(35) Approximate the ground state energy of the simple harmonic oscillator by using a trial wave fcn ($^{w/}$ A = const): $\phi(x) = A[1-(|x|/\alpha)]$, for $|x| \leq \alpha$, and $\phi(x) \equiv 0$, for $|x| > \alpha$. Find the energy corresponding to this ϕ, and -- for optimum α -- show that it lies not more than 10% above the exact value $E_0 = \frac{1}{2}\hbar\omega$.

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(36) A QM system has Hamiltonian $\mathcal{H}$, and eigenfcns Ψ_n & eigenenergies E_n, i.e. $\mathcal{H}\Psi_n = E_n \Psi_n$. To estimate the ground state energy E_0, use a trial fcn: $\underline{\underline{\Psi = \Psi_0 + \lambda\phi}}$, $^{w/}$ Ψ_0 = actual ground state wavefcn (not known), λ = small (real) parameter, and ϕ is an arbitrary fcn with expansion $\phi = \sum_n c_n \Psi_n$ ($\lambda\phi$ measures how far Ψ differs from Ψ_0). Show that if the approximate (variational) energy: $E(\lambda) = \langle\Psi|\mathcal{H}|\Psi\rangle / \langle\Psi|\Psi\rangle$, is expanded in a power series in λ: $\underline{\underline{E(\lambda) = E_0 + \lambda\mathcal{E}_1 + \lambda^2\mathcal{E}_2 + \lambda^3\mathcal{E}_3 + \ldots}}$, then $\mathcal{E}_1 = 0$, while $\mathcal{E}_2 = \sum_n |c_n|^2 (E_n - E_0) > 0$. <u>CONCLUSION</u>: any system perturbation shifting $\Psi_0 \to \Psi_0 + \lambda\phi$ by a term of $O(\lambda)$, will shift $E_0 \to E_0 + \lambda^2\mathcal{E}_2$ by <u>smaller</u> $O(\lambda^2)$ terms.

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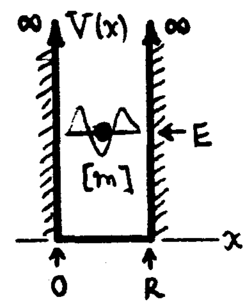
(37) For the well at right, the normalized eigenfcns (from prob.^m (34)) are: $\underline{\underline{\Psi_n(x) = \sqrt{2/R}\,\sin(n\pi x/R)}}$, $n = 1, 2, 3, \ldots$. And the energies E_n = ?.



(A) Show the $\Psi_n(x)$ are linearly <u>independent</u> and mutually <u>orthogonal</u>.

(B) Show the $\{\Psi_n(x)\}$ are a <u>complete</u> set for the expansion of any fcn $\Psi(x)$ obeying the same boundary conditions on $0 \leq x \leq R$ (viz. $\Psi(0) = 0 = \Psi(R)$), by proving closure: $\underline{\underline{\sum_n \Psi_n^*(x)\Psi_n(x') = \delta(x - x')}}$. HINT: consider the Fourier series expansion of $\delta(x - x')$ on the interval, $^{w/}$ $0 < x, x' < R$.

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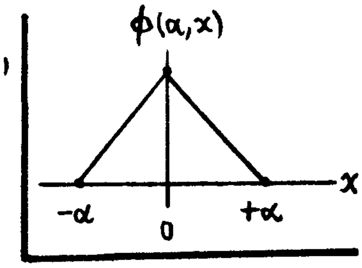
(38) Mass m is in the ground state $\Psi_0(x)$ of a SHO potential $V(x) = \frac{1}{2} m\omega^2 x^2$. Expand $\Psi_0(x)$ in terms of 1D free particle (momentum) eigenfcns $\phi_k(x)$, in the form $\int c(k)\phi_k(x)\,dk$. Find the spectrum fcn $c(k)$, and verify that $\int |c(k)|^2\,dk = 1$. What is the probability of finding m with a momentum <u>exceeding</u> the maximum classical value $p_0 = \sqrt{2mE_0}$, $^{w/}$ $E_0 = \frac{1}{2}\hbar\omega$ is the total energy in the state?

ϕ506 Solutions

(35) Estimate SHO groundstate energy w/ trial wavefcn: $\phi(\alpha,x) = A[1-(|x|/\alpha)]$.



1. A & α = cnsts, and: $\phi(\alpha,x) = A[1-(|x|/\alpha)]$ for $|x| \leq \alpha$; $\phi \equiv 0$, otherwise. Normalization integral is...

