Modern Physics: Physics 305, Section 1

NAME:

Homework 6: 1-Dimensional Applications of Non-Relativistic Quantum Mechanics: Homeworks are due as posted on the course web site. They are **NOT** handed in. The student reports that it is completed and receives one point for this. Solutions are already posted, but students are only permitted to look at the solutions after completion. The solutions are intended to be (but not necessarily are) super-perfect and go beyond a complete answer expected on a test.

Answer Table for the Multiple-Choice Questions

	a	b	c	d	e		a	b	c	d	e
1.	O	O	O	O	O	16.	O	O	O	O	O
2.	O	O	O	O	O	17.	O	O	O	O	O
3.	O	O	O	O	O	18.	O	O	O	O	O
4.	O	O	O	O	O	19.	O	O	O	O	O
5.	O	O	O	O	O	20.	O	O	O	O	O
6.	O	O	O	O	O	21.	O	O	O	O	O
7.	O	O	O	O	O	22.	O	O	O	O	O
8.	O	O	O	O	O	23.	O	O	O	O	O
9.	O	O	O	O	O	24.	O	O	O	O	O
10.	O	O	O	O	O	25.	O	O	O	O	O
11.	O	O	O	O	O	26.	O	O	O	O	O
12.	O	O	O	O	O	27.	O	O	O	O	O
13.	O	O	O	O	O	28.	O	O	O	O	O
14.	O	O	O	O	O	29.	O	O	O	O	O
15.	O	O	O	O	O	30.	O	O	O	O	O

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003 qmult 00050 1 1 1 easy memory: infinite square well

1. In quantum mechanics, the infinite square well can be regarded as the prototype of:

   a) all bound systems. b) all unbound systems. c) both bound and unbound systems. d) neither bound nor unbound systems. e) Prometheus unbound.

   SUGGESTED ANSWER: (a)

   Wrong answers:

   e) Prometheus was chained to a rock with vultures perpetually munching his innards for giving fire to mortals. Herakles freed him at last, reconciling revolution and order (i.e., Prometheus and Zeus).

   Redaction: Jeffery, 2001jan01

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003 qmult 00100 2 4 2 moderate deducto-memory: infinite square well BCs

2. In the infinite square well problem, the wave function and its first spatial derivative are:

   a) both continuous at the boundaries.
   b) continuous and discontinuous at the boundaries, respectively.
   c) both discontinuous at the boundaries.
   d) discontinuous and continuous at the boundaries, respectively.
   e) both infinite at the boundaries.

   SUGGESTED ANSWER: (b)

   Wrong Answers:

   e) Can this ever be arranged for any system?

   Redaction: Jeffery, 2001jan01

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003 qmult 00300 1 1 3 easy memory: boundary conditions

3. Meeting the boundary conditions of bound quantum mechanical systems imposes:

   a) Heisenberg's uncertainty principle. b) Schrödinger's equation. c) quantization. d) a vector potential. e) a time-dependent potential.

   SUGGESTED ANSWER: (c)

   Wrong answers:

   e) Nah.

   Redaction: Jeffery, 2001jan01

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003 qmult 00400 1 1 5 easy memory: continuum of unbound states

4. At energies higher than the bound stationary states there:

   a) are between one and several tens of unbound states. b) are only two unbound states. c) is a single unbound state. d) are no states. e) is a continuum of unbound states.

   SUGGESTED ANSWER: (e)

   Wrong answers:

   d) This is only true for infinitely deep potential wells and such systems are only idealizations. No infinitely deep wells exist: you can always get out of a well.

   Redaction: Jeffery, 2001jan01

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003 qmult 00500 1 4 2 easy deducto-memory: tunneling

5. "Let's play *Jeopardy*! For $100, the answer is: This effect occurs because wave functions can extend (in an exponentially decreasing way albeit) into the classically forbidden region: i.e., the region where a classical particle would have negative kinetic energy."

   What is ____________, Alex?

a) stimulated radiative emission b) quantum mechanical tunneling c) quantization
d) symmetrization e) normalization

SUGGESTED ANSWER: (b)

Wrong answers:
d) Symmetrization is another fundamental property of quantum systems—but beyond our scope.

