ϕ506 Final Exam Profile

Mon. 12/13/93

The ϕ506 Final will be given on Wed. 12/15/93, @ 7-10 P.M., in AJM 221.

The exam is open-book, open notes... with the following restrictions on the materials you bring to the exam:

1. The "book" is a copy of Davydov, or some other single QM text of your choice.
2. The "notes" are your (Xerox) class notes, or notes & summaries in your handwriting. Your solutions to problem sets and/or solution keys are also OK.
3. Also OK: one math reference table, a hand calculator, a dictionary.

The final exam is worth 315 points*, and consists of 8 problems with general descriptions as follows...

1. Momentum matrix elements for stationary states.
2. Spectral distribution fcn for a QM energy eigenstate.
3. A matrix multiplication rule for arbitrary QM operators.
4. Eigenstates & eigenvalues via annihilation & creation operators.
5. QM variances for eigenstates of the SHO.
6. Lifetime for trapping a particle in a semi-permeable box.
7. WKB analysis of a familiar bound state problem.
8. Variational estimate for binding energy of an "interesting" system.

Good luck in your studies. Best wishes for happy holidays, and may all your dreams be orthonormal.

Dick Robiscoe

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* Total points for course: 535 (problem sets) + 150 (midterm exam) + 315 (final exam) = 1000 pts.

ϕ 506 Final Exam (3hr.) Wed. 15 Dec. 1993

This exam is open-book, open-notes, and is worth 315 pts. There are 8 problems, with individual point values as marked. For each problem, $\boxed{\text{box}}$ your answer, $\boxed{\text{number}}$ your solution pages consecutively, write your $\boxed{\text{name}}$ on the cover page, & $\boxed{\text{staple}}$ the pages together before handing them in.

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① [30 pts]. Let the stationary states of a QM system be specified by a set of eigenfunctions $u_\alpha(x)$ with eigenenergies E_α (i.e. if $\mathcal{H}$ = system Hamiltonian: $\mathcal{H}u_\alpha = E_\alpha u_\alpha$). For a particle of mass m, and in 1D, let p be the momentum operator, and let x be the position coordinate. Prove the identity:

$$\boxed{\langle u_\alpha | p | u_\beta \rangle = \frac{im}{\hbar}(E_\alpha - E_\beta)\langle u_\alpha | x | u_\beta \rangle}.$$

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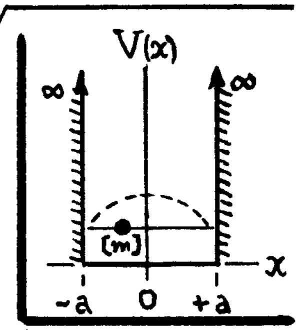
② [45 pts]. A particle of mass m is in the ground state of an infinitely deep 1D rectangular potential well of width $2a$ as shown. Find the probability distribution function for values of the particle momentum in this state. Sketch a graph of this function vs. momentum, and label the zeros and maxima. What is the most probable momentum in the ground state?



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③ [35 pts]. Given: arbitrary operators A & B, and a complete set of orthonormal eigenfcns $\{\Psi_n(x)\}$. If the matrix element $\langle k|A|l\rangle = \int dx\, \Psi_k^*(x) A \Psi_l(x) = A_{kl}$, prove the matrix multiplication rule: $(AB)_{km} = \sum_l A_{kl} B_{lm}$, i.e. show that:

$$\boxed{\langle k|AB|m\rangle = \sum_l \langle k|A|l\rangle\langle l|B|m\rangle}.$$

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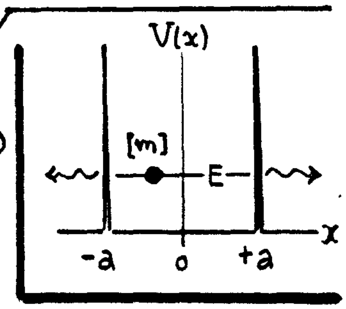
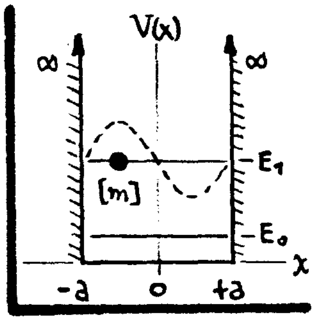
④ [45 pts]. Consider the operator: $\Lambda = a^\dagger a$, where a & $a^\dagger$ obey an anti-commutation rule: $aa^\dagger + a^\dagger a = 1$. Assume there exists a set of orthonormal eigenstates $|\lambda\rangle$ such that: $\Lambda|\lambda\rangle = \lambda|\lambda\rangle$. By calculating $a|\lambda\rangle$ and $a^\dagger|\lambda\rangle$ explicitly, show that in fact there are only two eigenstates of Λ. What are the allowed eigenvalues of Λ?

