Shankar 16.1.3

Trial function of $\psi(x) = e^{-\alpha x^2/2}$

for attractive delta function potential $V = -aV_0\delta(x)$

$$E(\alpha) = \frac{\int_{-\infty}^{\infty} e^{-\alpha x^2/2}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - aV_0\delta(x)\right)e^{-\alpha x^2/2}\,dx}{\int_{-\infty}^{\infty} e^{-\alpha x^2}\,dx}$$

$$= \frac{-\frac{\hbar^2}{2m}\left(-\frac{1}{2}\sqrt{\alpha}\sqrt{\pi}\right) - aV_0}{\sqrt{\frac{\pi}{\alpha}}}$$

$E(\alpha) = \frac{\hbar^2}{4m}\alpha - \frac{aV_0}{\sqrt{\pi}}\alpha^{1/2}$. Now minimize energy.

$$0 = \frac{dE}{d\alpha} = \frac{\hbar^2}{4m} - \frac{aV_0}{2\sqrt{\pi}}\frac{1}{\alpha_0^{1/2}}$$

$\alpha_0 = \frac{4m^2a^2V_0^2}{\hbar^4\,\pi}$ Plug back into $E(\alpha)$ to obtain energy:

$$E(\alpha_0) = \frac{\hbar^2}{4m}\left(\frac{4m^2a^2V_0^2}{\hbar^4\pi}\right) - \frac{aV_0}{\sqrt{\pi}}\left(\frac{2maV_0}{\hbar^2\sqrt{\pi}}\right)$$

$$E(\alpha_0) = -\frac{a^2V_0^2m}{\hbar^2\pi} > -\frac{a^2V_0^2m}{2\hbar^2}$$

gaussian estimate energy — exact bound state energy

Shankar 17.2.1 a) Consider $H' = \lambda x^4$ for the oscillator. Calculate E_n'

$$E_n' = \langle n^0 | H' | n^0 \rangle$$

Recall $x = \sqrt{\frac{\hbar}{2m\omega}}(a+a^\dagger)$, so $\lambda x^4 = \frac{\lambda \hbar^2}{4m^2\omega^2}(a+a^\dagger)^2(a+a^\dagger)^2$

Thus $E_n' = \frac{\lambda\hbar^2}{4m^2\omega^2}\langle n|(a+a^\dagger)^2 \cdot (a+a^\dagger)^2|n\rangle$

Let's split the inner product in two and evaluate: $(a+a^\dagger)^2|n\rangle$ and $\langle n|(a+a^\dagger)^2$ seperately...

$$(a+a^\dagger)^2|n\rangle = \sqrt{n(n-1)}\,|n-2\rangle + (2n+1)|n\rangle + \sqrt{(n+1)(n+2)}\,|n+2\rangle$$

simmilarly,

$$\langle n|(a+a^\dagger)^2 = \sqrt{n(n-1)}\,\langle n-2| \quad (2n+1)\langle n| + \sqrt{(n+1)(n+2)}\,\langle n+2|$$

Putting the inner product back together and taking advantage of orthogonality;

$$E_n' = \frac{\lambda\hbar^2}{4m^2\omega^2}\left(n(n-1) + (2n+1)^2 + (n+1)(n+2)\right)$$

$$E_n' = \frac{3\lambda\hbar^2}{4m^2\omega^2}\left(1 + 2n + 2n^2\right)$$

b) Recall that $E_n^0 = \hbar\omega(n+\frac{1}{2})$

The zeroth order energy (unperturbed) goes like n^1.
The first order energy correction goes like n^2.
Thus, regardless of the smallness of λ, for some large enough n, the higher order energies increase and pertubation theory fails. Physically, at high n's, the particle has a higher probability of being found at large x's so λx^4 is no longer a small pertubation

Shankar 17.2.4) Prove Thomas-Reiche-Kuhn sum rule.

$$\sum_{n'}(E_{n'}-E_n)|\langle n'|X|n\rangle|^2=\frac{\hbar^2}{2m}$$

We write the left hand side as

$$\sum_{n'}(E_{n'}-E_n)\langle n|X|n'\rangle\langle n'|X|n\rangle$$

$$=\sum_{n'}\left[\langle n|X|n'\rangle\langle n'|\quad X|n\rangle-\langle n|H\ X|n'\rangle\langle n'|X|n\rangle\right]$$

Eliminating the complete set of states,

$$=\langle n|X\,H\,X|n\rangle-\langle n|H\,X\,X|n\rangle$$

$$=-\langle n|[HX,X]|n\rangle \quad ①$$

Alternatively, if we switch where we place E_n

$$=\sum_{n'}[\langle n|X|n'\rangle\langle n'|HX|n\rangle-\langle n|X|n'\rangle\langle n'|XH\rangle$$

we obtain

$$=-\langle n|[X,XH]|n\rangle \quad ②$$

Since ① and ② are equal, their average is nothing but themself.

$$=-\tfrac{1}{2}([HX,X]+[X,XH]$$

$$=-\tfrac{1}{2}([[H,X],X]).$$ We are left to evaluate this commutator.