Redaction: Jeffery, 2001jan01

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003 qmult 00600 2 1 2 moderate memory: benzene ring model

6. A simple model of the outer electronic structure of a benzene molecule is a 1-dimensional infinite square well with:

a) vanishing boundary conditions. b) periodic boundary conditions.
c) aperiodic boundary conditions. d) no boundary conditions.
e) incorrect boundary conditions.

SUGGESTED ANSWER: (b)

Wrong Answers:
e) One can use incorrect boundary conditions as a simplification in cases where the boundary conditions have no significant effect. But in this case the system is small and correct boundary conditions are important.

Redaction: Jeffery, 2001jan01

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003 qfull 00100 2 3 0 moderate math: infinite square well in 1-d

7. You are given the time-independent Schrödinger equation

$$H\psi(x) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) = E\psi(x)$$

and the infinite square well potential

$$V(x) = \begin{cases} 0\,, & x \in [0,a]; \\ \infty & \text{otherwise.} \end{cases}$$

a) What must the wave function be outside of the well (i.e., outside of the region $[0,a]$) in order to satisfy the Schrödinger equation? Why?

b) What boundary conditions must the wave function satisfy? Why must it satisfy these boundary conditions?

c) Reduce Schrödinger's equation inside the well to an equation of the same form as the **CLASSICAL** simple harmonic oscillator equation with all the constants combined into a factor of $-k^2$, where k is newly defined constant. What is k's definition?

d) Solve for the general solution for a **SINGLE** k value, but don't impose boundary conditions or normalization yet. A solution by inspection is adequate. Why can't we allow solutions with $E \le 0$? Think carefully: it's not because k is imaginary when $E < 0$.

e) Use the boundary conditions to eliminate most of the solutions with $E > 0$ and to impose quantization on the allowed set of distinct solutions (i.e., on the allowed k values). Give the general wave function with the boundary conditions imposed and give the quantization rule for k in terms of a dimensionless quantum number n. Note that the multiplication of a wave function by an arbitrary global phase factor $e^{i\phi}$ (where ϕ is arbitrary) does not create a physically distinct wave function (i.e., does not create a new wave function as recognized by nature.) (Note the orthogonality relation used in expanding general functions in eigenfunctions also does not distinguish eigenfunctions that differ by global phase factors either: i.e., it gives the expansion coefficients only for distinct eigenfunctions. So the idea of distinct eigenfunctions arises in pure mathematics as well as in physics.)

f) Normalize the solutions.

g) Determine the general formula for the eigenenergies in terms of the quantum number n.

SUGGESTED ANSWER:

a) Outside the well any wave function is zero in order to satisfy the Schrödinger equation. This is because if the potential goes to infinity over a finite region, the only reasonable way to satisfy the Schrödinger equation is with a zero wave function in that region.

b) For a finite potential the wave function and its 1st derivative must be continuous: the 1st derivative is allowed to have kinks. If the potential becomes infinite at a point, then the first derivative is allowed to have finite discontinuities and the wave function is allowed to have kinks at that point. In our case, all the well walls require by themselves is that the wave function be continuous there and thus be zero there. It is known (but exactly how is seldom gone into) that in this case no condition is imposed on the continuity of the 1st derivative of the wave function and no condition is needed. I append a note discussing the continuity of the wave function and its 1st derivative below: it's prolix.

c) Inside the well one has

$$H\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi \ .$$

Defining

$$k = \frac{\sqrt{2mE}}{\hbar} \ ,$$

we obain

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi \ .$$

This last equation has the same form as the classical simple harmonic oscillator equation.

d) By inspection and lots of experience, the general solution for $E > 0$ is

$$\psi(x) = A\sin(kx) + B\cos(kx) \ ,$$

where A and B are constants. This solution, of course, only applies inside the well. Outside of the well $\psi = 0$ everywhere.