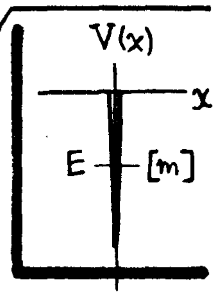
⑤ [40 pts]. Recall that for a QM operator A, the variance or uncertainty $(\Delta A)_n$ in an eigenstate n was defined by: $(\Delta A)_n^2 = \langle n|A^2|n\rangle - (\langle n|A|n\rangle)^2$. Calculate a value for the uncertainty product $\underline{(\Delta x)_n (\Delta p)_n}$ in the n^{th} eigenstate of the 1D simple harmonic oscillator. HINT: you already "know" the key matrix elements. What is the variance in the energy of the state $|n\rangle$?



⑥ [45 pts]. A particle of mass m and energy E is trapped in a 1D box of width $2a$ as shown. The walls of the box are potential barriers that are infinitely high, but they are not thick -- the wall potential is proportional to a delta function, so that m is initially moving inside the potential: $\underline{V(x) = C[\delta(x-a) + \delta(x+a)]}$, C = cnst. There is a finite probability that m can penetrate one of the walls and move off to the right or left. Find the lifetime of the particle in the box, i.e. how much time elapses between insertion of m in the box ($|x| < a$) and its appearance outside (@ $|x| > a$)?



⑦ [35 pts]. The energies & eigenfunctions of a particle (mass m) in an ∞ly deep 1D box are well-known [e.g. $\underline{E_n = (n+1)^2 E_0}$, w/ $n = 0, 1, 2, \ldots$, and $E_0 = (\hbar\pi/2a)^2/2m$ the ground state energy]. Use the WKB method to find approximate forms for the E_n and eigenfcns ψ_n. Then compare both the E_n(WKB) and the ψ_n(WKB) with the actual E_n and ψ_n. Show that the ψ_n(WKB) are not physical. So, what did you expect?



⑧ [40 pts]. For an attractive 1D delta-fcn potential well: $V(x) = -A\,\delta(x)$, you have shown (prob$^{\underline{m}}$ ㉘) that the single bound state energy is $\underline{E = -\frac{1}{2} m A^2/\hbar^2}$, for a particle of mass m. Now estimate E by a variational calculation, using the trial wavefcn: $\phi(x) = (a^2 - x^2)$, $|x| \leq a$, and zero otherwise. Why is this estimate so poor? How could it be improved?

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① [30pts]. Prove that: $\langle u_\alpha|p|u_\beta\rangle = \frac{im}{\hbar}(E_\alpha - E_\beta)\langle u_\alpha|x|u_\beta\rangle$, for stationary states.

1. In QM, momentum is defined in an expectation value sense: $\langle p\rangle = m\frac{d}{dt}\langle x\rangle$, and in the present case, this means...

$$\rightarrow \langle u_\alpha|p|u_\beta\rangle = m\frac{d}{dt}\langle u_\alpha|x|u_\beta\rangle. \tag{1}$$

In the same sense, the QM Eqtn-of-Motion (CLASS NOTES, p. Prop. 16, Eq. (15A)) specifies:

$$\rightarrow \frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\langle[\mathcal{H}, x]\rangle, \tag{2}$$

where $\mathcal{H}$ is the Hamiltonian that generates the stationary states of interest, viz: $\mathcal{H}|u_n\rangle = E_n|u_n\rangle$. When (2) is used in (1), we have:

$$\rightarrow \langle u_\alpha|p|u_\beta\rangle = \frac{im}{\hbar}\langle u_\alpha|[\mathcal{H}, x]|u_\beta\rangle. \tag{3}$$

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2. Keeping in mind that $\mathcal{H}$ is Hermitian, and $\mathcal{H}|u_n\rangle = E_n|u_n\rangle$, we can process the matrix element on the RHS of (3), viz...

