denoted by the eigenket $\left|n_x, n_y\right\rangle$ with the energy

$$E(n_x, n_y) = \hbar\omega_0(n_x + n_y + 1)$$

(i) The ground state: $|0,0\rangle$ (the nondegenerate state).

$$E_0 = E(0,0) = \hbar\omega_0$$

(ii) The first excited state: $|1,0\rangle$ and $|0,1\rangle$ (degenerate state).

$$E_1 = E(1,0) = E(0,1) = 2\hbar\omega_0$$

The second excited state: $|2,0\rangle$, $|1,1\rangle$, and $|0,2\rangle$ (degenerate state).

$$E_2 = E(2,0) = E(1,1) = E(0,2) = 3\hbar\omega_0$$

The third excited state: $|3,0\rangle, |2,1\rangle, |1,2\rangle, |0,3\rangle$ (degenerate state).

$$\hat{H}_1|n_x, n_y\rangle = a\hat{x}\hat{y}|n_x, n_y\rangle$$

Here we note that

$$\hat{x}|n_x\rangle = \frac{1}{\sqrt{2}\beta}(\sqrt{n_x}|n_x - 1\rangle + \sqrt{n_x + 1}|n_x + 1\rangle)$$

$$\hat{y}|n_y\rangle = \frac{1}{\sqrt{2}\beta}(\sqrt{n_y}|n_y - 1\rangle + \sqrt{n_y + 1}|n_y + 1\rangle)$$

Then

$$\hat{H}_1|1,1\rangle = a\hat{x}\hat{y}|1,1\rangle = \frac{a}{2\beta^2}(|0\rangle_x + \sqrt{2}|2\rangle_x)(|0\rangle_y + \sqrt{2}|2\rangle_y)$$

$$= \frac{a}{2\beta^2}(|0,0\rangle + \sqrt{2}|0,2\rangle + \sqrt{2}|2,0\rangle + \sqrt{2}|2,2\rangle)$$

$$\hat{H}_1|2,0\rangle = \frac{a}{2\beta^2}(\sqrt{2}|1\rangle_x + \sqrt{3}|3\rangle_x)|1\rangle_y$$

$$= \frac{a}{2\beta^2}(\sqrt{2}|1,1\rangle + \sqrt{3}|3,1\rangle)$$

$$\hat{H}_1|0,2\rangle = \frac{a}{2\beta^2}(\sqrt{2}|1,1\rangle + \sqrt{3}|1,3\rangle)$$

Matrix of $\hat{H}_1 = a\hat{x}\hat{y}$ in terms of the basis $\{|1,1\rangle, |2,0\rangle, |0,2\rangle\}$

$$\hat{H}_1 = \begin{pmatrix} 0 & \alpha & \alpha \\ \alpha & 0 & 0 \\ \alpha & 0 & 0 \end{pmatrix}$$

with

$$\alpha = \frac{a}{\sqrt{2}\beta^2}$$

We use the Mathematica to determine the eigenvalue;

Eigensystem[H_1]:

(i) $E_2^{(1)} = 3\hbar\omega_0 - \sqrt{2}\alpha$

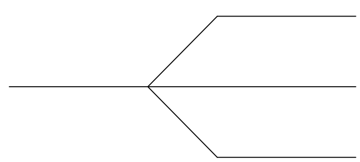
$$\left|\psi_{21}{}^{(0)}\right\rangle = \frac{1}{2}[-\sqrt{2}\left|1,1\right\rangle + \left|2,0\right\rangle + \left|0,2\right\rangle]$$

(ii) $E_2^{(2)} = 3\hbar\omega_0$

$$\left|\psi_{22}{}^{(0)}\right\rangle = \frac{1}{\sqrt{2}}[-\left|2,0\right\rangle + \left|0,2\right\rangle]$$

(iii) $E_2^{(3)} = 3\hbar\omega_0 + \sqrt{2}\alpha$

$$\left|\psi_{23}{}^{(0)}\right\rangle = \frac{1}{2}[\sqrt{2}\left|1,1\right\rangle + \left|2,0\right\rangle + \left|0,2\right\rangle]$$



23.4. Sakurai 5-12 (This is a tricky problem because the degeneracy between the first and the second state is not removed in first order. See also Gottfried 1966, 397, Problem 1.) This problem is from Schiff 1968, 295, Problem 4. A system that has three unperturbed states can be represented by the pertrurbed Hamiltonian matrix

$$\begin{pmatrix} E_1 & 0 & a \\ 0 & E_1 & b \\ a^* & b^* & E_2 \end{pmatrix}$$

where $E_2 > E_1$. The quantities a and b are to be regarded as perturbations that are of the same order and are small compared with $E_2 - E_1$. Use the second-order nondegenerate perturbation theory to calculate the perturbed eigenvalues. (Is this procedure correct?) Then diagonalize the matrix to find the exact eigenvalues. Finally, use the second-order degenerate perturbation theory. Compare the three results obtained.

