φ506 MidTerm Exam Preview

19 Oct, 1994

The φ506 MidTerm will be given 7-9 P.M. on Mon. 24 Oct. in AJM 221.

1. Material covered will be limited to that through the lecture of 10/17/94, i.e. from p. Intro. 1 through p. Sol^{n}s 14 of your CLASS NOTES. There will be 5 problems on the exam, worth 300 points total; the problems are ~ uniformly distributed over the topics we have studied.
2. There will be no class lecture on the day of the exam.
3. There is no problem set assigned for the week beginning 14 Oct. The next φ506 set (i.e. #8) will be handed out on 21 Oct. and due on 28 Oct.
4. A general description of the exam problems follows:

① What would Planck's contribution to QM have been had he known too much?
② Scales of QM effects, via estimates by de Broglie & Uncertainty Relations.
③ Use of a given wave function to calculate expectation values.
④ Another QM analogue to a theorem from classical mechanics.
⑤ Particle moving in 1D and reflected from a barrier.

NOTE: problem ② involves the calculation of actual numbers. You will need, and should bring to the exam, a calculator and a table of physical constants.

The exam is open-book, open-notes. What you bring to the exam is limited to:
1) one textbook of your choice (e.g. Davydov, or any book by Lewis Carroll);
2) Class Notes, problems & solutions (yours and/or keys), notes in your handwriting;
3) a math reference/tables, a calculator, physical constants table, & dictionary.

May your studies obey the limit that $\hbar \to 0$.

Good Luck // Dick Robiscoe

ϕ506 Mid Term Exam (2 hr., in-class) — Mon. 24 Oct 1994

This exam is open-book, open notes, and is worth 300 points. There are 5 problems on 2 pages, with point values as marked. For each problem, box your answer, number your solution pages in sequence, write your name on the cover sheet, and staple the pages together before handing them in.

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(1) [60 pts.]. In deriving his famous blackbody radiation law, Planck assumed that the atomic oscillators in the walls of the blackbody cavity could absorb and radiate energy only in quantized units, viz. $E_n = nh\nu$, w/ $n = 0, 1, 2, \ldots, \infty$, at given (linear) frequency ν. From our study of QM oscillators, however, we know that the energies are quantized as $E_n = (n+s)h\nu$, where $s = \frac{1}{2}$ is in place in order to satisfy the position-momentum uncertainty relation. Generalize Planck's calculation from $s = 0$ (as he assumed) to $s > 0$ (as he should have known(?)), and discuss what happens to the radiation law.

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(2) [60 pts.] The advent of QM effects is semi-quantitatively governed by criteria associated with de Broglie's relation ($\lambda = h/p$), and/or the Uncertainty Relations ($\Delta x \Delta p \gtrsim \frac{\hbar}{2}$, etc.). State the criterion, and find numbers, for the following cases:

(A) When will an electron (mass m_e), moving at velocity $v \ll c$, show distinct wave properties upon scattering from a crystal of lattice spacing $a = 1$ Å (10^{-8} cm)? Calculate a nominal electron energy in eV where QM shows up.

(B) The position of the center-of-mass of a liquid droplet of mass $m = 1\,\mu$g (microgram) can be determined to an accuracy of $1\,\mu$ (i.e. 10^{-4} cm). Is there a need to apply QM in describing the droplet's motion? Why or why not?

(C) On a metal surface, to see whether an electron belongs to a given atom, one must determine the electron's position to an accuracy $d \sim 1$ Å (i.e. to ~ one atomic diameter). Compare the random energy imparted to the electron by this measurement to the ionization energy of an atom in the metal -- typically 6-8 eV. What conclusion can you draw?

③ [60pts.]. In 3D, a spherically symmetric system is described by a wavefcn: $\Psi(r) = Ne^{-\alpha r}$, w// N & α = (+)ve cnsts, & // r is the radial coordinate, with range $0 \leq r \leq \infty$. "Spherically symmetric" means that there is no angular dependence in Ψ, and the 3D volume element is $d^3x = 4\pi r^2 dr$. Incidently, this form of Ψ specifies the ground state of the hydrogen atom.

(A) Find the average size of the system described by $\Psi(r)$. Call it a.

(B) Calculate the probability $P(\geq a)$ that a measurement of the system's size will yield a value larger than (or equal to) the average a. NOTE: you can and should get an actual number for $P(\geq a)$.