$$\begin{aligned}\rightarrow \langle u_\alpha|[\mathcal{H}, x]|u_\beta\rangle &= \langle u_\alpha|\mathcal{H}x|u_\beta\rangle - \langle u_\alpha|x\mathcal{H}|u_\beta\rangle \\ &= E_\alpha\langle u_\alpha|x|u_\beta\rangle - E_\beta\langle u_\alpha|x|u_\beta\rangle \\ &= (E_\alpha - E_\beta)\langle u_\alpha|x|u_\beta\rangle.\end{aligned} \tag{4}$$

Use of this result in Eq. (3) gives the required identity...

$$\boxed{\langle u_\alpha|p|u_\beta\rangle = \frac{im}{\hbar}(E_\alpha - E_\beta)\langle u_\alpha|x|u_\beta\rangle.} \quad \text{QED} \tag{5}$$

NOTE: If $\beta=\alpha$, so we are calculating the expected value of p within a given stationary state, Eq. (5) $\Rightarrow \langle u_\alpha|p|u_\alpha\rangle \equiv 0$. This adds force to the name "stationary state"... it doesn't go anywhere, on average.

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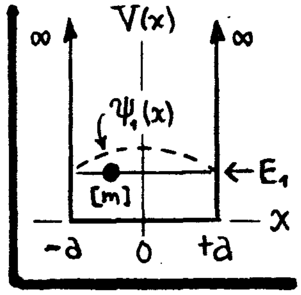
② [45 pts]. **Momentum distribution for ground state of a deep rectangular well.**



1. Consult Eqs. (10) & (11) on p. Sol^{n}s 4 of CLASS NOTES. The normalized wave fcn in the ground state (corresponding to energy $E_1 = \frac{1}{2m}(\hbar k_1)^2$, with $k_1 = \pi/2a$) is given by... (note--norm per Prob. ㉔)...

$\rightarrow \psi_1(x) = (1/\sqrt{a})\cos(\pi x/2a)$, for $|x| \leq a$; $\psi_1(x) \equiv 0$, otherwise. (1)

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2. With $k = p/\hbar$, the required momentum spectrum fcn is...

$$\rightarrow \phi_1(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi_1(x)e^{-ikx}dx = \frac{1}{\sqrt{2\pi a}}\int_{-a}^{+a}e^{-ikx}\cos k_1 x\,dx, \quad \text{w/ } \underline{k_1 = \pi/2a} \quad (2)$$

$$= \frac{1}{\sqrt{2\pi a}}\cdot\frac{1}{2}\int_{-a}^{+a}\left[e^{-i(k-k_1)x} + e^{-i(k+k_1)x}\right]dx \quad \int \text{use integration formula: } \int_{-a}^{+a}e^{-ikx}dx = \frac{2}{k}\sin ka$$

so/

$$\phi_1(k) = \sqrt{\frac{a}{2\pi}}\left[\frac{\sin(k-k_1)a}{(k-k_1)a} + \frac{\sin(k+k_1)a}{(k+k_1)a}\right]. \quad (3)$$

The momentum probability distribution fcn is $|\phi_1(k)|^2$. Notice that as $k \rightarrow k_1$, the [ ] $\rightarrow$ [1+0], since $\sin(k_1+k_1)a = \sin\pi = 0$. A similar result holds as $k \rightarrow (-)k_1$, and we can state: $\underline{|\phi_1(k = \pm k_1)|^2 = a/2\pi}$.

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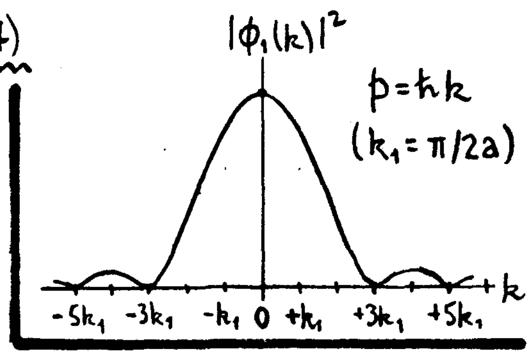
3. In Eq. (3), have $\sin(k \mp k_1)a = \sin(ka \mp \frac{\pi}{2}) = \mp\cos ka$, so we can write...