((**Exact solution**))

$$H = \begin{pmatrix} E_1 & 0 & a \\ 0 & E_1 & b \\ a^* & b^* & E_2 \end{pmatrix}$$

Det[H - λI] = 0

$\lambda = E_1$,

$$\lambda = \frac{E_1 + E_2}{2} \pm \frac{1}{2}\sqrt{(E_2 - E_1)^2 + 4(|a|^2 + |b|^2)}$$

$$= \frac{E_1 + E_2}{2} \pm \frac{1}{2}(E_2 - E_1)[1 + \frac{4(|a|^2 + |b|^2)}{(E_2 - E_1)^2}]^{1/2}$$

When $|a| << E_2 - E_1, |b| << E_2 - E_1$,

$$\lambda = \frac{E_1 + E_2}{2} \pm [\frac{E_2 - E_1}{2} + \frac{(|a|^2 + |b|^2)}{(E_2 - E_1)}]$$

or

$$\lambda = E_1 - \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

$$\lambda = E_2 + \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

((**Perturbation theory**))

$$H_0 = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_1 & 0 \\ 0 & 0 & E_2 \end{pmatrix}, \qquad H_1 = \begin{pmatrix} 0 & 0 & a \\ 0 & 0 & b \\ a^* & b^* & 0 \end{pmatrix}$$

$$\hat{H}_0|\phi_\alpha\rangle = E_1|\phi_\alpha\rangle, \qquad |\phi_\alpha\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\hat{H}_0|\phi_\beta\rangle = E_1|\phi_\beta\rangle, \qquad |\phi_\beta\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\hat{H}_0|\phi_\gamma\rangle = E_2|\phi_\gamma\rangle, \qquad |\phi_\gamma\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\hat{H}_1|\phi_\alpha\rangle = \begin{pmatrix} 0 \\ 0 \\ a^* \end{pmatrix} = a^*|\phi_\gamma\rangle$$

$$\hat{H}_1|\phi_\beta\rangle = \begin{pmatrix} 0 \\ 0 \\ b^* \end{pmatrix} = b^*|\phi_\gamma\rangle$$

$$\hat{H}_1|\phi_\gamma\rangle = \begin{pmatrix} a \\ b \\ 0 \end{pmatrix} = a|\phi_\alpha\rangle + b|\phi_\beta\rangle$$

$|\phi_\gamma\rangle$ is the eigenket of $\hat{H}_0$ with the energy E_2. Since this state is non-degenerate, we can apply the perturbation theory (non-degenerate case) to calculate the energy

The resulting energy is

$$E_\gamma = E_2 + \langle\phi_\gamma|\hat{H}_1|\phi_\gamma\rangle + \frac{|\langle\phi_\alpha|\hat{H}_1|\phi_\gamma\rangle|^2}{E_2 - E_1} + \frac{|\langle\phi_\beta|\hat{H}_1|\phi_\gamma\rangle|^2}{E_2 - E_1} = E_2 + \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

$\left|\phi_\alpha\right\rangle$ and $\left|\phi_\beta\right\rangle$ are degenerate.

This is the degenerate case.

(i) The First order:

The matrix element of H_1 in the basis of $\left|\phi_\alpha\right\rangle$ and $\left|\phi_\beta\right\rangle$ is equal to zero. So we need to calculate the second order

(ii) The second order

$$\sum_{\nu=1}^{g}\left\langle\varphi_{n,\mu}{}^{(0)}\right|\hat{\Lambda}\left|\varphi_{n,\nu}{}^{(0)}\right\rangle\left\langle\varphi_{n,\nu}{}^{(0)}\right|\left.\psi_n{}^{(0)}\right\rangle = E_n{}^{(2)}\left\langle\varphi_{n,\mu}{}^{(0)}\right|\left.\psi_n{}^{(0)}\right\rangle.$$

$$\hat{\Lambda} = \sum_{k\neq n}\frac{\hat{H}_1\left|\psi_k{}^{(0)}\right\rangle\left\langle\psi_k{}^{(0)}\right|\hat{H}_1}{E_n{}^{(0)} - E_k{}^{(0)}} = \frac{\hat{H}_1\left|\phi_\gamma\right\rangle\left\langle\phi_\gamma\right|\hat{H}_1}{E_1 - E_2}$$

The matrix element

$$\Lambda = \begin{pmatrix} \dfrac{\langle\phi_\alpha|\hat{H}_1|\phi_\gamma\rangle\langle\phi_\gamma|\hat{H}_1|\phi_\alpha\rangle}{E_1 - E_2} & \dfrac{\langle\phi_\alpha|\hat{H}_1|\phi_\gamma\rangle\langle\phi_\gamma|\hat{H}_1|\phi_\beta\rangle}{E_1 - E_2} \\ \dfrac{\langle\phi_\beta|\hat{H}_1|\phi_\gamma\rangle\langle\phi_\gamma|\hat{H}_1|\phi_\alpha\rangle}{E_1 - E_2} & \dfrac{\langle\phi_\beta|\hat{H}_1|\phi_\gamma\rangle\langle\phi_\gamma|\hat{H}_1|\phi_\beta\rangle}{E_1 - E_2} \end{pmatrix} = \begin{pmatrix} \dfrac{|a|^2}{E_1 - E_2} & \dfrac{ab^*}{E_1 - E_2} \\ \dfrac{a^*b}{E_1 - E_2} & \dfrac{|b|^2}{E_1 - E_2} \end{pmatrix}$$

Det[Λ-λI] = 0.

