Wigner - Brillouin perturbation theory

recall our previous work

$$\hat{H}|n\rangle = E_n|n\rangle$$

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

$$\hat{H}_0|n\rangle_0 = E_n^0|n\rangle_0$$

write $\hat{H}|n\rangle = E_n|n\rangle$ as

$$(E_n - \hat{H}_0)|n\rangle = \hat{V}|n\rangle$$

define $\hat{P}_n = |n\rangle_0\,{}_0\langle n|$ $\quad \hat{Q}_n = 1 - \hat{P}_n$ as before

Now recall $\hat{Q}_n|n\rangle = \dfrac{\hat{Q}_n}{E_n - \hat{H}_0}\hat{V}|n\rangle$ caveat - $\hat{Q}_n$ protects $\dfrac{1}{E_n - \hat{H}_0}$ only when $\hat{V} = 0$

since $|n\rangle = (\hat{P}_n + \hat{Q}_n)|n\rangle = \hat{P}_n|n\rangle + \dfrac{\hat{Q}_n}{E_n - \hat{H}_0}\hat{V}|n\rangle$

~~multiply by ${}_0\langle n|$~~

$$\cancel{{}_0\langle n|}\left(1 - \frac{\hat{Q}_n}{E_n - \hat{H}_0}\hat{V}\right)|n\rangle = \hat{P}_n|n\rangle = |n\rangle_0 \underbrace{{}_0\langle n|n\rangle}_{=1}$$

$$\text{So } |n\rangle = \left[1 - \frac{\hat{Q}_n}{E_n - \hat{H}_0}\hat{V}\right]^{-1}|n\rangle_0$$

$$= |n\rangle_0 + \frac{\hat{Q}_n}{E_n - \hat{H}_0}\hat{V}|n\rangle_0 + \frac{\hat{Q}_n}{E_n - \hat{H}_0}\hat{V}\frac{\hat{Q}_n}{E_n - \hat{H}_0}\hat{V}|n\rangle_0 + \cdots$$

To find E_n, multiply $(E_n - \hat{H}_0)|n\rangle = \hat{V}|n\rangle$ by ${}_0\langle n|$

$$E_n - E_n^0 = {}_0\langle n|\hat{V}|n\rangle$$

So we get

$$E_n = E_n^0 + {}_0\langle n|\hat{V}|n\rangle_0 + {}_0\langle n|\hat{V}\frac{\hat{Q}}{E_n-\hat{H}_0}\hat{V}|n\rangle_0 + \cdots$$

$$E_n = E_n^0 + V_{nn} + \sum_{m\neq n}\frac{V_{nm}V_{mn}}{E_n-E_m^0} + \cdots$$

Note E_n appears on RHS and LHS. $\Rightarrow$ This creates a new equation for E_n

But the series is much simpler than for the non degenerate case and we did not need to assume that the system was non degenerate.

On the down side, it often is less accurate than R-S perturbation theory.

The full series for $|n\rangle$ becomes

$$|n\rangle = \sum_{m=0}^{\infty}\left(\frac{\hat{Q}}{E_n-\hat{H}_0}\hat{V}\right)^m |n\rangle_0$$

$$E_n = E_n^0 + V_{nn} + \sum_{m\neq n}\frac{V_{nm}V_{mn}}{E_n-E_m^0} + \sum_{m\neq n}\sum_{m'\neq n}\frac{V_{nm}V_{mm'}V_{m'n}}{(E_n-E_m^0)(E_n-E_{m'}^0)}$$

$$+\cdots+\sum_{m_1\neq n}\sum_{m_2\neq n}\cdots\sum_{m_\ell\neq n}\frac{V_{nm_1}V_{m_1m_2}V_{m_2m_3}\cdots V_{m_{\ell-1}m_\ell}V_{m_\ell n}}{(E_n-E_{m_1}^0)(E_n-E_{m_2}^0)\cdots(E_n-E_{m_\ell}^0)}$$

example:

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}K\hat{x}^2 \qquad \hat{V} = c\hat{x}$$

exact solution

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}K\hat{x}^2 + c\hat{x} = \frac{\hat{p}^2}{2m} + \frac{1}{2}K\left(\hat{x} + \frac{c}{K}\right)^2 - \frac{c^2}{2K}$$

define $\hat{x}' = \hat{x} + \frac{c}{K} \qquad [\hat{x}', \hat{p}] = i\hbar$

so $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}K\hat{x}'^2 - \frac{c^2}{2K}$

$$\Rightarrow \boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{c^2}{2K}}$$

The energy is shifted to second order only!

$$c\hat{x} = c\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^+ + \hat{a}\right)$$

$$V_{nn} = \langle n | c\hat{x} | n \rangle = 0$$

$V_{nm} = 0$ except $m = n \pm 1$

$$V_{n\,n+1} = c\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n+1} \qquad E_n^0 - E_{n+1}^0 = -\hbar\omega$$

$$V_{n\,n-1} = c\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n} \qquad E_n^0 - E_{n-1}^0 = \hbar\omega$$

Rayleigh-Schrodinger

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) + 0 + \frac{|V_{n\,n+1}|^2}{E_n^0 - E_{n+1}^0} + \frac{|V_{n\,n-1}|^2}{E_n^0 - E_{n-1}^0} =$$

$$= \hbar\omega\left(n + \frac{1}{2}\right) + c^2\frac{\hbar}{2m\omega}\frac{1}{\hbar\omega}\left(-(n+1) + n\right) = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{c^2}{2m\omega^2}$$

so

$$E_n = \hbar\omega\left(n+\tfrac{1}{2}\right) - \frac{c^2}{2k} \quad \checkmark$$

as a check, look at the third-order correction

$$\Delta E_n^{(3)} = \sum_m{}' \sum_{m'}{}' \frac{V_{nm}V_{mm'}V_{m'n}}{(E_n^0 - E_m^0)(E_n^0 - E_{m'}^0)} - V_{nn} \sum_m{}' \frac{|V_{nm}|^2}{(E_n^0 - E_m^0)^2}$$

but $V_{nn} = 0$ and

$V_{nm}V_{mm'}V_{m'n} = 0$ since $m = n \pm 1$

$m' = n \pm 1$

in all cases $V_{mm'} = 0$

so $\Delta E_n^{(3)} = 0$ similarly, all $\Delta E_n^{(m)} = 0$ for $m \geq 3$

~~Rayleigh Schrodinger~~

Wigner-Brillouin

$$E_n = \hbar\omega\left(n+\tfrac{1}{2}\right) + 0 + c^2 \frac{\hbar}{2m\omega}\left[\frac{n+1}{E_n - \hbar\omega(n+\frac{3}{2})} + \frac{n}{E_n - \hbar\omega(n-\frac{1}{2})}\right]$$

multiply by $\left(E_n - \hbar\omega(n+\tfrac{3}{2})\right)\left(E_n - \hbar\omega(n-\tfrac{1}{2})\right)$ to get

$$E_n\left(E_n - \hbar\omega(n+\tfrac{3}{2})\right)\left(E_n - \hbar\omega(n-\tfrac{1}{2})\right) = \hbar\omega\left(n+\tfrac{1}{2}\right)\left(E_n - \hbar\omega(n+\tfrac{3}{2})\right)\left(E_n - \hbar\omega(n-\tfrac{1}{2})\right)$$

$$+ \frac{c^2\hbar}{2m\omega}\left[(n+1)\left(E_n - \hbar\omega(n-\tfrac{1}{2})\right) + n\left(E_n - \hbar\omega(n+\tfrac{3}{2})\right)\right]$$

$$E_n^3 + E_n^2\left[-\hbar\omega(2n+1) - \hbar\omega\left(n+\tfrac{1}{2}\right)\right] + E_n\left[(\hbar\omega)^2\left(n^2+n-\tfrac{3}{4}+2n^2+2n+\tfrac{1}{2}\right) - \frac{c^2\hbar}{2m\omega}(2n+1)\right]$$