We cannot allow $E \leq 0$ as we show in the following. If we did allow $E \leq 0$, we would have the differential equation

$$\frac{\partial^2\psi}{\partial x^2} = \kappa^2\psi \ ,$$

where

$$\kappa = \frac{\sqrt{2m|E|}}{\hbar} \ .$$

Note by our definition, k would be imaginary in this case, but that has no consequence since the eigenvalues in our Hermitian operator equation for $E \leq 0$ are still real.

For $E < 0$, the general solution is

$$\psi = Ae^{\kappa x} + Be^{-\kappa x} \ ,$$

where A and B are constants. Neither of the terms of this solution are ever zero (unless $A = B = 0$) and since one term is strictly increasing and the other strictly decreasing, only one zero can be created by linear combination. The linear combination that gives the one zero at any x satisfies the ratio

$$\frac{A}{B} = -e^{-2\kappa x} \ .$$

Because there is only one zero at most, the $E < 0$ solution cannot satisfy the boundary conditions and must be ruled out. For $E = 0$, the general solution is

$$\psi = Ax + B \ ,$$

where A and B are constants. This solution can only be zero at one point (unless $A = B = 0$), and thus cannot satisfy the boundary conditions and must be ruled out. If $A = B = 0$ for

$E \leq 0$, the boundary conditions are satisfied, but the solutions cannot be normalized, and so must be ruled out. So all cases of $E \leq 0$ give physically invalid solutions.

Note there is a general proof that $E > V_{\rm min}$, except that $E = V_{\rm min}$ is allowed for a constant wave function solution to a system with periodic boundary conditions: see the solution to the problem suggested by Griffiths's problem Gr-24:2.2. For the infinite square well, the boundary conditions are not periodic and $V_{\rm min} = 0$. Thus we find that solutions must have $E > 0$ by the general proof.

e) To satisfy the boundary conditions (ψ continuous, but no continuity constraint on $\partial\psi/\partial x$ because of the infinite potential), we must have $\psi(0) = \psi(ka) = 0$. Thus, $B = 0$ (i.e., no cosine solutions are allowed) and

$$k = \frac{n\pi}{a} ,$$

where n must be an integer. The fact that n must be an integer gives the quantization of allowed states: the boundary conditions have imposed this quantization, in fact. The number n is the dimensionless quantum number.

The $n = 0$ case gives a zero eigenfunction which cannot be normalized and the negative n values because of the oddness of the sine function do not give physically distinct solutions from their positive counterparts (i.e, the $-n$ values). Recall wave functions that differ by a global phase factor (i.e., $e^{i\phi}$ where ϕ is any number) are not physically distinct: nature does not recognize them as different states. There are actually infinitely many mathematical states for each physically distinct state.

Finally, we find that n runs over all positive integers only: $n = 1, 2, 3, \ldots$ The allowed solutions are

$$\psi_n(x) = A \sin\left(\frac{n\pi}{a}x\right) .$$

A few other remarks can be made. We can see that k is in fact a wavenumber since the solution is periodic for every $\Delta x = 2\pi/k$. The wavelength λ is in fact that Δx:

$$\lambda = \frac{2\pi}{k} = \frac{2a}{n} .$$

Consequently, we find

$$n\frac{\lambda}{2} = a$$

which implies that the nth wave function will have n antinodes and $n + 1$ nodes. Two of the nodes are on the boundaries, of course.

f) For normalization we require

$$\begin{aligned}
1 &= A^2 \int_0^a \sin^2(kx)\,dx = A^2 \frac{1}{k} \int_0^{ka} \sin^2(y)\,dy \\
&= A^2 \frac{1}{2k} \int_0^{ka} [1 - \cos(2y)]\,dy \\
&= A^2 \frac{1}{2k} \left[y - \frac{\sin(2y)}{2} \right] \Bigg|_0^{ka=n\pi} \\
&= A^2 \frac{1}{2k}(ka) \\
&= A^2 \frac{a}{2} ,
\end{aligned}$$

and thus

$$A = \sqrt{\frac{2}{a}} ,$$

where we have chosen A to be pure real. Thus the normalized general solution is

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) .$$

g) The energy of the nth eigenstate is given by

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2 \ .$$

Thus the energies are quantized with n being the quantum number. The quantization is imposed by the boundary conditions and the requirement of normalizability. All bound quantum states are in fact quantized. But we won't prove that here.