$u = x/\alpha$.

$$\rightarrow \langle\phi|\phi\rangle = A^2 \int_{-\alpha}^{+\alpha} \left(1-\frac{|x|}{\alpha}\right)^2 dx = 2\alpha A^2 \int_0^1 (1-u)^2 du$$

$$\text{so } \langle\phi|\phi\rangle = \tfrac{2}{3}\alpha A^2 = 1 \Rightarrow \underline{\underline{A^2 = 3/2\alpha}}. \qquad (1)$$

---

2. The SHO Ham^n is; $\mathcal{H}(\text{SHO}) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$, where m = SHO mass and ω is its natural freq. Then, with value of A in Eq. (1), the energy for ϕ is

$$\rightarrow E(\alpha) = \langle\phi|\mathcal{H}(\text{SHO})|\phi\rangle = \frac{3}{2\alpha}\int_{-\alpha}^{+\alpha}\left(1-\frac{|x|}{\alpha}\right)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right]\left(1-\frac{|x|}{\alpha}\right)dx. \qquad (2)$$

To evaluate $E(\alpha)$, we need to notice that $\frac{d^2}{dx^2}|x|$ generates a δ-fcn. Because...

$$\int_{-\epsilon}^{+\epsilon}\left(\frac{d^2}{dx^2}|x|\right)dx = \int_{-\epsilon}^{+\epsilon}\frac{d}{dx}\left(\frac{d|x|}{dx}\right)dx = \left(\frac{d|x|}{dx}\right)\Bigg|_{x=+\epsilon} - \left(\frac{d|x|}{dx}\right)\Bigg|_{x=-\epsilon} = (+1)-(-1) = 2,$$

$$\text{so } \underline{\underline{\frac{d^2}{dx^2}|x| = 2\delta(x)}}. \qquad (3)$$

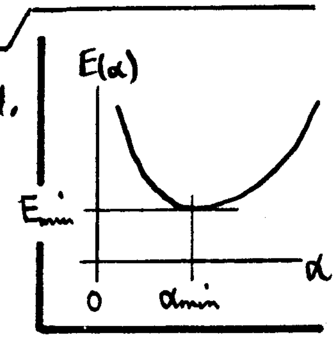
Use this fact in Eq. (2) to calculate...

$$\rightarrow E(\alpha) = \frac{3}{2\alpha}\left\{\int_{-\alpha}^{+\alpha}\left(1-\frac{|x|}{\alpha}\right)\frac{\hbar^2}{2m}\frac{1}{\alpha}\cdot 2\delta(x)\,dx + \frac{1}{2}m\omega^2\int_{-\alpha}^{+\alpha}x^2\left(1-\frac{|x|}{\alpha}\right)^2 dx\right\}$$

$$E(\alpha) = \frac{3}{2\alpha}\left\{\frac{\hbar^2}{m\alpha} + m\omega^2\alpha^3\underbrace{\int_0^1 u^2(1-u)^2 du}_{=1/30}\right\} = \frac{3}{2}\frac{\hbar^2}{m\alpha^2} + \frac{1}{20}m\omega^2\alpha^2. \qquad (4)$$

---

3. As a fcn of the parameter α, $E(\alpha)$ looks like the graph sketched. The minimum is at...



$$\frac{\partial E}{\partial \alpha} = 0 \Rightarrow \alpha^2 = \sqrt{30}\,(\hbar/m\omega) = \alpha_{min}^2; \qquad (5)$$

$$\text{so } \boxed{E_{min} = E(\alpha_{min}) = \sqrt{\frac{6}{5}}\left(\frac{1}{2}\hbar\omega\right) = 1.095\,E_0}. \qquad (6)$$

E_{min} is the best estimate for the groundstate energy $E_0 = \frac{1}{2}\hbar\omega$ for this type of trial ϕ.

(36) For ground state (ψ_0, E_0), $\mathcal{O}(\lambda)$ perturbation on wavefcn $\psi_0 \Rightarrow \mathcal{O}(\lambda^2)$ correction to energy E_0.

1) Calculation is best done by putting in $\phi = \sum_n c_n \psi_n$ at the very end. Straightforwardly:

$$E(\lambda) = \langle\psi|\mathcal{H}|\psi\rangle / \langle\psi|\psi\rangle = \langle\psi_0+\lambda\phi|\mathcal{H}|\psi_0+\lambda\phi\rangle / \langle\psi_0+\lambda\phi|\psi_0+\lambda\phi\rangle$$

or

$$\rightarrow E(\lambda) = \frac{\overset{①}{\langle\psi_0|\mathcal{H}|\psi_0\rangle} + \lambda[\overset{②}{\langle\psi_0|\mathcal{H}|\phi\rangle} + \overset{③}{\langle\phi|\mathcal{H}|\psi_0\rangle}] + \lambda^2\langle\phi|\mathcal{H}|\phi\rangle}{\underset{④}{\langle\psi_0|\psi_0\rangle} + \lambda\underbrace{[\langle\psi_0|\phi\rangle + \langle\phi|\psi_0\rangle]}_{N} + \lambda^2\langle\phi|\phi\rangle}. \tag{1}$$