$$\phi_1(k) = \sqrt{\frac{a}{2\pi}}\left[\frac{1}{(k_1-k)a} + \frac{1}{(k_1+k)a}\right]\cos ka = \sqrt{\frac{\pi a}{2}}\,\frac{\cos ka}{(k_1^2-k^2)a^2}$$

so/

$$\boxed{|\phi_1(k)|^2 = \frac{\pi a}{2}\cos^2 ka\Big/\left[(ka)^2 - (\pi/2)^2\right]^2} \quad (4)$$



This is the required distribution. It is symmetric in k, and falls off as k^4 for $k \gg k_1$. The max. is at $k=0$, where $|\phi_1(0)|^2 = (8/\pi^3)a = 0.258\,a$. As shown above $|\phi_1(\pm k_1)|^2 = (1/2\pi)a = 0.159\,a$ is regular. Zeros occur at $k = \pm 3k_1, \pm 5k_1$, etc. The subsidiary maxima at $k \simeq \pm 4k_1$ are only about $(1/225)\times$ central max. $\pm k$ values are equally likely $\Rightarrow$ most probable k, i.e. $\langle k \rangle$, is zero.

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3 [35 pts]. For a complete set, prove: $\langle k|AB|m\rangle = \sum_\ell \langle k|A|\ell\rangle\langle \ell|B|m\rangle$.

1. The RHS of the required identity involves...

$$\rightarrow \sum_\ell \langle k|A|\ell\rangle\langle \ell|B|m\rangle = \sum_\ell \int dx\, \psi_k^*(x) A \psi_\ell(x) \int dx'\, \psi_\ell^*(x') B' \psi_m(x'), \quad (1)$$

where B' means the operator B defined in terms of primed coordinates. By changing the order of integration and summation, we can write...

$$\rightarrow \sum_\ell \langle k|A|\ell\rangle\langle \ell|B|m\rangle = \int dx\, \psi_k^*(x) A \int dx' \underbrace{\Big[\sum_\ell \psi_\ell(x)\psi_\ell^*(x')\Big]}_{\text{call this } \Delta(x,x')} B'\psi_m(x'). \quad (2)$$

2. By the fact that the $\{\psi_n(x)\}$ are a complete set, $\Delta(x,x')$ is a Dirac delta fcn [see CLASS NOTES, p. Comp$\frac{1}{2}$ 2, Eq. (5)], i.e.

$$\Delta(x,x') = \sum_\ell \psi_\ell(x)\psi_\ell^*(x') = \delta(x-x') \leftarrow \text{the } \{\psi_\ell(x)\} \text{ are complete}. \quad (3)$$

Then, in Eq. (2), we have...

$$\sum_\ell \langle k|A|\ell\rangle\langle \ell|B|m\rangle = \int dx\, \psi_k^*(x) A \int dx'\, \delta(x-x') B'\psi_m(x')$$

$$= \int dx\, \psi_k^*(x) AB \psi_m(x) = \langle k|AB|m\rangle. \quad \text{QED} \quad (4)$$

The identity is proved.

Interesting feature of bra-ket notation. The relation in (4) is...

$$\sum_\ell \langle k|A|\ell\rangle\langle \ell|B|m\rangle = \langle k|A \underbrace{\Big(\sum_\ell |\ell\rangle\langle \ell|\Big)}_{I} B|m\rangle = \langle k|AB|m\rangle.$$

The quantity $I = \sum_\ell |\ell\rangle\langle \ell|$ is acting like an identity operator; in fact, this is the equivalent of a closure relation in the bra-ket scheme. Note that: $I|n\rangle = \sum_\ell |\ell\rangle\langle \ell|n\rangle = \sum_\ell |\ell\rangle \delta_{\ell n} = |n\rangle$, in fact just multiplies $|n\rangle$ by one.

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④ [45 pts]. For $\Lambda = a^\dagger a$, and $aa^\dagger + a^\dagger a = 1$, find eigenstates & eigenvalues for $\Lambda|\lambda\rangle = \lambda|\lambda\rangle$.

1. This problem is done by the same sort of manipulations we used in "QM SHO by Operator Techniques" (CLASS NOTES, pp. SHO 1-4). Only change is that now we have $aa^\dagger + a^\dagger a = 1$, rather than the previous $aa^\dagger - a^\dagger a = 1$.