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④ [60pts.]. (A) In 1D, and for Ψ a general QM state fcn, find an expression for: $(d/dt)\langle\Psi|px|\Psi\rangle$, w// x = position, and p = momentum (operator). The system Hamiltonian (operator) is, as usual: $\mathcal{H} = (p^2/2m) + V(x)$.

(B) Now, if $\Psi \to \Psi_E$, a stationary eigenstate of energy E, show that:

$$\boxed{\langle\Psi_E|K|\Psi_E\rangle = \tfrac{1}{2}\langle\Psi_E|x(\partial V/\partial x)|\Psi_E\rangle}, \quad K = \frac{p^2}{2m} = \text{K.E. (operator)}.$$

This is the QM counterpart of the Virial Theorem from classical mechanics.

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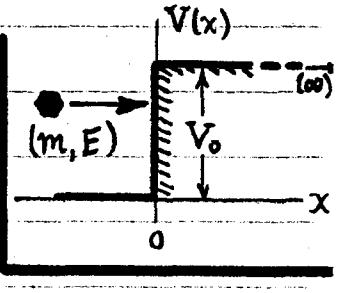
⑤ [60pts.]. A QM particle of mass m and total energy E moves to the right along the x-axis, and encounters a step-function potential at the origin, i.e.

$V(x) = 0$, for $x < 0$; $V(x) = V_o$, for $x > 0$.



Calculate the reflection coefficient $R(E)$ for m in this encounter, for both $0 \leq E < V_o$, and $V_o \leq E$. Sketch $R(E)$ vs. E for both cases ($E < V_o$ & $V_o < E$), on one graph. Finally, what feature of your solution is non-classical?

φ506 MidTerm Solutions (Oct. '94).

(1) [60 pts.]. Had he known about the QM SHO, what would Planck have done?

1. If his system had had quantized energies $E_n = (n+s)h\nu$, Planck would have calculated the average energy @ freq. ν as (ref CLASS NOTES, p. Intro. 5, Eq. (11)):

$$\rightarrow \bar{E} = \frac{\sum_{n=0}^{\infty} E_n e^{-E_n/kT}}{\sum_{n=0}^{\infty} e^{-E_n/kT}} = h\nu \frac{\sum_n (n+s) e^{-(n+s)\epsilon}}{\sum_n e^{-(n+s)\epsilon}}, \quad \text{w// } \epsilon = h\nu/kT$$

(cancel)

$$\text{so// } \bar{E}/h\nu = \sum_n (n+s) e^{-n\epsilon} / \sum_n e^{-n\epsilon} = \left(\sum_n n e^{-n\epsilon} / \sum_n e^{-n\epsilon}\right) + s \,. \qquad (1)$$

The first term RHS here just sums to Planck's result, viz $1/(e^{\epsilon}-1)$, while s is only a simple add-on. Thus we get ...

$$\rightarrow \underline{\bar{E} = h\nu/(e^{h\nu/kT}-1) + sh\nu}. \qquad (2)$$

No problem here; $s>0$ just gives a simple and finite addition to $\bar{E}$.

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2. An apparent problem arises with the <u>total</u> BB energy, however. By Eq. (13) of p. Intro 6, and with the mode density $dp/d\nu = \frac{8\pi}{c^3}\nu^2$, the energy density at frequency ν is $U_\nu = \bar{E}\, dp/d\nu$, or

$$\rightarrow \underline{U_\nu = \frac{8\pi h}{c^3}\nu^3\left[(e^{h\nu/kT}-1)^{-1} + s\right]}. \qquad (3)$$

For U_ν, the 1st term RHS gives Planck's Law, but now it is offset by s. Still no worry; $s>0$ would only be detectable in U_ν at high freqs. ν. BUT... the total system energy $\int_0^\infty U_\nu\, d\nu$ will now contain a term $\propto s\int_0^\infty \nu^3 d\nu$, which diverges violently as $\nu\to\infty$. Apparently, for $s>0$, we have a brand new version of the <u>UV catastrophe</u>, which Planck had avoided.

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3. BUT... this calc^n applies to the <u>oscillators</u> per se, and <u>not</u> the cavity radiation. The absorption/emission of radiation still occurs in <u>units</u> $nh\nu$, as an oscillator changes state $n_1 \to n_2$, w// $n = n_1 - n_2$. Planck's hypothesis & radiation law are <u>still</u> true.

φ506 MidTerm Solutions (Oct.'94)

(2) [60 pts.]. Estimate advent of QM effects in three different situations.