$$-(\hbar\omega)^3\left(n^3+\tfrac{3}{2}n^2-\tfrac{1}{4}n-\tfrac{3}{8}\right) + \frac{c^2\hbar}{2m\omega}\hbar\omega\left(n^2+\tfrac{1}{2}n-\tfrac{1}{2}+n^2+\tfrac{3}{2}n\right) = 0$$

$$E_n^3 + E_n^2\left[-\hbar\omega\left(3n+\tfrac{3}{2}\right)\right] + E_n\left[(\hbar\omega)^2\left(3n^2+3n-\tfrac{1}{4}\right) - \frac{c^2\hbar}{2m\omega}(2n+1)\right]$$
$$-(\hbar\omega)^3\left[n^3+\tfrac{3}{2}n^2-\tfrac{1}{4}n-\tfrac{3}{8}\right) + \frac{c^2\hbar^2}{2m}\left(2n^2+2n-\tfrac{1}{2}\right) = 0$$

this should factorize if it gives the exact answer

but

$$\left(E_n - \hbar\omega\left(n+\tfrac{1}{2}\right) + \frac{c^2}{2m\omega^2}\right)\left(E_n^2 + E_n\left(-\hbar\omega(2n+1) - \frac{c^2}{2m\omega^2}\right)\right.$$
$$\left. + (\hbar\omega)^2\left(n^2+n-\tfrac{3}{4}\right) - \frac{c^2\hbar}{2m\omega}\left(n+\tfrac{1}{2}\right) + \frac{c^4}{(2m\omega^2)^2}\right)$$

which is off by an extra term $\dfrac{c^6}{(2m\omega^2)^3}$

$\Rightarrow$ result will have an error $O\left(\dfrac{c^6}{(2m\omega^2)^3}\right)$

also note we have 3 roots not one

$\Rightarrow$ some roots of W-B PT are unphysical.

In general, one often finds W-B PT is less accurate than Rayleigh-Schroedinger PT as shown here.

$\Rightarrow$ higher order terms must contribute to cancel extra terms and ultimately give us the exact answer.

check $n=0$ energy

$$E_0 = \frac{\hbar\omega}{2} + \frac{c^2\hbar}{2m\omega}\,\frac{1}{E_0 - \frac{3}{2}\hbar\omega}$$

$$E_0^2 - E_0\,\tfrac{3}{2}\hbar\omega = \frac{\hbar\omega}{2}\left(E_0 - \tfrac{3}{2}\hbar\omega\right) + \frac{c^2\hbar}{2m\omega}$$

$$E_0^2 - E_0\,2\hbar\omega + \tfrac{3}{4}(\hbar\omega)^2 - \frac{c^2\hbar}{2m\omega} = 0$$

$$E_0 = \hbar\omega \pm \tfrac{1}{2}\sqrt{4(\hbar\omega)^2 - 3(\hbar\omega)^2 + \frac{2c^2\hbar}{m\omega}}$$

$$= \hbar\omega \pm \tfrac{1}{2}\sqrt{(\hbar\omega)^2 + \frac{2c^2\hbar}{m\omega}}$$

take $-$ root

$$= \hbar\omega - \tfrac{1}{2}\hbar\omega\sqrt{1 + 2\frac{c^2}{K}\,\frac{1}{\hbar\omega}}$$

$$= \hbar\omega - \tfrac{1}{2}\hbar\omega\left(1 + \frac{c^2}{K}\,\frac{1}{\hbar\omega} - \frac{4}{8}\left(\frac{c^2}{K}\,\frac{1}{\hbar\omega}\right)^2 + \cdots\right)$$

$$= \tfrac{1}{2}\hbar\omega - \frac{c^2}{2K} + \frac{1}{4}\,\frac{c^4}{K^2}\,\frac{1}{\hbar\omega} + \cdots$$

note the error at order V^4 !