2. With the assumption of eigenstates $|\lambda\rangle$, we calculate...

$$a|\lambda\rangle = \overbrace{(aa^\dagger + a^\dagger a)}^{(\ )=1} a|\lambda\rangle = a\Lambda|\lambda\rangle + \Lambda a|\lambda\rangle = (\lambda + \Lambda)a|\lambda\rangle,$$

or// $\Lambda(a|\lambda\rangle) = (1-\lambda)(a|\lambda\rangle)$, so// $a|\lambda\rangle = A|1-\lambda\rangle$ ✓ $a|\lambda\rangle$ belongs to eigenvalue $(1-\lambda)$. (1)

Find the cnst A by imposing normalization...

$$\rightarrow |A|^2 \underbrace{\langle 1-\lambda|1-\lambda\rangle}_{1} = \langle a\lambda|a\lambda\rangle = \langle\lambda|a^\dagger a|\lambda\rangle = \lambda, \text{ so// } \boxed{a|\lambda\rangle = \sqrt{\lambda}\,|1-\lambda\rangle}. \quad (2)$$

Treating $a^\dagger$ similarly... (insert "1" to the right of $a^\dagger$)...

$$a^\dagger|\lambda\rangle = a^\dagger(aa^\dagger + a^\dagger a)|\lambda\rangle = (\Lambda + \lambda)a^\dagger|\lambda\rangle$$

or// $\Lambda(a^\dagger|\lambda\rangle) = (1-\lambda)(a^\dagger|\lambda\rangle)$, so// $a^\dagger|\lambda\rangle = B|1-\lambda\rangle$ ✓ $a^\dagger|\lambda\rangle$ also belongs to $(1-\lambda)$. (3)

$$|B|^2 \underbrace{\langle 1-\lambda|1-\lambda\rangle}_{1} = \langle a^\dagger\lambda|a^\dagger\lambda\rangle = \langle\lambda|\underbrace{aa^\dagger}_{=1-\Lambda}|\lambda\rangle = (1-\lambda), \text{ so } \boxed{a^\dagger|\lambda\rangle = \sqrt{1-\lambda}\,|1-\lambda\rangle}. \quad (4)$$

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3. The annihilation & creation operator a & $a^\dagger$ thus generate only two eigenstates for $\Lambda = a^\dagger a$, viz. $|\lambda\rangle$ & $|1-\lambda\rangle$. Repeated operations by a & $a^\dagger$ do not get you out of this small space: $a^2|\lambda\rangle = \sqrt{\lambda(1-\lambda)}\,|\lambda\rangle = a^{\dagger 2}|\lambda\rangle$. The two allowed eigenvalues, λ & $(1-\lambda)$, are sometimes assigned the values 1 & 0. Then: $a|1\rangle = |0\rangle$, $a^\dagger|0\rangle = |1\rangle$, and: $\langle 1|\Lambda|1\rangle = 1$, $\langle 0|\Lambda|0\rangle = 0$.

NOTE: operators obeying $aa^\dagger + a^\dagger a = 1$, and allowing only 2 states per mode, characterize fermion fields. When $aa^\dagger - a^\dagger a = 1$, there are an ∞ # of states per mode $\Rightarrow$ boson fields.

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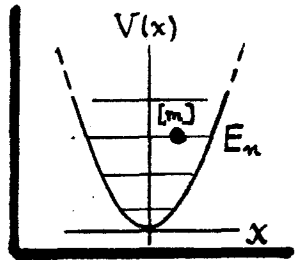
⑤ [40pts]. Find a value for the uncertainty product in the n^{th} state of a QM SHO.



1. The expectation values $\langle n|x|n\rangle$ and $\langle n|p|n\rangle$ are both zero in eigenstate $|n\rangle$ of the SHO -- by symmetry arguments (both x & p have odd parity), or by actual calculation [see Eq. (2), p. SHO 1 of CLASS NOTES: $x \propto (a+a^\dagger)$ & $p \propto (a-a^\dagger)$, and $\langle n|a|n\rangle = 0$ & $\langle n|a^\dagger|n\rangle = 0$]. This means the variances in question are...

$$\rightarrow (\Delta x)_n^2 = \langle n|x^2|n\rangle, \quad (\Delta p)_n^2 = \langle n|p^2|n\rangle. \tag{1}$$