NOTE: Herein we consider the continuity properties of the wave function and its 1st derivative at some length. This note has never been perfected. Once we go to the infinite potential case, it's just maundering on and has to be all cleaned up when I get a chance.

First note that the time independent Schrödinger equation leads directly to the following integral

$$\left.\frac{\partial\psi}{\partial x}\right|_{a+\epsilon} - \left.\frac{\partial\psi}{\partial x}\right|_{a-\epsilon} = \int_{a-\epsilon}^{a+\epsilon} dx\,\frac{\partial^2\psi}{\partial x^2} = \int_{a-\epsilon}^{a+\epsilon} dx\,\frac{2m}{\hbar^2}\left[V(x)-E\right]\psi(x) \ ,$$

where a is any point and ϵ is a small displacement parameter. It is a given that E is finite or zero. If the potential and wave function are finite or zero everywhere, we find

$$\lim_{\epsilon\to 0}\left[\left.\frac{\partial\psi}{\partial x}\right|_{a+\epsilon} - \left.\frac{\partial\psi}{\partial x}\right|_{a-\epsilon}\right] = 0 \ .$$

This result follows even V or $\psi(x)$ is discontinuous at a: the integral is still of a finite integrand over a zero area in the limit that $\epsilon \to 0$.

Thus the 1st derivative of the wave function must be continuous at points of finite potential and wave function: kinks in the 1st derivative are allowed in principle. But if the 1st derivative is continuous, then the wave function itself must be continuous and kink-free. A kink in the wave function causes a discontinuity in the 1st derivative and a discontinuity in the wave function causes an infinite discontinuity in the 1st derivative.

To sum up, if V is finite or zero, then the wave function must be continuous and kink-free. The 1st derivative is allowed have kinks. Note V can be discontinuous.

Now what if potential goes to positive infinity? First let us consider the case where there is an infinite potential over a finite region. We set one boundary of the infinite wall at $x = 0$ for convenience.

To find the solution let us first allow the potential to be a finite constant V for $x < 0$. For $x > 0$, we set the potential to 0. I think we can always consider zones close enough to the wall that the potential on either side can be considered as constants. We assume $0 < E < V$: I don't think this is unduly restrictive: recall $E > V_{\text{mininim}}$, except for periodic boundary condition cases (Gr-24). The solutions close the wall are

$$\psi(x) = Ae^{\kappa x} \qquad \text{and} \qquad \psi(x) = B\sin(kx) + C\cos(kx) \ ,$$

where

$$\kappa = \pm\sqrt{\frac{2m}{\hbar^2}(V-E)} \qquad \text{and} \qquad k = \pm\sqrt{\frac{2m}{\hbar^2}E} \ .$$

Only the positive solution for κ is allowed by the normalizability condition. We cannot specify A, B, and C exactly without defining the whole potential and finding an expression for the whole wave function. We don't want to do that since we are trying to see if can get a general understanding.

Since we are first considering a finite wall, we require continuous wave function and its 1st derivative. Thus at $x = 0$ we demand

$$A = C \qquad \text{and} \qquad A\kappa = Bk \ .$$

Now if we let V become large, $\psi(x < 0)$ must become small and thus A and C must become small. But nothing demands that Bk become small since κ is growing large as V grows large. If we let $V \to \infty$, then A and C go to zero, but Bk can stay non-zero since $A\kappa$ can stay non-zero and finite. In this way wave function stays continuous at $x = 0$ and in a limiting sense so does its 1st derivative even though in direct sense there is discontinuity in the 1st derivative.

But does nature take the limit such that $A\kappa$ stays finite non-zero? Well nature certainly doesn't let $A\kappa$ go to infinity since that would make Bk go to infinity which seems implausible. If $A\kappa$ goes to zero, then either B or k goes to zero and then the wave function and its 1st derivative are both zero at $x = 0$. If one requires the wave function and its 1st derivative to be zero at the wall, then there are no solutions to the infinite square well problem. We know in nature that systems approaching the infinite square well do have a spectrum of solutions, and so conclude that does take the limit such that Bk stays finite non-zero.

