Phys 506 lecture 15: Wigner-Brillouin perturbation theory

1 Formalism for the series for the perturbed states

Recall from our previous work that we wish to solve the general energy eigenvalue problem with $\hat{H}|n\rangle = E_n|n\rangle$, with the Hamiltonian able to be proken into an unperturbed and perturbed part via $\hat{H} = \hat{H}_0 + \hat{V}$, and the unperturbed energy eigenvalue problem is given by $\hat{H}_0|n\rangle_0 = E_n^0|n\rangle_0$. This implies that $\hat{H}|n\rangle = E_n|n\rangle$ can be written as

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

Therefore, let's define, as before the two following projection operators (onto and perpendicular to the unperturbed ground state):

$$\hat{P}_n|n\rangle_0\,{}_0\langle n| \text{ and } \hat{Q}_n = 1 - \hat{P}_n.$$

Now recall that we previously found that

$$\hat{Q}_n|n\rangle = \frac{\hat{Q}_n}{E_n - \hat{H}_0}\hat{V}|n\rangle.$$

However, beware that there is a caveat to this—namely that $\hat{Q}_n$ projects $\frac{1}{E_n - \hat{H}_0}$ perpendicular to the unperturbed ground state only when $\hat{V} = 0$, because the denominator has an E_n in it instead of an $E_N^{(0)}$. Now note that:

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

So we write:

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

using the same normalization as we did before. Then we have that

$$|n\rangle = \left[1 - \frac{\hat{Q}_n\hat{V}}{E_n - \hat{H}_0}\right]^{-1}|n\rangle_0 = |n\rangle_0 + \frac{\hat{Q}_n\hat{V}}{E_n - \hat{H}_0}|n\rangle_0 + \frac{\hat{Q}_n\hat{V}\hat{Q}_n\hat{V}}{(E_n - \hat{H}_0)^2}|n\rangle_0 + \cdots$$

2 Formalism to find the perturbed energy

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

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

So we find that

$$\begin{aligned} E_n &= E_n^{(0)} + {}_0\langle n|\hat{V}|n\rangle_0 + {}_0\langle n|\hat{V}\frac{\hat{Q}_n}{E_n - \hat{H}_0}\hat{V}|n\rangle_0 + \cdots \\ &= E_n^{(0)} + V_{nn} + \sum_{m\neq n}\frac{V_{nm}V_{mn}}{E_n - E_m^{(0)}} + \cdots \end{aligned}$$

Note that E_n appears on both the RHS and LHS. This generates 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 downside, it is often less accurate than Rayleigh-Schrödinger perturbation theory. The full series for $|n\rangle$ becomes:

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

For E_n, we have:

$$\begin{aligned} E_n =& E_n^{(0)} + V_{nn} + \sum_{m\neq n}\frac{V_{nm}V_{mn}}{E_n - E_m^{(0)}} + \sum_{m\neq n}\sum_{m'\neq n}\frac{V_{nm}V_{mm'}V_{m'n}}{(E_n - E_m^{(0)})(E_n - E_{m'}^{(0)})} + \cdots \\ &+ \sum_{m_1\neq n}\sum_{m_2\neq n}\cdots\sum_{m_\ell\neq n}\frac{V_{nm_1}V_{m_1m_2}V_{m_2m_3}\cdots V_{m_{\ell-1}m_\ell}V_{m_\ell n}}{(E_n - E_{m_1}^{(0)})(E_n - E_{m_2}^{(0)})\cdots(E_n - E_{m_\ell}^{(0)})}. \end{aligned}$$

This leads to a high-order polynomial equation for E_n. Usually, only one root is the physical root in this polynomial equation.

3 Example: Shifting the simple harmonic oscillator

Let's consider an example to see this process in action. Consider the following one-dimensional Hamiltonian:

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

where $\hat{V} = c\hat{x}$. This corresponds to a linear shift of the harmonic-oscillator Hamiltonian. The full Hamiltonian is then:

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

Now, define $\hat{x}' = \hat{x} + \frac{c}{k}$ to find that

$$[\hat{x}', \hat{p}] = i\hbar$$

and

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

and we get that

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

This means the energy is shifted to second order only!

Now, we calculate energies with perturbation theory. First we determine all of the quantities we will need. We rewrite $\hat{V}$ as $\hat{V} = c\hat{x} = c\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right)$. Then, we find that $V_{nn} = \langle n|c\hat{x}|n\rangle = 0$, $V_{mn} = 0$ unless $m = n \pm 1$. Then, we have that

$$V_{n,n+1} = c\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n+1} \text{ and } V_{n,n-1} = c\sqrt{\frac{\hbar}{2m\omega}}\sqrt{n}.$$

We also have that $E_n^{(0)} - E_{n+1}^{(0)} = -\hbar\omega$ and $E_n^{(0)} - E_{n-1}^{(0)} = \hbar\omega$.