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2. The SHO Hamiltonian is $\mathcal{H} = p^2/2m + \frac{1}{2}m\omega^2x^2$, so $p^2 = 2m\mathcal{H} - m^2\omega^2x^2$. Since $\langle n|\mathcal{H}|n\rangle = E_n = (n+\frac{1}{2})\hbar\omega$, we have that...

$$\rightarrow \langle n|p^2|n\rangle = 2mE_n - m^2\omega^2\langle n|x^2|n\rangle. \tag{2}$$

Then both variances $(\Delta x)_n$ & $(\Delta p)_n$ in Eq. (1) are specified once we find the matrix element $\langle n|x^2|n\rangle$. In fact, we calculated this quantity in ϕ 506 Prob^m #33, while we were showing $\langle n|V|n\rangle = \frac{1}{2}E_n$. Result:

$$\underline{\underline{\langle n|x^2|n\rangle = E_n/m\omega^2}}. \tag{3}$$

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3. By using (3) in (1) & (2), we find...

$$\left.\begin{array}{l}(\Delta x)_n^2 = E_n/m\omega^2 \\ (\Delta p)_n^2 = mE_n\end{array}\right\} \text{ so } (\Delta x)_n^2(\Delta p)_n^2 = (E_n/\omega)^2 \tag{4}$$

With $E_n = (n+\frac{1}{2})\hbar\omega$, this gives the required uncertainty product:

$$\boxed{(\Delta x)_n(\Delta p)_n = (n+\tfrac{1}{2})\hbar \geq \tfrac{1}{2}\hbar}, \quad \text{for } n = 0, 1, 2, \ldots \tag{5}$$

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4. The energy $E = E_n = (n+\frac{1}{2})\hbar\omega$ is an eigenvalue of the state n, so the variance $(\Delta E)_n^2 = \langle n|E^2|n\rangle - (\langle n|E|n\rangle)^2 = E_n^2 - (E_n)^2 \equiv 0$, as should be.

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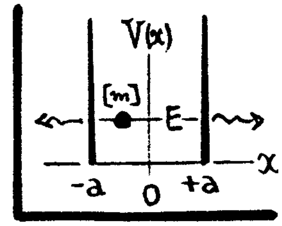
⑥ [45 pts]. Lifetime for a particle trapped in a semi-permeable box.

1. The decay rate for trapping is: $\Gamma = \left(\frac{1}{\tau/2}\right) T$, where τ is the natural period of m's motion inside the box, and T is the transmission coefficient at one of the walls. The required lifetime is: $\Delta t = 1/\Gamma$. Since m is free inside the box, we can write: $\tau = 2\cdot(2a)/v$, where m's velocity $v = \sqrt{2E/m}$. So: $\tau/2 = \sqrt{2ma^2/E}$, and the trapping lifetime is:



$$\rightarrow \Delta t = \frac{\tau}{2}/T = \sqrt{\frac{2ma^2}{E}}/T. \qquad (1)$$

If the wall transmission coefficient $T \to 0$, $\Delta t \to \infty$ and m remains forever trapped in the box. BUT, as we show below, T is finite for a δ-fcn wall.

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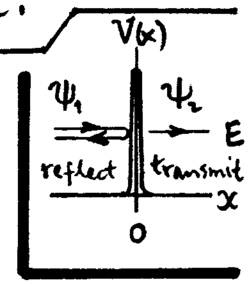
2. Find T for a δ-fcn wall, with potential $V = C\,\delta(x)$. If m is incident at energy E, with momentum $\hbar k = \sqrt{2mE}$, wavefcns are:



$$\rightarrow x<0:\ \psi_1(x) = e^{ikx} + A e^{-ikx};\quad x>0:\ \psi_2(x) = B e^{ikx}. \qquad (2)$$

We want $T = |B|^2$. Impose the continuity conditions (see prob$^{\underline{m}}$ ㉘ for II)...