But one doesn't really like to appeal to observation. Isn't there some general mathematical argument? Since for any specific system, there is a mathematical solution for A and if it always gives $A\kappa = Bk$ for when $V \to \infty$ (as we seem to think nature demands), then there must be some general mathematical proof that $A\kappa = Bk$ for when $V \to \infty$. But I can't see what it could be?

Maybe I'm being over-idealizing. There are no infinite potentials nor even any finite, sharp wall potentials. Maybe nearly sharp finite wall potential approximated as sharp infinite wall potential just allows one to use only the continuity condition on the wave function because one is admitting at the outset one isn't treating the wave function in the neighborhood of the nearly sharp wall at all correctly. Anyway Gr-60 treats the finite square well, but that doesn't elucidate the general sharp wall case for me.

The following may be gibberish: I've no patience right now to figure out if I was talking sense when I wrote it.

So far so good: now on to the pathological cases. Can the wave function be infinite? Not over a finite region for that would give an infinite probability of finding the particle in that region: a probability greater than 1 is not allowed. Can we allow a Dirac delta region of the wave function? In the limiting sense of a very highly peaked wave function region I don't see why not, but I confess I don't know how to treat a Dirac delta function magnitude squared (which is probability density). The 1st derivative could be discontinuous across the Dirac delta function region, but only by a finite amount. Thus the wave function will be continuous if kinked across the Dirac delta region (not counting where it shoots to "infinity"). So in a sense the wave function must be continuous even if it shoots at a point to a Dirac delta infinity.

What if the potential shoots to a Dirac delta infinity at point a? Well the 1st derivative can have a finite discontinuity, but the wave function must stay continuous. But the wave function doesn't have to go to zero at a. What if the potential shoots to more than a Dirac delta infinity at a point. Well this is a physically impossible case. No potential is really ever infinite and a Dirac delta infinity is just a way of compress a very high potential that acts over a small region into a neat mathematical form.
We leave further thought on this *sine die*.

We have considered an infinite wall, but what a about an infinite drop potential. Well below the drop the drop looks like an infinite wall. So this case reduces to the last. The particle is always on the drop side.

We could go on considering pathological cases all night, but enough already. Infinite potentials are an idealization anyway. Still it's necessary to know how to treat them in the correct limiting way.

Redaction: Jeffery, 2001jan01

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003 qfull 00450 2 3 0 moderate math: infinie square well features

8. The one-dimensional infinite square well with a symmetric potential and width a is

$$V = \begin{cases} 0 & \text{for } |x| \le a/2; \\ \infty & \text{for } |x| > a/2. \end{cases}$$

The eigenstates for infinite square well are given by

$$\psi_n(x) = \sqrt{\frac{2}{a}} \times \begin{cases} \cos(kx) & \text{for } n = 1, 3, 5 \ldots; \\ \sin(kx) & \text{for } n = 2, 4, 6 \ldots, \end{cases}$$

where

$$\frac{ka}{2} = \frac{n\pi}{2} \qquad \text{and} \qquad k = \frac{n\pi}{a} \; .$$

The n is the quantum number for eigenstates. The eigenstates have been normalized and are guaranteed orthogonal by the mathematics of Hermitian operators of the which the Hamiltonian is one. A quantum number is a dimensionless index (usually integer or half-integer) that specifies the eigenstates and eigenvalues somehow. The eigen-energies are given by

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2 .$$

a) Verify the normalization of eigenstates.

b) Determine $\langle x \rangle$ for the eigenstates.

c) Determine $\langle p_{\rm op} \rangle$ for the eigenstates. **HINT:** Recall

$$p_{\rm op} = \frac{\hbar}{i}\frac{\partial}{\partial x} .$$

d) Determine $\langle p_{\rm op}^2 \rangle$ and the momentum standard deviation $\sigma_{\rm p}$ for the eigenstates.