3.1 Rayleigh-Schrödinger perturbation theory

We now compute the Rayleigh-Schrödinger perturbation theory:

$$\begin{aligned}
E_n &= \hbar\omega\left(n + \frac{1}{2}\right) + 0 + \frac{|V_{n,n+1}|^2}{E_n^{(0)} - E_{n+1}^{(0)}} + \frac{|V_{n,n-1}|^2}{E_n^{(0)} - E_{n-1}^{(0)}} \\
&= \hbar\omega\left(n + \frac{1}{2}\right) + \frac{c^2}{2m\omega}\frac{\hbar}{\hbar\omega}\left(-(n+1) + n\right) \\
&= \hbar\omega\left(n + \frac{1}{2}\right) - \frac{c^2}{2m\omega^2}.
\end{aligned}$$

Hence, $E_n = \hbar\omega(n + \frac{1}{2}) - \frac{c^2}{2k}$. This agrees with the exact answer.

As a further check, let's 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 $m = n \pm 1$ and $m' = n \pm 1$ in all cases implies that we must also have that $V_{mm'} = 0$. Thus, $\Delta E_n^{(3)} = 0$ and similarly for all $m \geq 3$, we have $\Delta E_n^{(m)} = 0$.

3.2 Wigner-Brillouin perturbation theory

Let's now turn to Wigner-Brillouin perturbation theory. Here we have:

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

Multiply by $(E_n - \hbar\omega(n+\frac{3}{2}))(E_n - \hbar\omega(n-\frac{1}{2}))$ to get:

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

Expanding, we find that

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

Simplifying, we find that

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

This should factorize if it gives the exact answer. But, we have that

$$\begin{aligned} &\left(E_n - \hbar\omega\left(n+\frac{1}{2}\right) + \frac{c^2}{2m\omega^2}\right) \\ &\quad\times\left(E_n^2 + E_n\left[-\hbar\omega(2n+1) - \frac{c^2}{2m\omega^2}\right]\right. \\ &\qquad\left. + (\hbar\omega)^2\left(n^2+n-\frac{3}{4}\right) - \frac{c^2\hbar}{2m\omega}\left(n+\frac{1}{2}\right) + \frac{c^4}{(2m\omega^2)^2}\right) \end{aligned}$$

is off by an extra term $\frac{c^6}{(2m\omega^2)^3}$, which means that the result will have an error of order $\mathcal{O}\left(\frac{c^6}{(2m\omega^2)^3}\right)$. Also note that we have 3 roots, not one. This means that some roots ofthe Wigner-Brillouin perturbation theory are unphysical. In general, one often finds that Wigner-Brillouin perturbation theory is less accurate than Rayleigh-Schrödinger perturbation theory, as shown here, which further implies that higher order terms must contribute to cancel extra terms and ultimately give us the exact answer.

3.3 Special case of $n = 0$

Lastly, let's check the energy for $n = 0$, where we can solve the polynomial equation exactly:

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

This then becomes

$$\begin{aligned} E_0^2 - E_0 \cdot \frac{3}{2}\hbar\omega = \hbar\omega\left(E_0 - \frac{3}{2}\hbar\omega\right) + \frac{c^2\hbar}{2m\omega}, \\ 0 = E_0^2 - E_0 \cdot 2\hbar\omega + \frac{3}{4}(\hbar\omega)^2 - \frac{c^2\hbar}{2m\omega}, \end{aligned}$$

The solutions are

$$\begin{aligned} E_0 &= \hbar\omega + \frac{1}{2}\sqrt{4(\hbar\omega)^2 - 3(\hbar\omega)^2 + \frac{2c^2\hbar}{m\omega}}, \\ &= \hbar\omega \pm \frac{1}{2}\sqrt{(\hbar\omega)^2 + \frac{2c^2\hbar}{m\omega}}. \end{aligned}$$

Now take the root:

$$\begin{aligned} E_0 &= \hbar\omega - \frac{1}{2}\hbar\omega\sqrt{1 + \frac{2c^2}{k\hbar\omega}} \\ &= \hbar\omega - \frac{1}{2}\hbar\omega\left(1 + \frac{c^2}{k\hbar\omega} - \frac{4}{8}\left(\frac{c^2}{k\hbar\omega}\right)^2 + \cdots\right) \\ &= -\frac{1}{2}\hbar\omega - \frac{c^2}{2k} + \frac{1}{4}\frac{c^4}{k^2\hbar\omega} + \cdots \end{aligned}$$

Note the error that we have at order V^4! This will be canceled by higher-order terms.