I. ψ continuous @ $x=0$: $1 + A = B$. (3)

II. ψ' discontinuous @ $x=0$: $\psi_2'(0+) - \psi_1'(0-) = \frac{2mC}{\hbar^2}\psi(0)$,

i.e.// $ik[B-(1-A)] = \left(\frac{2mC}{\hbar^2}\right)B$, or// $1 - A = \left(1 - \frac{2mC}{ik\hbar^2}\right)B$. (4)

Add (3) & (4) to eliminate A. Get: $B = 1/[1 + i(mC/\hbar^2 k)]$. Then, using $(\hbar k)^2 = 2mE$, we find the transmission coefficient...

$$\rightarrow T = |B|^2 = 1/[1 + (mC^2/2\hbar^2 E)]. \qquad (5)$$

Put T of Eq.(5) to find the required trapping lifetime...

$$\boxed{\Delta t = \sqrt{\frac{2ma^2}{E}}\left[1 + (mC^2/2\hbar^2 E)\right]} \qquad (6)$$

As $E \to$ large, $\Delta t \to 0$... m escapes rapidly. $E \to 0 \Rightarrow$ trapping forever.

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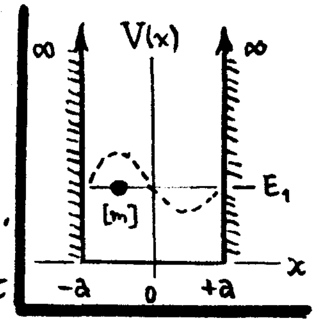
⑦ [35 pts]. WKB "treatment" of bound states in a very deep rectangular well.



1. WKB approxns should not work very well in this case, because the wave # $k=\sqrt{(2m/\hbar^2)[E-V(x)]}$ becomes ∞ at the turning pts $x=\pm a$ (i.e. the walls), and likewise the slope dk/dx is singular. The WKB parameter $\left|\frac{1}{k^2}(dk/dx)\right|$ is undefined at the walls. But we proceed anyway. We can compare WKB with known results (CLASS NOTES, p. Solns 4):

$$\left[\begin{array}{l} \text{energies}: E_n=\frac{1}{2m}(\hbar k_n)^2, \\ \text{w/ } k_n=(n+1)\frac{\pi}{2a};\ n=0,1,2,\ldots \end{array}\right\| \begin{array}{l} \text{even states}\ \}\ \psi_n(x)=\frac{1}{\sqrt{a}}\cos k_n x;\ n=0,2,4,\ldots \\ \text{odd states}\ \}\ \psi_n(x)=\frac{1}{\sqrt{a}}\sin k_n x;\ n=1,3,5,\ldots \end{array} \tag{1}$$

Notice that we have stepped down n by one; the ground state is labelled $n=0$.

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2. For use of the Bohr-Sommerfeld rule: $\int_{-a}^{+a} k(x)\,dx=(n+\frac{1}{2})\pi$, we note that inside the well, $k(x)=\sqrt{(2m/\hbar^2)E}$ is cnst (over $|x|<a$), so the WKB energies are →

$$\int_{-a}^{+a}\sqrt{(2m/\hbar^2)E}\,dx=(n+\tfrac{1}{2})\pi \Rightarrow \boxed{E_n(\text{WKB})=(n+\tfrac{1}{2})^2\frac{(\hbar k_0)^2}{2m}}. \tag{2}$$

where $k_0=\pi/2a$, and $n=0,1,2,\ldots$ In the same notation, the true energies are: $\underline{E_n(\text{true})=(n+1)^2(\hbar k_0)^2/2m}$, so $E_n(\text{WKB})=\left(\frac{n+1/2}{n+1}\right)^2 E_n(\text{true})$ is low. The difference is marked in the ground state: $E_0(\text{WKB})=\frac{1}{4}E_0(\text{true})$, but for $n\geq 9$, $E_n(\text{WKB})$ is 90% or better of $E_n(\text{true})$. Not too bad.

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3. The situation with the WKB wavefcns $\psi(x)=\frac{\text{cnst}}{\sqrt{k(x)}}\left\{\begin{matrix}\cos\\ \sin\end{matrix}\right\}\left(\int k(x)\,dx\right)$ is not too good. With $k(x)=$ cnst inside the well, we will just skip the cnst outside. Then for the quantized WKB wave #: $k_n^{\text{WKB}}=(n+\frac{1}{2})k_0$, (per Eq. (2)), we can write

$$\rightarrow \psi_n^{\text{WKB}}(x)\propto\left\{\begin{matrix}\cos\\ \sin\end{matrix}\right\}(k_n^{\text{WKB}}x)=\left\{\begin{array}{l}\cos(n+\frac{1}{2})\pi x/2a,\ \text{even states } (n=0,2,4,\ldots)\\ \sin(n+\frac{1}{2})\pi x/2a,\ \text{odd states } (n=1,3,5,\ldots)\end{array}\right. \tag{3}$$

These $\psi_n^{\text{WKB}}(x)$ have the correct (and required) reflection symmetry, but they do <u>not</u> vanish at the walls $\left[|\psi_n^{\text{WKB}}(x=\pm a)|\propto\frac{1}{\sqrt{2}}\right]$. So ψ_n^{WKB} is <u>discontinuous</u> @ $x=\pm a$. Not physical!