We've used λ = real here. Term ① $\equiv E_0$, and in terms ② & ③, use $\langle\psi_0|\mathcal{H} = E_0\langle\psi_0|$ & $\mathcal{H}|\psi_0\rangle = E_0|\psi\rangle$, resp. ($\mathcal{H}$ is Hermitian). Term ④ $\equiv 1$, by normalization. With the shorthand notation $N = \langle\psi_0|\phi\rangle + \langle\phi|\psi_0\rangle$, Eq. (1) becomes...

$$\underline{\underline{E(\lambda) = [(1+\lambda N)E_0 + \lambda^2\langle\phi|\mathcal{H}|\phi\rangle] / [(1+\lambda N) + \lambda^2\langle\phi|\phi\rangle]}}. \tag{2}$$

---

2) In Eq. (2), $\lambda \to$ small. If we define the quantity: $\kappa = \lambda^2/(1+\lambda N)$, then

$$\left[\begin{aligned} &E(\lambda) = E_0\left[1 + \frac{\kappa}{E_0}\langle\phi|\mathcal{H}|\phi\rangle\right] / [1 + \kappa\langle\phi|\phi\rangle], \\ &\text{w/ } \kappa = \lambda^2/(1+\lambda N) \simeq \lambda^2[1 - \lambda N + (\lambda N)^2 - \cdots]. \end{aligned}\right. \tag{3}$$

The leading term in κ is $\mathcal{O}(\lambda^2)$ in smallness. To $\mathcal{O}(\lambda^2)$, $E(\lambda)$ expands to...

$$E(\lambda) \simeq E_0\left[1 + \frac{\lambda^2}{E_0}\langle\phi|\mathcal{H}|\phi\rangle\right][1 - \lambda^2\langle\phi|\phi\rangle] \simeq E_0 + \lambda^2\mathcal{E}_2,$$

$$\text{w/ } \underline{\underline{\mathcal{E}_2 = \langle\phi|\mathcal{H}|\phi\rangle - E_0\langle\phi|\phi\rangle}}. \tag{4}$$

As advertised, the first correction to E_0 is $\mathcal{O}(\lambda^2)$, not $\mathcal{O}(\lambda)$.

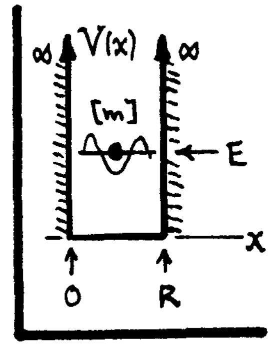
---

3) Calculate $\mathcal{E}_2$ in Eq. (4) by putting in $\phi = \sum_n c_n\psi_n$. Since $\{\psi_n\}$ is an orthonormal set: $\langle\psi_m|\psi_n\rangle = \delta_{mn}$, we get...

$$\underline{\underline{\mathcal{E}_2}} = \sum_{m,n} c_m^* c_n [\langle\psi_m|\mathcal{H}|\psi_n\rangle - E_0\langle\psi_m|\psi_n\rangle] = \underline{\underline{\sum_n |c_n|^2(E_n - E_0)}}, \tag{5}$$

as required. $\mathcal{E}_2 \geqslant 0$, since $E_n - E_0 \geqslant 0$. So $E(\lambda)$ in Eq. (4) lies above E_0.

(37) Orthogonality & completeness for eigenfcns ψ_n in a rigid box.



From problem (34), the normed eigenfcns for the rigid 1D box shown at right are: $\psi_n(x) = \sqrt{2/R}\,\sin k_n x$, w/ $k_n = n\pi/R$. Eigenenergies are: $E_n = \hbar^2 k_n^2/2m = (\pi^2\hbar^2/2mR^2)n^2$, w/ $n = 1, 2, 3, \ldots$

(A) **1.** For orthonormality, we need the integral ...

$$\rightarrow \langle m|n\rangle = \int_0^R \psi_m^*(x)\psi_n(x)\,dx = \frac{2}{R}\int_0^R \sin k_m x \,\sin k_n x\,dx \quad \text{let } u = \pi x/R$$

or/

$$\underline{\underline{\langle m|n\rangle}} = \frac{2}{\pi}\int_0^\pi \sin mu \,\sin nu\,du = \left\{\begin{matrix} 0, & m \neq n \\ 1, & m = n\end{matrix}\right\} = \underline{\underline{\delta_{mn}}}. \quad \text{QED} \tag{1}$$

This result follows from tabulated integrals (e.g. Dwight # (858.516)).