$$\begin{vmatrix} \dfrac{|a|^2}{E_1 - E_2} - \lambda & \dfrac{ab^*}{E_1 - E_2} \\ \dfrac{a^*b}{E_1 - E_2} & \dfrac{|b|^2}{E_1 - E_2} - \lambda \end{vmatrix} = 0$$

$$\left(\frac{|a|^2}{E_2 - E_1} + \lambda\right)\left(\frac{|b|^2}{E_2 - E_1} + \lambda\right) - \frac{|a|^2|b|^2}{(E_1 - E_2)^2} = 0$$

or

$$\lambda\left[\lambda + \frac{|a|^2 + |b|^2}{E_2 - E_1}\right] = 0$$

Then we have

$$\lambda = 0 \text{ and } \lambda = -\frac{|a|^2 + |b|^2}{E_2 - E_1}$$

The final result is

$$\tilde{E}_a = E_1$$

$$\tilde{E}_\beta = E_1 - \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

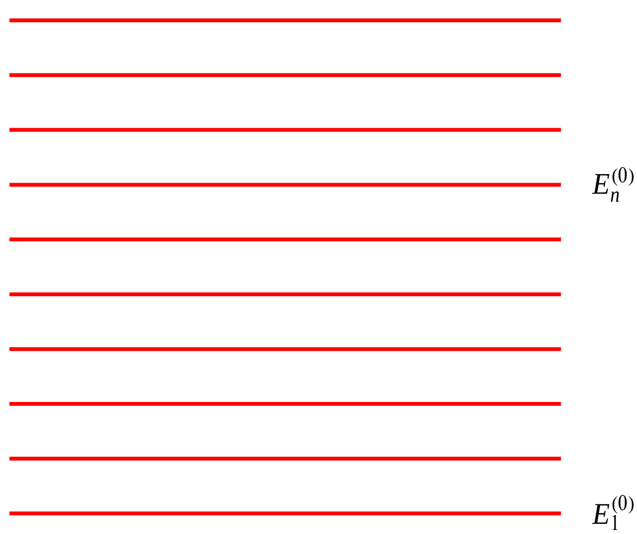
$$\tilde{E}_\gamma = E_2 + \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

24. Diagram of the Purturbation by Mathematica

Here we present a method how to solve the problem of the perturbation theory (time-independent) by using the Mathematica. We consider the two cases; (i) the non-degenerate case, and (ii) the degenerate case.

24.1 Non-degenerate system

In the presence of only a unperturbed Hamiltonian $\hat{H}_0$



(i) Eigensystem[H_0]
(ii) Normalize[eigenket]

(iii) The eigenvalues are different.

Eigen values $E_n^{(0)}$

Eigenkets: $\left|\psi_n^{(0)}\right\rangle$

(iii) Unitary operator $\hat{U}_a$

$\hat{U}_a{}^T = \{\left|\psi_1^{(0)}\right\rangle, \left|\psi_2^{(0)}\right\rangle, ..., \left|\psi_n^{(0)}\right\rangle, ...\}$

$\hat{U}_a = Transpose[\{\left|\psi_1^{(0)}\right\rangle, \left|\psi_2^{(0)}\right\rangle, ..., \left|\psi_n^{(0)}\right\rangle, ... \}]$

In the presence of the perturbation $\hat{H}_1$, we need to calculate the matrix element of $\hat{H}_1$

$$\left\langle\psi_k^{(0)}\right|\hat{H}_1\left|\psi_l^{(0)}\right\rangle$$

The first order

$$E_n^{(1)} = \left\langle\psi_n^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle$$

$$\left|\psi_n^{(1)}\right\rangle = \sum_{k\neq n}\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\middle|\psi_n^{(1)}\right\rangle = \sum_{k\neq n}\left|\psi_k^{(0)}\right\rangle\frac{\left\langle\psi_k^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle}{E_n^{(0)} - E_k^{(0)}}$$

The second order

$$E_n^{(2)} = \sum_{k\neq n}\frac{\left|\left\langle\psi_n^{(0)}\right|\hat{H}_1\left|\psi_k^{(0)}\right\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}} = \sum_{k\neq n}\frac{\left\langle\psi_n^{(0)}\right|\hat{H}_1\left|\psi_k^{(0)}\right\rangle\left\langle\psi_k^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle}{E_n^{(0)} - E_k^{(0)}}$$

$$\left|\psi_n^{(2)}\right\rangle = \sum_{k\neq n}\left|\psi_k^{(0)}\right\rangle[\sum_{l\neq n}\frac{\left\langle\psi_k^{(0)}\right|\hat{H}_1\left|\psi_l^{(0)}\right\rangle\left\langle\psi_l^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_l^{(0)})} - \frac{\left\langle\psi_k^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle\left\langle\psi_n^{(0)}\right|\hat{H}_1\left|\psi_n^{(0)}\right\rangle}{(E_n^{(0)} - E_k^{(0)})^2}]$$

24.2 Degenerate case (consisting of non-degenerate and degenerate states for H_0)

Fig. The degenerate energy level ($E_k^{(0)}$) and the non-degenerate energy level ($E_n^{(0)}$) with $n \neq k$.

(a) Non-degenerate states ($E_n^{(0)}$) with $n \neq k$.