ϕ506 Final Exam Solutions (1993)

(8) [40 pts]. Variational estimate of binding energy in the 1D potential $V(x) = -A\delta(x)$.

1. Let $\mathcal{N}$ be the norm cnst for the trial fcn, so: $\phi(x) = \mathcal{N}(a^2 - x^2)$. Then...

$$\rightarrow \langle\phi|\phi\rangle = \mathcal{N}^2 \int_{-a}^{+a} (a^2 - x^2)^2 dx = \mathcal{N}^2 a^5 \int_{-1}^{+1} (1-u^2)^2 du$$

$$= 2\mathcal{N}^2 a^5 \int_0^1 (1 - 2u^2 + u^4) du = 2\mathcal{N}^2 a^5 \left(1 - \tfrac{2}{3} + \tfrac{1}{5}\right)$$

So// $\langle\phi|\phi\rangle = \frac{16}{15}\mathcal{N}^2 a^5$. (1)

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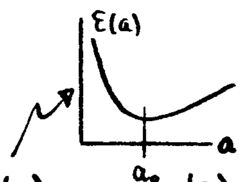
2. The system Hamiltonian is: $\mathcal{H} = \frac{1}{2m}p^2 + V(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - A\delta(x)$, and the variational estimate for the ground state (only) energy is...

$$\rightarrow \mathcal{E} = \langle\phi|\mathcal{H}|\phi\rangle / \langle\phi|\phi\rangle = \frac{15}{16a^5}\int_{-a}^{+a} (a^2 - x^2)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - A\delta(x)\right](a^2 - x^2)dx$$

i.e.// $$\mathcal{E} = \frac{15}{16a^5}\left\{\frac{\hbar^2}{m}\int_{-a}^{+a}(a^2 - x^2)dx - A\int_{-a}^{+a}(a^2-x^2)^2 dx\right\}$$



or// $$\mathcal{E} = \frac{15}{16a^5}\left\{\frac{4}{3}\frac{\hbar^2 a^3}{m} - Aa^4\right\} = \frac{5}{4}(\hbar^2/ma^2) - \frac{15}{16}\frac{A}{a} = \mathcal{E}(a).$$ (2)

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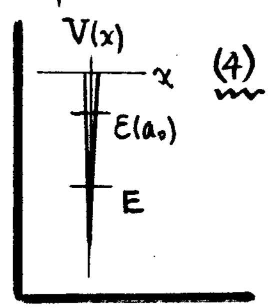
3. Now minimize $\mathcal{E}(a)$ w.r.t. the adjustable width parameter a...

$$\frac{\partial}{\partial a}\mathcal{E}(a) = -\frac{5}{2a^3}\left[\frac{\hbar^2}{m} - \frac{3}{8}Aa\right] = 0 \Rightarrow a = \frac{8}{3}\hbar^2/mA = a_0.$$ (3)

The best variational estimate of the binding energy for the given ϕ is then:

$$\boxed{\mathcal{E}(a_0) = -\frac{5}{4}\left[\frac{3}{4}\frac{A}{a_0} - \frac{\hbar^2}{ma_0^2}\right] = -(45/128)\cdot\frac{1}{2}mA^2/\hbar^2}.$$ (4)



The variational binding $\mathcal{E}(a_0)$ lies well above the known binding energy $E = -\frac{1}{2}(mA^2/\hbar^2)$; in fact $|\mathcal{E}(a_0)|$ is only 35% of $|E|$. The problem is that $\phi(x) = \mathcal{N}(a^2 - x^2)$ is too smooth near $x = 0$ and it is too wide... it does not match the actual wavefcn $\psi(x) = \mathcal{N}e^{-(mA/\hbar^2)|x|}$ very well. Presumably the variational $\mathcal{E}$ would be improved by choosing ϕ to be more sharply peaked near $x = 0$. $\phi(x) = \mathcal{N}e^{-|x|/a}$ would work just fine.