2. To establish linear independence, we have to show that if $\sum_{n=1}^\infty c_n\psi_n(x) = 0$, then all the coefficients $c_n \equiv 0$. With orthonormality of the $\{\psi_n\}$, per Eq. (1), this is easy: we operate on $0 = \sum_n c_n|n\rangle$ with $\langle m| = \int_0^R dx\,\psi_m^*(x)\cdot$, so

$$0 = \sum_n c_n\langle m|n\rangle = \sum_n c_n\delta_{mn} = c_m, \quad \text{so/} \quad \underline{\underline{c_m = 0 \text{ for all } m}} \quad \text{QED} \tag{2}$$

(B) **3.** To demonstrate completeness of the $\{\psi_n\}$, we must show that the series...

$$\rightarrow \sum_n \psi_n^*(x')\psi_n(x) = \frac{2}{R}\sum_{n=1}^\infty \sin k_n x' \sin k_n x, \quad \text{w/ } k_n = n\pi/R, \tag{3}$$

sums to a Dirac delta fcn $\delta(x-x')$. Consider that fcn generally, i.e.

$$\rightarrow f(x) = \delta(x-x'), \quad \text{on } 0 < x, x' < R, \quad \text{w/ } f(0) = 0 = f(R). \tag{4}$$

By Fourier's Theorem, $f(x)$ will have a Fourier sine series on the interval:

$$f(x) = \sum_{n=1}^\infty a_n \sin k_n x, \quad \text{w/ } a_n = (2/R)\int_0^R f(\xi)\sin k_n\xi\,d\xi$$

$$\ldots \text{ but } f(\xi) = \delta(\xi - x') \Rightarrow a_n = (2/R)\sin k_n x'$$

$$\text{so/ } f(x) = \frac{2}{R}\sum_{n=1}^\infty \sin k_n x' \sin k_n x, \quad \text{i.e./ } \boxed{\delta(x-x') = \sum_n \psi_n^*(x')\psi_n(x)}. \quad \text{QED} \tag{5}$$

(38) Expand SHO wavefcn $\psi_0(x)$ in momentum eigenstates $\phi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$.

1. The SHO ground state wavefcn is (CLASS NOTES, p. Solns 18, Eq. (41)):

$$\to \psi_0(x) = (\alpha/\sqrt{\pi})^{1/2} e^{-\frac{1}{2}\alpha^2 x^2}, \quad \text{w/ } \alpha = \sqrt{m\omega/\hbar}. \tag{1}$$

An expansion in terms of momentum eigenfcns $\phi_k(x)$ means the Fourier integral:

$$\to \psi_0(x) = \int_{-\infty}^{+\infty} c(k)\phi_k(x)\,dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} c(k) e^{ikx}\,dk, \tag{2}$$

where we use the ∞ box normalization for the $\phi_k(x)$ (NOTES, p. Comp$^{\underline{l}}$ 8).

2. The Fourier inverse of Eq. (2) gives the spectral amplitude $C(k)$ as...

$$\to C(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi_0(x) e^{-ikx}\,dx = \frac{1}{\sqrt{2\pi}}\left(\frac{\alpha}{\sqrt{\pi}}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\alpha^2 x^2 - ikx}\,dx. \tag{3}$$

The integral is tabulated (e.g. Gradshteyn & Ryzhik, # (3.323.2)), with result:

$$\boxed{C(k) = (1/\alpha\sqrt{\pi})^{1/2} e^{-k^2/2\alpha^2}}. \tag{4}$$

3. $|c(k)|^2 dk$ is the probability of finding m in the SHO ground state with momentum in the range k to $k+dk$. Over all possible momenta, we have:

$$\to \int_{-\infty}^{\infty} |c(k)|^2 dk = \frac{1}{\alpha\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-k^2/\alpha^2} dk = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-z^2} dz = 1. \tag{5}$$

This result verifies Parseval's Theorem, and conservation of probability.

4. The probability of finding m with momentum: $p \geqslant p_0 = \sqrt{2mE_0} = \sqrt{m\hbar\omega}$, i.e.: $k = p/\hbar \geqslant \sqrt{m\omega/\hbar} = \alpha$, is found by calculating...

$$\underline{\underline{P(|k| \geq \alpha)}} = \int_{-\infty}^{-\alpha} |c(k)|^2 dk + \int_{\alpha}^{\infty} |c(k)|^2 dk = 2\cdot\frac{1}{\alpha\sqrt{\pi}} \int_{\alpha}^{\infty} e^{-k^2/\alpha^2} dk$$

$$= \frac{2}{\sqrt{\pi}} \int_{1}^{\infty} e^{-u^2} du = 1 - \mathrm{erf}(1) = 1 - 0.842 = \underline{0.158} \tag{6}$$

So, m in an SHO potential spends almost 16% of its time traveling at momenta exceeding the maximum classical value.