(i) Eigensystem[H_0]
(ii) Normalize[eigenket]
(iii) Non-degenerate case.
Eigenvalues $E_n^{(0)}$
Eigenkets: $\left|\psi_n^{(0)}\right\rangle$

(b) Degenerate case ($E_k^{(0)}$)

Eigenvalues $E_k^{(0)}$

Suppose that there are g independent eigenstates with the same energy $E_k^{(0)}$.

Eigensystem[H_0]

We get the eigenkets: $\{\left|\phi_{k1}^{(0)}\right\rangle, \left|\phi_{k2}^{(0)}\right\rangle, \left|\phi_{k3}^{(0)}\right\rangle, ..., \left|\phi_{kg}^{(0)}\right\rangle\}$. We need to check whether the the condition of orthogonality is satisfied;

$$\{\left|\phi_{k1}^{(0)}\right\rangle, \left|\phi_{k2}^{(0)}\right\rangle, \left|\phi_{k3}^{(0)}\right\rangle, ..., \left|\phi_{kg}^{(0)}\right\rangle\}$$

If these do not form the orthonormal kets, we need to obtain the appropriate orthnormal eigenkets by using the Mathematica program such that

Orthogonalize and Normalize[$\{\left|\phi_{k1}{}^{(0)}\right\rangle, \left|\phi_{k2}{}^{(0)}\right\rangle, \left|\phi_{k3}{}^{(0)}\right\rangle, ..., \left|\phi_{kg}{}^{(0)}\right\rangle\}$]

the normalized eigenstates (orthogonal to each other) thus obtained are

$$\{\left|\psi_{k1}{}^{(0)}\right\rangle, \left|\psi_{k2}{}^{(0)}\right\rangle, \left|\psi_{k3}{}^{(0)}\right\rangle, ..., \left|\psi_{kg}{}^{(0)}\right\rangle\}$$

In the presence of the perturbation H_1, we need to calculate the matrix.

(i) The first order

$$(H_1)_{k\mu,k\nu} = \left\langle \psi_{k\mu}{}^{(0)} \right| \hat{H}_1 \left| \psi_{k\nu}{}^{(0)} \right\rangle$$

(i) Eigensystem[$(H_1)_{k\mu,k\nu}$]

(ii) Normalize[eigenket]

(iii)

Eigen values $E_{k\nu}{}^{(1)}$

Eigenkets: $\left|\Phi_{k\nu}^{(1)}\right\rangle$

(iv) Unitary operator $\hat{U}$

$$\hat{U}_b{}^T = \{\left|\Phi_{k1}^{(1)}\right\rangle, \left|\Phi_{k1}^{(1)}\right\rangle, ..., \left|\Phi_{kg}^{(1)}\right\rangle..\}$$

$$\hat{U}_b = Transpose[\{\left|\Phi_1^{(1)}\right\rangle, \left|\Phi_2^{(1)}\right\rangle, ..., \left|\Phi_{kg}^{(1)}\right\rangle\}]$$

(ii) The second order

Suppose that

$$(H_1)_{k\mu,k\nu} = \left\langle \psi_{k\mu}{}^{(0)} \right| \hat{H}_1 \left| \psi_{k\nu}{}^{(0)} \right\rangle = 0 \qquad (\mu \neq \nu)$$

$$(H_1)_{k\mu,k\mu} = \left\langle \psi_{k\mu}{}^{(0)} \right| \hat{H}_1 \left| \psi_{k\mu}{}^{(0)} \right\rangle = a : \text{independent of } \mu \qquad (\mu = 1, 2, ..., g).$$

In other words,

$$H_1 = \begin{pmatrix} a & 0 & 0 & 0 & \cdot & \cdot & 0 \\ 0 & a & 0 & 0 & \cdot & \cdot & 0 \\ 0 & 0 & a & 0 & 0 & \cdot & 0 \\ 0 & 0 & 0 & a & 0 & \cdot & \cdot \\ \cdot & \cdot & 0 & 0 & a & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & 0 & a & 0 \\ 0 & 0 & 0 & \cdot & 0 & 0 & a \end{pmatrix}$$

In this case, the degeneracy cannot be removed under the first order perturbation. So we need to go to the second order correction.

$$\hat{\Lambda} = \sum_{n \neq k} \frac{\hat{H}_1 \left|\psi_n{}^{(0)}\right\rangle \left\langle \psi_n{}^{(0)}\right| \hat{H}_1}{E_k{}^{(0)} - E_n{}^{(0)}}$$

where $E_k{}^{(0)}$ is the energy of the degenerate state and $E_n{}^{(0)}$ us the energy of the nondegenerate state. Calculate the matrix element defined by

$$\Lambda_{k\mu,k\nu} = \left\langle \varphi_{k,\mu}{}^{(0)} \right| \hat{\Lambda} \left| \varphi_{k,\nu}{}^{(0)} \right\rangle.$$

(i) Eigensystem[$\Lambda_{k\mu,k\nu}$]

(ii) Normalize[eigenket]

(iii)