e) Determine $\langle x^2 \rangle$ and the position standard deviation σ_x in the large n limit. **HINT:** Assume x^2 can be approximated constant over one complete cycle of the probability density $\psi_n^*\psi_n$

f) Now for the boring part. Determine $\langle x^2 \rangle$ and the position standard deviation σ_x exactly now. **HINT:** There probably are several different ways of doing this, but there seem to be no quick tricks to the answer. The indefinite integral

$$\int x^2 \cos(bx)\,dx = \frac{x^2}{b}\sin(bx) + \frac{2}{b^2}x\cos(bx) - \frac{2}{b^3}\sin(bx)$$

might be helpful.

g) Verify that the Heisenberg uncertainty principle

$$\Delta x \Delta p = \sigma_x \sigma_p \geq \frac{\hbar}{2}$$

is satisfied for the infinite square well case.

SUGGESTED ANSWER:

a) Behold:

$$\begin{aligned} 1 &= A^2 \int_{-a/2}^{a/2} \left\{ \begin{array}{c} \cos^2(kx) \\ \sin^2(kx) \end{array} \right\} dx = A^2(2)\int_0^{a/2} \frac{1}{2}\left[1 \pm \cos(2kx)\right] dx \\ &= A^2 \left[x \pm \frac{\sin(2kx)}{2k} \right] \Bigg|_0^{a/2} = A^2 \left[\frac{a}{2} \pm \frac{\sin(2ka)}{2k} \right] \\ &= A^2 \frac{a}{2} , \end{aligned}$$

where we have used the evenness of the integrands and the fact that $2ka = n(2\pi)$. We find that the normalization factor is

$$A = \sqrt{\frac{2}{a}}$$

for all n.

b) Well

$$\langle x \rangle = \frac{2}{a}\int_{-a/2}^{a/2} x \left\{ \begin{array}{c} \cos^2(kx) \\ \sin^2(kx) \end{array} \right\} dx = 0$$

in all cases by the oddness of the integrands.

c) Well

$$\langle p_{\rm op}\rangle = \frac{2}{a}\int_{-a/2}^{a/2} \left\{ \begin{array}{c} \cos(kx)p_{\rm op}\cos(kx) \\ \sin(kx)p_{\rm op}\sin(kx) \end{array} \right\} dx$$

must be zero in any right-thinking universe since the expectation values are guaranteed real for a Hermitian operator like $p_{\rm op}$ and integrands are pure imaginary if they are not zero. But to be explicit

$$\langle p_{\rm op}\rangle = \frac{2}{a}\frac{\hbar k}{i}\int_{-a/2}^{a/2} \left\{ \begin{array}{c} -\cos(kx)\sin(kx) \\ \sin(kx)\cos(kx) \end{array} \right\} dx = 0$$

by the oddness of the integrands.

d) Behold:

$$\langle p_{\rm op}^2\rangle = \int_{-a/2}^{a/2} \psi_n^* p_{\rm op}^2 \psi_n\, dx = \frac{\hbar^2}{-1}(-k^2)\int_{-a/2}^{a/2} \psi_n^*\psi_n\, dx = \hbar^2 k^2 \ ,$$

where we have used normalization. The standard deviation of $p_{\rm op}$ is

$$\sigma_p = \sqrt{\langle p_{\rm op}^2\rangle - \langle p_{\rm op}\rangle^2} = \hbar k = \hbar\frac{n\pi}{a} \ .$$

e) In the large n limit, we can assume that x^2 is constant over the scale of a complete cycle of the probability density $\psi_n^*\psi_n$. Well the average probability density over a cycle is

$$\begin{aligned} \frac{1}{\lambda/2}\int_0^{\lambda/2} \frac{2}{a}\left\{ \begin{array}{c} \cos^2(kx) \\ \sin^2(kx) \end{array} \right\} dx &= \frac{1}{\pi}\int_0^{\pi} \frac{2}{a}\left\{ \begin{array}{c} \cos^2(y) \\ \sin^2(y) \end{array} \right\} dy = \frac{1}{\pi}\int_0^{\pi} \frac{2}{a}\frac{1}{2}\left[1 \pm \cos(2y)\right] dy \\ &= \frac{1}{\pi}\frac{1}{a}\left[x \mp \frac{\sin(2y)}{2}\right]\Bigg|_0^{\pi} \\ &= \frac{1}{a} \ . \end{aligned}$$

This is result is—and maybe it should have not been a surprise—the probability of a flat probability density over the well.