(A) As for the scattering of light, we will see wave-like diffraction effects when the (electron) wavelength $\underline{\lambda = h/m_e v \sim a}$, i.e. when the (electron) velocity $v \sim h/m_e a$. The electron energy in these circumstances will be:

$$\rightarrow K = \tfrac{1}{2} m_e v^2 \sim h^2/2m_e a^2 \quad \text{[multiply \& divide by rest energy } m_e c^2\text{]} \Rightarrow \underline{\underline{K \sim \frac{m_e c^2}{2}(\lambda_c/a)^2}}. \quad (1)$$

$\lambda_c = h/m_e c$ is the electron Compton wavelength. For a numerical value...

$$\left[\begin{array}{l} m_e c^2 = 0.511\ \text{MeV, and:} \\ \lambda_c = 2.43\times10^{-10}\ \text{cm},\ a = 10^{-8}\ \text{cm} \end{array}\right\} \boxed{K \sim 150\ \text{eV}} \quad (2)$$

The diffraction effects increase as $K \lesssim$ such energies.

(B) The QM effect of localizing the droplet's position to an accuracy of Δx will be the generation of random momentum components in the droplet's motion, of size: $\underline{m\Delta v \sim h/\Delta x}$, w/ m = droplet mass. QM will apply here if Δv is "appreciable" compared to a typical (measurable) droplet velocity. For numbers:

$$\left[\begin{array}{l} h = 1.05\times10^{-27}\ \text{cgs, and:} \\ m = 10^{-6}\ \text{gm},\ \Delta x = 10^{-4}\ \text{cm} \end{array}\right\} \boxed{\Delta v \sim \frac{h}{m\Delta x} = 1.05\times10^{-17}\ \frac{\text{cm}}{\text{sec}}} \quad (3)$$

Such a small velocity ($\sim \frac{1}{3}$ of a nuclear diameter per hour) is basically undetectable; any measurable droplet motion will not be affected by QM in this case.

(C) As in part (B), localization to $\Delta x = d$ generates random velocity components of size: $\underline{\Delta v \sim h/m_e d}$, and hence a random kinetic energy $\underline{\Delta K = \tfrac{1}{2} m_e \Delta v^2}$ for the measured electron. Do the same trick as in part (A) to write: $\underline{\Delta K} \sim \tfrac{1}{2} m_e (h/m_e d)^2 = \underline{\tfrac{1}{2} m_e c^2 (\lambda\!\!\!^{-}_c/d)^2}$, w/ $\lambda\!\!\!^{-}_c = \lambda_c/2\pi$ (circular λ_c). Numbers:

$$\left[\begin{array}{l} m_e c^2 = 0.511\ \text{MeV, and} \\ \lambda\!\!\!^{-}_c = \lambda_c/2\pi,\ d = 10^{-8}\ \text{cm} \end{array}\right\} \boxed{\Delta K \sim 3.8\ \text{eV}} \quad (4)$$

In trying for a localization to better than 1 Å (say to 0.7 Å), we will induce ionization and thereby lose track of the original electron.

ϕ506 MidTerm Solutions (Oct. '94)

(3) [60 pts.]. Calculate "size" of 3D system w/ $\psi(r) = Ne^{-\alpha r}$. Also $P(r \geq a)$.

It is convenient to normalize ψ at the outset, i.e. impose:

$$\rightarrow 1 = \int_\infty |\psi|^2 d^3x = 4\pi |N|^2 \int_0^\infty r^2 e^{-2\alpha r} dr = 4\pi |N|^2 \cdot \frac{2!}{(2\alpha)^3} \Rightarrow \underline{\underline{N = \left(\frac{\alpha^3}{\pi}\right)^{\frac{1}{2}}}}. \quad (1)$$

We've used the tabulated integral: $\int_0^\infty u^n e^{-ku} du = \frac{n!}{k^{n+1}}$, $k > 0$ [Dwight (860.07)].

(A) The simplest "size" to associate with ψ's system is the expectation value of r:

$$\langle r \rangle = \int_\infty \psi^* \{r\} \psi \, d^3x \overset{\text{use Eq. (1)}}{=} 4\pi |N|^2 \int_0^\infty r^3 e^{-2\alpha r} dr = 4\alpha^3 \cdot \frac{3!}{(2\alpha)^4},$$

so // $\boxed{\langle r \rangle = 3/2\alpha = a}$, simple average size (2)

This is what we'll call the average size a. It is not unique... we could have put the "size" $= \langle r^n \rangle^{\frac{1}{n}} = (3/2\alpha)\left[\frac{(n+2)!}{3!}/3^{n-1}\right]^{\frac{1}{n}}$, but the $[\,]^{\frac{1}{n}}$ doesn't change radically with n (e.g. for $n=2$: $\langle r^2 \rangle^{\frac{1}{2}} = (3/2\alpha) \cdot 1.1547$). So $\langle r \rangle$ suffices.