Eigen values $E_{k\nu}{}^{(2)}$

Eigenkets: $\left|\Phi_{k\nu}^{(2)}\right\rangle$

(iv) Unitary operator $\hat{U}$

$\hat{U}_c{}^T = \{\left|\Phi_{k1}^{(2)}\right\rangle, \left|\Phi_{k1}^{(2)}\right\rangle, \ldots, \left|\Phi_{kg}^{(2)}\right\rangle ..\}$

$\hat{U}_c = Transpose[\{\left|\Phi_1^{(2)}\right\rangle, \left|\Phi_2^{(2)}\right\rangle, \ldots, \left|\Phi_{kg}^{(2)}\right\rangle\}]$

REFERENCES

L. Schiff, *Quantum Mechanics*, 3rd edition (McGraw-Hill, New York, 1968).

E. Merzbacher, *Quantum Mechanics*, 3rd edition (John Wiley & Sons, New York, 1998).

J.J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, second edition (Addison-Wesley, New York, 2011).

APPENDIX-A: **Example of simple harmonics**

A.1. Simple harmonics

$$\hat{a} = \frac{\beta}{\sqrt{2}}(\hat{x} + \frac{i\hat{p}}{m\omega}) = \frac{1}{\sqrt{2}}(\sqrt{\frac{m\omega}{\hbar}}\hat{x} + \frac{i\hat{p}}{\sqrt{m\hbar\omega}}),$$

$$\hat{a}^{+} = \frac{\beta}{\sqrt{2}}(\hat{x} - \frac{i\hat{p}}{m\omega}) = \frac{1}{\sqrt{2}}(\sqrt{\frac{m\omega}{\hbar}}\hat{x} - \frac{i\hat{p}}{\sqrt{m\hbar\omega}}),$$

The operators $\hat{x}$ and $\hat{p}$ are given by

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\left(\hat{a} + \hat{a}^{+}\right) = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\hat{a} + \hat{a}^{+}\right)$$

$$\hat{p} = \frac{1}{\sqrt{2}\beta}\frac{m\omega_0}{i}\left(\hat{a} - \hat{a}^{+}\right) = \frac{1}{i}\sqrt{\frac{m\hbar\omega_0}{2}}\left(\hat{a} - \hat{a}^{+}\right)$$

where

$$[\hat{x}, \hat{p}] = \frac{1}{\left(\sqrt{2}\beta\right)^2}\frac{m\omega_0}{i}[\hat{a} + \hat{a}^{+}, \hat{a} - \hat{a}^{+}] = -\frac{\hbar}{i}[\hat{a}, \hat{a}^{+}].$$

Since $\left[\hat{x}, \hat{p}\right] = i\hbar\hat{1}$, the commutation relation $\left[\hat{a}, \hat{a}^{+}\right]$ is obtained as

$$[\hat{a}, \hat{a}^{+}] = \hat{1}.,$$

$$\hat{a}^{+}\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle$$

$$\hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle$$

$$\hat{x}\left|n\right\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\hat{a} + \hat{a}^{+}\right)\left|n\right\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\sqrt{n+1}\left|n+1\right\rangle + \sqrt{n}\left|n-1\right\rangle\right)$$

$$\hat{p}\left|n\right\rangle = \sqrt{\frac{m\hbar\omega_0}{2}}i\left(\hat{a}^{+} - \hat{a}\right)\left|n\right\rangle = \sqrt{\frac{m\hbar\omega_0}{2}}i\left(\sqrt{n+1}\left|n+1\right\rangle - \sqrt{n}\left|n-1\right\rangle\right)$$

A.2 Exact solution

The one-dimensional harmonic oscillator consists of a particle of mass *m* having a potential energy. Assume, in addition, that this particle has a charge *q* that it is placed in a uniform electric field ε parallel to the *x* axis. What are its new stationary states and the corresponding energies.

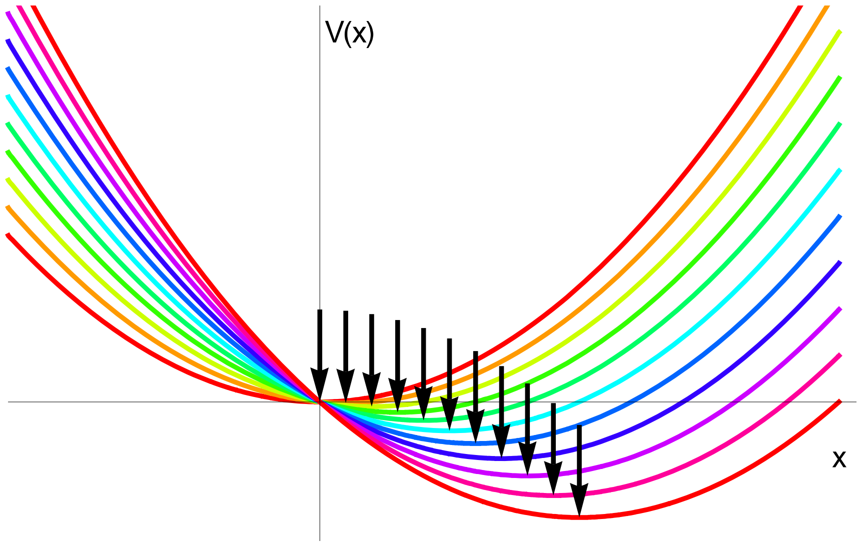


Fig. The potential energy $V(x) = \frac{1}{2} m\omega^2 x^2 - q\varepsilon x$. The potential takes a minimum at $x_0 = \mu = \frac{q\varepsilon}{m\omega_0^{\,2}}$. The minimum position of the potential energy shifts to the larger x as the electric field increases.