Now we find for the large n limit

$$\langle x^2\rangle = \int_{-a/2}^{a/2} \frac{x^2}{a}\, dx = 2\int_0^{a/2} \frac{x^2}{a}\, dx = 2\frac{x^3}{3a}\Bigg|_0^{a/2} = \frac{a^2}{12} \ .$$

The standard deviation of x in the large n limit is

$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \frac{a}{\sqrt{12}} = \frac{a}{2\sqrt{3}} \ .$$

f) Behold:

$$\begin{aligned} \langle x^2\rangle &= \frac{2}{a}(2)\int_0^{a/2} x^2 \left\{ \begin{array}{c} \cos^2(kx) \\ \sin^2(kx) \end{array} \right\} dx \\ &= \frac{4}{ak^3}\int_0^{n\pi/2} y^2 \left\{ \begin{array}{c} \cos^2(y) \\ \sin^2(y) \end{array} \right\} dy \\ &= \frac{2}{ak^3}\int_0^{ka/2} y^2\left[1 \pm \cos(2y)\right] dy \\ &= \frac{a^2}{12} \pm \frac{2}{ak^3}\int_0^{ka/2} y^2\cos(2y)\, dy \\ &= \frac{a^2}{12} \pm \frac{2}{ak^3}\left[\frac{x^2}{2}\sin(2x) + \frac{2}{2^2}x\cos(2x) - \frac{2}{2^3}\sin(2x)\right]\Bigg|_0^{ka/2=n\pi/2} \end{aligned}$$

$$
\begin{aligned}
&= \frac{a^2}{12} \pm \frac{2}{ak^3}\frac{1}{2}ka/2\cos(n\pi) \\
&= \frac{a^2}{12} \pm \frac{a^2}{2\pi^2 n^2}(-1)^n \\
&= \frac{a^2}{12} + (-1)^{n+1}\frac{a^2}{2\pi^2 n^2}(-1)^n \\
&= \frac{a^2}{12} - \frac{a^2}{2\pi^2 n^2}(-1)^n \\
&= \frac{a^2}{12}\left[1 - \frac{6}{\pi^2 n^2}\right]
\end{aligned}
$$

which isn't half bad to look at. Compactly

$$
\langle x^2\rangle = \frac{a^2}{12}\begin{cases} 1 - \dfrac{6}{\pi^2 n^2} & \text{in general;} \\ 1 - \dfrac{6}{\pi^2} \approx \dfrac{1}{3} & \text{for } n = 1; \\ 1 - \dfrac{3}{2\pi^2} \approx \dfrac{5}{6} & \text{for } n = 2; \\ 1 & \text{for } n \text{ large.} \end{cases}
$$

The standard deviation of x

$$
\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \frac{a}{2\sqrt{3}}\sqrt{1 - \frac{6}{\pi^2 n^2}} \ .
$$

g) Behold:

$$
\Delta x \Delta p = \sigma_x \sigma_p = \frac{a}{2\sqrt{3}}\sqrt{1 - \frac{6}{\pi^2 n^2}}\,\hbar\frac{n\pi}{a} = \hbar\frac{n\pi}{2\sqrt{3}}\sqrt{1 - \frac{6}{\pi^2 n^2}} \geq= \hbar\frac{\pi}{2\sqrt{3}}\sqrt{1 - \frac{6}{\pi^2}} \approx \hbar\frac{\pi}{6} =\approx \frac{\hbar}{2} \ ,
$$

where the inequality is for $n = 1$ which clearly gives the smallest case. A more exact calculation of the $n = 1$ case gives

$$
\Delta x \Delta p = \sigma_x \sigma_p \geq \hbar \times 0.567861808386611\ldots > \frac{\hbar}{2}
$$

Thus, the infinite square well is consistent with the uncertainty principle.

It can, in fact, be shown that only a Gaussian wave function gives

$$
\Delta x \Delta p = \sigma_x \sigma_p = \frac{\hbar}{2}
$$

(Gr-111—112).