Shankar 17.2.4) Prove Thomas-Reiche-Kuhn sum rule.

$$\sum_{n'}(E_{n'}-E_n)|\langle n'|X|n\rangle|^2 = \frac{\hbar^2}{2m}$$

We write the left hand side as

$$\sum_{n'}(E_{n'}-E_n)\langle n|X|n'\rangle\langle n'|X|n\rangle$$

$$= \sum_{n'}\left[\langle n|X|n'\rangle\langle n'| \quad X|n\rangle - \langle n|H \quad X|n'\rangle\langle n'|X|n\rangle\right]$$

Eliminating the complete set of states,

$$= \langle n|X H X|n\rangle - \langle n|H X X|n\rangle$$

$$= -\langle n|[HX, X]|n\rangle \quad (1)$$

Alternatively, if we switch where we place E_n

$$= \sum_{n'}[\langle n|X|n'\rangle\langle n'|HX|n\rangle - \langle n|X|n'\rangle\langle n'|XH\rangle$$

we obtain

$$= -\langle n|[X, XH]|n\rangle \quad (2)$$

Since (1) and (2) are equal, their average is nothing but themself.

$$= -\tfrac{1}{2}([HX, X] + [X, XH]$$

$$= -\tfrac{1}{2}([[H,X],X]).$$ We are left to evaluate this commutator.

Shankar (17.2.4 cont) $[H, X] = \left[\frac{P^2}{2m}, X\right] + \left[V(x), X\right]^{\to 0}$

$$= -\frac{\hbar^2}{m}\frac{d}{dx}$$

and then

$$[[H, X], X] = -\frac{\hbar^2}{m}$$

so

$$= -\frac{1}{2}([[H, X], X]) = \frac{\hbar^2}{2m}. \quad QED.$$

(4a) $\hat{H}_0 = \frac{\hat{P}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 \qquad \hat{H}' = \kappa\hat{x}^2$

Define ω' such that $\left(\frac{m\omega^2}{2} + \kappa\right) \equiv \frac{m\omega'^2}{2}$

$$\Rightarrow \omega'^2 = \omega^2 + \frac{2\kappa}{m}$$

$$\omega' = \sqrt{\omega^2 + \frac{2\kappa}{m}}$$

So full Hamiltonian is $\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega'^2\hat{x}^2$, and this is ~~simply~~ a harmonic oscillator.

So $E_n = \left(n + \frac{1}{2}\right)\hbar\omega'$.

(4b) $E_n^{(1)} = \langle n^{(0)}|\hat{H}'|n^{(0)}\rangle$

$$= \kappa\langle n^{(0)}|\hat{x}^2|n^{(0)}\rangle$$

$$= \kappa\frac{\hbar}{2m\omega}\langle n^{(0)}|(\hat{a} + \hat{a}^\dagger)^2|n^{(0)}\rangle$$

$$= \kappa\frac{\hbar}{2m\omega}\langle n^{(0)}|(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})|n^{(0)}\rangle$$

$$= \kappa\frac{\hbar}{2m\omega}\left[(n+1)^2 + (n)^2\right]\langle n^{(0)}|n^{(0)}\rangle$$

$$= \kappa\frac{\hbar}{2m\omega}\left(3n^2 + 2n + 1\right)$$

$$= \kappa\frac{\hbar}{2m\omega} \quad \text{for ground state } (n=0).$$

Compare to exact:

Expand E_0 to first order in κ:

$$E_0 = \frac{1}{2}\hbar\sqrt{\omega^2 + \frac{2\kappa}{m}} = \frac{1}{2}\hbar\omega\left(1 + \frac{2\kappa}{m\omega^2}\right)^{\frac{1}{2}} \approx \frac{1}{2}\hbar\omega\left(1 + \frac{\kappa}{m\omega^2}\right)$$

$$= E_0^{(0)} + \frac{\kappa\hbar}{2m\omega} = E_0^{(0)} + E_0^{(1)} \text{ from perturbation theory.}$$

(5) Liboff 13.4

$$E_2^{(0)} = \langle 2^{(0)} | \hat{H}_0 | 2^{(0)} \rangle = \frac{2\hbar^2\pi^2}{mL^2}$$

$$E_2^{(1)} = \langle 2^{(0)} | \hat{H}' | 2^{(0)} \rangle = \int_{-\frac{a}{2}}^{\frac{a}{2}} dx\, \psi_2^{(0)*}(x)\, V_0\, \psi_2^{(0)}(x) = V_0 \int_{-\frac{a}{2}}^{\frac{a}{2}} dx \left[\frac{2}{L} \sin^2\left(\frac{2\pi x}{L}\right)\right]$$

Take $\xi = \frac{2\pi x}{L}$

$$= \frac{2V_0}{L} \int_{-\frac{a\pi}{L}}^{\frac{a\pi}{L}} \frac{L}{2\pi} \sin^2\xi\, d\xi = \frac{V_0}{\pi} \left[\frac{1}{2}\xi - \frac{1}{4}\sin 2\xi\right]_{-\frac{a\pi}{L}}^{\frac{a\pi}{L}}$$

$$= \frac{V_0}{\pi}\left(\frac{a\pi}{L} - \frac{1}{2}\sin\frac{2a\pi}{L}\right)$$

(b) Small correction if $\frac{a\pi}{L}$ is small.

(c) even parity (odd n) eigenstates have peaks in their probability density at the origin – i.e. they "see" more of the perturbation than do the odd parity states (which go to zero in the vicinity of the perturbation.)