The Hamiltonian of a particle placed in a uniform electric field ε is given by

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2} m\omega^2 \hat{x}^2 - q\varepsilon\hat{x}$$

The new Hamiltonian under the translation operator can be rewritten as

$$\begin{aligned}
\hat{H}' &= \hat{T}_\mu \hat{H} \hat{T}_\mu^{\,+} \\
&= \hat{T}_\mu \left(\frac{1}{2m}\hat{p}^2 + \frac{1}{2} m\omega^2 \hat{x}^2 - q\varepsilon\hat{x}\right)\hat{T}_\mu^{\,+} \\
&= \frac{1}{2m}\hat{p}^2 + \frac{1}{2} m\omega^2 \hat{T}_\mu \hat{x}^2 \hat{T}_\mu^{\,+} - q\varepsilon \hat{T}_\mu \hat{x} \hat{T}_\mu^{\,+} \\
&= \frac{1}{2m}\hat{p}^2 + \frac{1}{2} m\omega^2 (\hat{x} - \mu\hat{1})^2 - q\varepsilon(\hat{x} - \mu\hat{1}) \\
&= \frac{1}{2m}\hat{p}^2 + \frac{1}{2} m\omega^2 \hat{x}^2 - (q\varepsilon + m\omega^2\mu)\hat{x} \\
&\quad + \frac{1}{2} m\omega^2 \mu^2 + q\varepsilon\mu
\end{aligned}$$

where

$$\hat{T}_\mu \hat{p}^2 \hat{T}_\mu^{\ +} = \hat{p}^2, \qquad \hat{T}_\mu \hat{p} \hat{T}_\mu^{\ +} = \hat{p}$$

$$\hat{T}_\mu \hat{x}^2 \hat{T}_\mu^{\ +} = (\hat{x} - \mu\hat{1})^2, \qquad \hat{T}_\mu \hat{x} \hat{T}_\mu^{\ +} = (\hat{x} - \mu\hat{1})$$

We choose μ as follows.

$$q\varepsilon + m\omega^2\mu = 0, \qquad \mu = -\frac{q\varepsilon}{m\omega^2}$$

Then we have

$$\hat{H}' = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 - \frac{q^2\varepsilon^2}{2m\omega^2}\hat{1} = \hat{H}_0 - \frac{q^2\varepsilon^2}{2m\omega^2}\hat{1}$$

Suppose that $|n\rangle$ is the eigenket of $\hat{H}_0$ with the eigenvalue $E_n = \hbar\omega_0(n+\frac{1}{2})$,

$$\hat{H}_0|n\rangle = \hbar\omega_0(n+\frac{1}{2})|n\rangle,$$

Then we have

$$\hat{H}'|n\rangle = (\hat{H}_0 - \frac{q^2\varepsilon^2}{2m\omega^2}\hat{1})|n\rangle = [\hbar\omega(n+\frac{1}{2}) - \frac{q^2\varepsilon^2}{2m\omega^2}]|n\rangle$$

$|n\rangle$ is the eigenket of $\hat{H}'$ with the energy eigenvalue of $\hat{H}'$ given by

$$E_n' = \hbar\omega(n+\frac{1}{2}) - \frac{q^2\varepsilon^2}{2m\omega^2}$$

Since

$$\hat{T}_\mu \hat{H} \hat{T}_\mu^{\ +}|n\rangle = E_n'|n\rangle$$

or

$$\hat{H}\hat{T}_\mu^{\ +}|n\rangle = E_n'\hat{T}_\mu^{\ +}|n\rangle$$

$\hat{T}_\mu^{+}|n\rangle$ is the eigenket of $\hat{H}$ with the energy eigenvalue E_n'

The $|x\rangle$ representation of the eigenket $\hat{T}_\mu^{+}|n\rangle$ is

$$\langle x|\hat{T}_\mu^{+}|n\rangle = \langle x+\mu|n\rangle = \left\langle x - \frac{q\varepsilon}{m\omega_0^{2}}\middle|n\right\rangle$$

where

$$\hat{T}_\mu|x\rangle = |x+\mu\rangle, \qquad \langle x+\mu| = \langle x|\hat{T}_\mu^{+}$$

and

$$\mu = -\frac{q\varepsilon}{m\omega^2}$$

We note

$$\begin{aligned}
\hat{T}_\mu^{+} &= \exp[\frac{i}{\hbar}\mu\hat{p}_x] \\
&\approx \hat{1} + \frac{i}{\hbar}\mu\hat{p}_x \\
&= \hat{1} + \frac{i}{\hbar}(-\frac{q\varepsilon}{m\omega^2})\frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a}-\hat{a}^{+}\right) \\
&= \hat{1} - \frac{q\varepsilon}{\omega}\sqrt{\frac{1}{2m\hbar\omega}}\left(\hat{a}-\hat{a}^{+}\right)
\end{aligned}$$

$$\begin{aligned}
\hat{T}_\mu^{+}|n\rangle &= [\hat{1} - \frac{q\varepsilon}{\omega}\sqrt{\frac{1}{2m\hbar\omega}}\left(\hat{a}-\hat{a}^{+}\right)]|n\rangle \\
&= |n\rangle + \frac{q\varepsilon}{\omega}\sqrt{\frac{1}{2m\hbar\omega}}[\sqrt{n+1}|n+1\rangle - \sqrt{n}|n-1\rangle
\end{aligned}$$

where

$$\hat{p}_x = \frac{1}{\sqrt{2}\beta}\frac{m\omega}{i}\left(\hat{a}-\hat{a}^{+}\right) = \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a}-\hat{a}^{+}\right)$$