(B) The probability of measuring the system size in $0 \leq r \leq \infty$ is $\int_\infty |\psi|^2 d^3x = 1$, by Eq. (1). If the range is restricted to finding the system in $a \leq r \leq \infty$, * i.e. at some size (any size) $r \geq a$, then the probability of that occurring is:

$$\rightarrow P(\geq a) = \int_{r \geq a} |\psi|^2 d^3x = 4\pi |N|^2 \int_a^\infty r^2 e^{-2\alpha r} dr = \frac{1}{2} \int_{u_0}^\infty u^2 e^{-u} du. \quad (3)$$

We've put $u = 2\alpha r$, and the (finite) lower limit is $u_0 = 2\alpha a = 3$, according to Eq. (2). Integral is again tabulated [Dwight #(567.2)], and we get:

$$\rightarrow P(\geq a) = \frac{1}{2}(u_0^2 + 2u_0 + 2) e^{-u_0} \Big|_{u_0 = 3}, \text{ or // } \boxed{P(\geq a) = \frac{17}{2} e^{-3} = 0.4232}. \quad (4)$$

It would be interesting to see how $P(\geq a)$ changes numerically were we to define "size" by $\langle r^n \rangle^{\frac{1}{n}}$, as noted above.

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* Relevant notion is that $|\psi|^2 d^3x$ is the probability that the system is found in d^3x.

ϕ506 MidTerm Solutions (Oct.'94)

④ [60 pts.]. Prove the QM version of the Virial Theorem: $\langle K\rangle = \frac{1}{2}\langle x(\partial V/\partial x)\rangle$.

A) 1. With $\langle Q\rangle = \langle\Psi|Q|\Psi\rangle$ denoting an expectation value, the QM Eq. of Motion gives:

$$\rightarrow \frac{d}{dt}\langle px\rangle = \frac{i}{\hbar}\langle[\mathcal{H}, px]\rangle + \cancel{\left\langle\frac{\partial}{\partial t}(px)\right\rangle}^{\,0} = \frac{i}{\hbar}\left\langle \frac{1}{2m}\underbrace{[p^2, px]}_{①} + \underbrace{[V, px]}_{②}\right\rangle. \quad (1)$$

The $\frac{\partial}{\partial t}$ vanishes because px does not depend explicitly on time. Commutators are:

$$① = [p^2, px] = p[p^2, x] + \cancel{[p^2, p]}^{\,0\text{(obvious)}}x = p\{p\underbrace{[p,x]}_{-i\hbar} + \underbrace{[p,x]}_{-i\hbar}p\}$$

$$\text{so// } \underline{① = -2i\hbar p^2} \quad (2)$$

We've used standard identities for commutators involving product operators [ref. prob$^{\text{m}}$ #⑳]. For commutator ②, use abbreviation: $\partial_x = \partial/\partial x$, and operate on some wavefcn $\phi(x)$ to be certain to catch all terms. Thus...

$$② = [V, px] = p\cancel{[V,x]}^{\,0\text{(obvious)}} + [V,p]x = -i\hbar[V, \partial_x]x$$

$$\text{so// } [V, px]\phi = -i\hbar[V, \partial_x](x\phi) = -i\hbar\{V\partial_x(x\phi) - \partial_x V(x\phi)\}$$

$$= -i\hbar\{\cancel{V\phi} + \cancel{Vx\partial_x\phi} - (\partial_x V)x\phi - \cancel{V\phi} - \cancel{Vx\partial_x\phi}\}$$

(cancel: $V\phi$ with $-V\phi$; $Vx\partial_x\phi$ with $-Vx\partial_x\phi$)

$$\text{or// } [V, px]\phi = +i\hbar\{x(\partial_x V)\}\phi, \text{ i.e.// } \underline{② = i\hbar\, x(\partial V/\partial x)}. \quad (3)$$