A.3. Perturbation theory

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 - q\varepsilon\hat{x}$$

$$\hat{H}_0 = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2, \qquad \hat{H}_1 = -q\varepsilon\hat{x} = -q\varepsilon\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^+\right)$$

where

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\left(\hat{a} + \hat{a}^+\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^+\right)$$

The zero-th order

$$E_n^{(0)} = (n + \frac{1}{2})\hbar\omega$$

The first order:

$$E_n^{(1)} = \left\langle n\middle|\hat{H}_1\middle|n\right\rangle = -q\varepsilon\sqrt{\frac{\hbar}{2m\omega}}\left\langle n\middle|\hat{a} + \hat{a}^+\middle|n\right\rangle = 0$$

The second order

$$\begin{aligned} E_n^{(2)} &= \sum_{k\neq n}\frac{\left|\left\langle k\middle|H\middle|n\right\rangle\right|^2}{E_n^0 - E_k^{(0)}} = \frac{\left|\left\langle n-1\middle|H\middle|n\right\rangle\right|^2}{E_n^0 - E_{n-1}^{(0)}} + \frac{\left|\left\langle n+1\middle|H\middle|n\right\rangle\right|^2}{E_n^0 - E_{n+1}^{(0)}} \\ &= q^2\varepsilon^2\frac{\hbar}{2m\omega}\left(\frac{n}{\hbar\omega} - \frac{n+1}{\hbar\omega}\right) \\ &= -\frac{q^2\varepsilon^2}{2m\omega^2} \end{aligned}$$

leading to

$$E_n = (n + \frac{1}{2})\hbar\omega - \frac{q^2\varepsilon^2}{2m\omega^2}$$

since

$$\langle k|\hat{H}_1|n\rangle = -q\varepsilon\sqrt{\frac{\hbar}{2m\omega}}\langle k|\hat{a}+\hat{a}^+|n\rangle$$

$$= -q\varepsilon\sqrt{\frac{\hbar}{2m\omega}}\langle k|(\sqrt{n}|n-1\rangle + \sqrt{n+1}|n+1\rangle)$$

$$= -q\varepsilon\sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n}\delta_{k,n-1} + \sqrt{n+1}\delta_{k,n+1})$$

$$\langle n+1|\hat{H}_1|n\rangle = -q\varepsilon\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n+1}$$

$$\langle n-1|\hat{H}_1|n\rangle = -q\varepsilon\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n}$$

–

$$|\psi_n\rangle = |\psi_n{}^{(0)}\rangle + \lambda|\psi_n{}^{(1)}\rangle + \lambda^2|\psi_n{}^{(2)}\rangle + ...$$

$$= |n\rangle + \frac{q\varepsilon}{\omega}\sqrt{\frac{1}{2m\hbar\omega}}(\sqrt{n+1}|n+1\rangle - \sqrt{n}|n-1\rangle$$

where

$$|\psi_n{}^{(1)}\rangle = \sum_{k\neq n}\frac{|k\rangle\langle k|\hat{H}_1|n\rangle}{E_n^{(0)} - E_k^{(0)}}$$

$$= \frac{|n+1\rangle\langle n+1|\hat{H}_1|n\rangle}{E_n^{(0)} - E_{n+1}^{(0)}} + \frac{|n-1\rangle\langle n-1|\hat{H}_1|n\rangle}{E_n^{(0)} - E_{n-1}^{(0)}}$$

$$= -\frac{|n+1\rangle\langle n+1|\hat{H}_1|n\rangle}{\hbar\omega} + \frac{|n-1\rangle\langle n-1|\hat{H}_1|n\rangle}{\hbar\omega}$$

$$= \frac{q\varepsilon}{\omega}\sqrt{\frac{1}{2m\hbar\omega}}(\sqrt{n+1}|n+1\rangle - \sqrt{n}|n-1\rangle$$

REFERENCES

J.J. Sakurai and J. Napolitano, Modern Quantum Mechanics, 2nd edition (Pearson, 2011).
B.G. Englert, Lectures on Quantum Mechanics vol.2 Simple Systems (World Scientific, 2006).
J.M. Ziman Elements of Advanced Quantum Theory (Cambridge, 1969)

APPENDIX-II
Mathematica program

HermitianMatrixQ

`HermitianMatrixQ[m]`
tests whether *m* is a Hermitian matrix.

MORE INFORMATION

- `HermitianMatrixQ[m]` gives `True` if *m* is explicitly Hermitian, and gives `False` if it is a matrix that is not Hermitian.
- `HermitianMatrixQ[m]` is effectively equivalent to *m* `==` `ConjugateTranspose[m]`.
- `HermitianMatrixQ` works with `SparseArray` objects.
- `HermitianMatrixQ` works for symbolic as well as numerical matrices.

Eigensystem

`Eigensystem[`*m*`]`
gives a list {*values*, *vectors*} of the eigenvalues and eigenvectors of the square matrix *m*.

`Eigensystem[{`*m*, *a*`}]`
gives the generalized eigenvalues and eigenvectors of *m* with respect to *a*.

`Eigensystem[`*m*, *k*`]`
gives the eigenvalues and eigenvectors for the first *k* eigenvalues of *m*.

`Eigensystem[{`*m*, *a*`}, `*k*`]`
gives the first *k* generalized eigenvalues and eigenvectors.

MORE INFORMATION

- `Eigensystem` finds numerical eigenvalues and eigenvectors if *m* contains approximate real or complex numbers.
- For approximate numerical matrices *m*, the eigenvectors are normalized.
- All the non-zero eigenvectors given are independent. If the number of eigenvectors is equal to the number of non-zero eigenvalues, then corresponding eigenvalues and eigenvectors are given in corresponding positions in their respective lists.
- If there are more eigenvalues than independent eigenvectors, then each extra eigenvalue is paired with a vector of zeros. »
- `Eigensystem[`*m*`, ZeroTest -> `*test*`]` applies *test* to determine whether expressions should be assumed to be zero. The default setting is `ZeroTest -> Automatic`.
- The eigenvalues and eigenvectors satisfy the matrix equation `m.Transpose[`*vectors*`] == Transpose[`*vectors*`].DiagonalMatrix[`*values*`]`. »
- Generalized eigenvalues and eigenvectors satisfy `m.Transpose[`*vectors*`] == a.Transpose[`*vectors*`].DiagonalMatrix[`*values*`]`.
- {*vals*, *vecs*} = `Eigensystem[`*m*`]` can be used to set *vals* and *vecs* to be the eigenvalues and eigenvectors respectively. »
- `Eigensystem[`*m*, *spec*`]` is equivalent to applying `Take[…, `*spec*`]` to each element of `Eigensystem[`*m*`]`.
- The option settings `Cubics -> True` and `Quartics -> True` can be used to specify that explicit radicals should be generated for all cubics and quartics.
- `SparseArray` objects can be used in `Eigensystem`. »

Normalize

`Normalize[v]`
gives the normalized form of a vector *v*.

`Normalize[z]`
gives the normalized form of a complex number *z*.

`Normalize[expr, f]`
normalizes with respect to the norm function *f*.

MORE INFORMATION

- `Normalize[v]` is effectively *v* / `Norm[v]`, except that zero vectors are returned unchanged.
- Except in the case of zero vectors, `Normalize[v]` returns the unit vector in the direction of *v*.
- For a complex number *z*, `Normalize[z]` returns *z* / `Abs[z]`, except that `Normalize[0]` gives `0`.
- `Normalize[expr, f]` is effectively *expr* / *f*[*expr*], except when there are zeros in *f*[*expr*].

Orthogonalize

Orthogonalize[{v_1, v_2, …}]
gives an orthonormal basis found by orthogonalizing the vectors v_i.

Orthogonalize[{e_1, e_2, …}, f]
gives a basis for the e_i orthonormal with respect to the inner product function f.

MORE INFORMATION

- Orthogonalize[{v_1, v_2, …}] uses the ordinary scalar product $\overline{v_1}.v_2$ as an inner product.
- The output from Orthogonalize always contains the same number of vectors as the input. If some of the input vectors are not linearly independent, the output will contain zero vectors.
- All nonzero vectors in the output are normalized to unit length.
- The inner product function f is applied to pairs of linear combinations of the e_i.
- The e_i can be any expressions for which f always yields real results.
- Orthogonalize[{v_1, v_2, …}, Dot] effectively assumes that all elements of the v_i are real.
- Orthogonalize by default generates a Gram-Schmidt basis.
- Other bases can be obtained by giving alternative settings for the Method option. Possible settings include: "GramSchmidt", "ModifiedGramSchmidt", "Reorthogonalization" and "Householder".
- Orthogonalize[*list*, Tolerance -> t] sets to zero elements whose relative norm falls below t.

Transpose

`Transpose[list]`
transposes the first two levels in *list*.

`Transpose[list, {n1, n2, …}]`
transposes *list* so that the k^{th} level in *list* is the $n_k{}^{th}$ level in the result.

MORE INFORMATION

- `Transpose` gives the usual transpose of a matrix.
- `Transpose[m]` can be input as $m^{\top}$.
- $^{\top}$ can be entered as Esc tr Esc or `\[Transpose]`.
- Acting on a tensor $T_{i_1 i_2 i_3 \ldots}$ `Transpose` gives the tensor $T_{i_2 i_1 i_3 \ldots}$. »
- `Transpose[list, {n1, n2, …}]` gives the tensor $T_{i_{n_1} i_{n_2} \ldots}$.
- So long as the lengths of the lists at particular levels are the same, the specifications n_k do not necessarily have to be distinct.
- `Transpose` works on `SparseArray` objects.