2. Put results ① & ② into Eq. (1) above to get... w// $K = p^2/2m$...

$$\boxed{\frac{d}{dt}\langle px\rangle = \frac{i}{\hbar}\left\langle -\frac{1}{2m}2i\hbar p^2 + i\hbar\, x\frac{\partial V}{\partial x}\right\rangle = 2\langle K\rangle - \langle x(\partial V/\partial x)\rangle}. \quad (4)$$

(B) 3. Eq. (4) holds for any QM state Ψ. For energy eigenstates $\Psi_E(x,t) = \phi_E(x)e^{-\frac{i}{\hbar}Et}$, the expectation value: $\langle px\rangle = \int_\infty \phi_E^*\{px\}\phi_E\,dx$, is time-indept., so $\frac{d}{dt}\langle px\rangle \equiv 0$. The LHS of (4) vanishes, and for the Ψ_E's, we can write, as required...

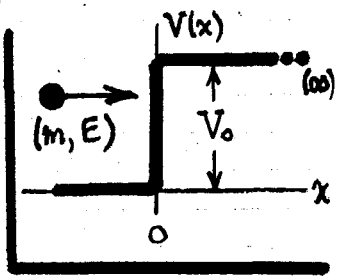
$$\boxed{\langle\Psi_E|K|\Psi_E\rangle = \frac{1}{2}\langle\Psi_E|x(\partial V/\partial x)|\Psi_E\rangle} \text{ , } \Psi_E \text{ an energy eigenstate} \quad (5)$$

NOTE: for a 1D SHO, $V = \frac{1}{2}kx^2$, and (5) gives the equipartition: $\langle K\rangle = \langle V\rangle$.

ϕ506 MidTerm Solutions (Oct '94)

(5) [60pts.]. Reflection of a particle from a 1D step-function potential barrier.

1) For the encounter shown at right, and with $E>0$, define...



→ $k=\sqrt{\frac{2mE}{\hbar^2}}$, free particle wave#; $\kappa=\sqrt{\frac{2m}{\hbar^2}(E-V_0)}$, interactive wave#. (1)

NOTE: when $E>V_0$, κ is real; when $E<V_0$, κ is imaginary.

Then m's wavefcns to the left and right of the step @ $x=0$ are...

$$\underline{x<0}: \psi(x) = e^{ikx} + Be^{-ikx} \quad \| \quad \underline{x>0}: \psi(x) = Ce^{i\kappa x} \qquad (2)$$

(e^{ikx}: unit (rightward) ampl.; $Ce^{i\kappa x}$: possible (rightward) ampl.)

These are plausible solns to $\psi'' + \frac{2m}{\hbar^2}(E-V)\psi = 0$ in the regions $x \lessgtr 0$. The QM enters by imposing that ψ & ψ' be <u>continuous</u> @ $x=0$.

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2) Imposition of continuity requires...

$$\left[\begin{array}{l} \psi \text{ cont}^{s} @\ x=0 \Rightarrow 1+B=C; \\ \psi' \text{ cont}^{s} @\ x=0 \Rightarrow ik(1-B)=i\kappa C; \end{array}\right] \quad \text{i.e.,} \quad \begin{array}{l} 1+B=C, \\ 1-B=\frac{\kappa}{k}C. \end{array} \qquad (3)$$

Add & subtract these last eqtns to find B & C, with result...

→ $C = 2k/(k+\kappa)$, $B = (k-\kappa)/(k+\kappa)$. (4)

This solution holds no matter whether κ is { real ($E>V_0$), or imag. ($E<V_0$).

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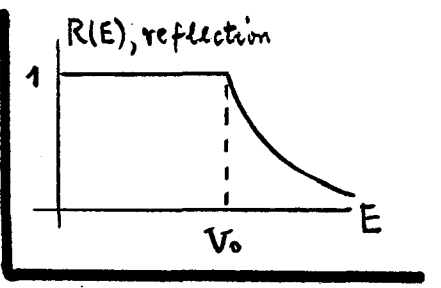
3) Define: $\mu = \sqrt{1-(V_0/E)}$. Then: $B = (1-\mu)/(1+\mu)$, and the reflection coefficient for this problem = leftward wave intensity @ $x<0$, i.e.

$$\boxed{R = |B|^2 = \left|\frac{1-\mu}{1+\mu}\right|^2, \quad \mu = \sqrt{1-(V_0/E)}} \qquad (5)$$



for $E>V_0$, μ is real, and $R<1$; ∴ some reflection at all finite E's; non-classical.

for $E<V_0$, μ is imag. and $R \equiv 1$ ∴ this means no transmission (obvious).