Fortran-95 Code

```
        print*
        con=(pi/(2.d0*sqrt(3.d0)))*sqrt(1.d0-6.d0/(pi**2))
        print*,'con'
        print*,con
!   0.5678618083866119
```

Redaction: Jeffery, 2008jan01

Equation Sheet for Modern Physics

These equation sheets are intended for students writing tests or reviewing material. Therefore they are neither intended to be complete nor completely explicit. There are fewer symbols than variables, and so some symbols must be used for different things: context must distinguish.

The equations are mnemonic. Students are expected to understand how to interpret and use them.

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1 Geometrical Formulae

$$C_{\rm cir} = 2\pi r \qquad A_{\rm cir} = \pi r^2 \qquad A_{\rm sph} = 4\pi r^2 \qquad V_{\rm sph} = \frac{4}{3}\pi r^3$$

---

2 Trigonometry

$$\frac{x}{r} = \cos\theta \qquad \frac{y}{r} = \sin\theta \qquad \frac{y}{x} = \tan\theta \qquad \cos^2\theta + \sin^2\theta = 1$$

$$\sin(a+b) = \sin(a)\cos(b) + \cos(a)\sin(b) \qquad \cos(a+b) = \cos(a)\cos(b) - \sin(a)\sin(b)$$

$$\cos^2\theta = \frac{1}{2}[1+\cos(2\theta)] \qquad \sin^2\theta = \frac{1}{2}[1-\cos(2\theta)] \qquad \sin(2\theta) = 2\sin(\theta)\cos(\theta)$$

$$\cos(a)\cos(b) = \frac{1}{2}\left[\cos(a-b)+\cos(a+b)\right] \qquad \sin(a)\sin(b) = \frac{1}{2}\left[\cos(a-b)-\cos(a+b)\right]$$

$$\sin(a)\cos(b) = \frac{1}{2}\left[\sin(a-b)+\sin(a+b)\right]$$

---

3 Blackbody Radiation

$$B_\nu = \frac{2h\nu^3}{c^2}\frac{1}{\left[e^{h\nu/(kT)}-1\right]} \qquad B_\lambda = \frac{2hc^2}{\lambda^5}\frac{1}{\left[e^{hc/(kT\lambda)}-1\right]}$$

$$B_\lambda\,d\lambda = B_\nu\,d\nu \qquad \nu\lambda = c \qquad \frac{d\nu}{d\lambda} = -\frac{c}{\lambda^2}$$

$$k = 1.3806505(24)\times10^{-23}\,\text{J/K} \qquad c = 2.99792458\times10^{8}\,\text{m}$$

$$h = 6.6260693(11)\times10^{-34}\,\text{J s} = 4.13566743(35)\times10^{-15}\,\text{eV s}$$

$$\hbar = \frac{h}{2\pi} = 1.05457168(18)\times10^{-34}\,\text{J s}$$

$$hc = 12398.419\,\text{eV Å} \approx 10^4\,\text{eV Å} \qquad E = h\nu = \frac{hc}{\lambda} \qquad p = \frac{h}{\lambda}$$

$$F = \sigma T^4 \qquad \sigma = \frac{2\pi^5}{15}\frac{k^4}{c^2h^3} = 5.670400(40) \times 10^{-8}\,\mathrm{W/m^2/K^4}$$

$$\lambda_{\max} T = \text{constant} = \frac{hc}{kx_{\max}} \approx \frac{1.4387751 \times 10^{-2}}{x_{\max}}$$

$$B_{\lambda,\mathrm{Wien}} = \frac{2hc^2}{\lambda^5} e^{-hc/(kT\lambda)} \qquad B_{\lambda,\mathrm{Rayleigh-Jeans}} = \frac{2ckT}{\lambda^4}$$

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{c}\nu = \frac{\omega}{c} \qquad k_i = \frac{\pi}{L} n_i \quad \text{standing wave BCs} \qquad k_i = \frac{2\pi}{L} n_i \quad \text{periodic BCs}$$

$$n(k)\,dk = \frac{k^2}{\pi^2}\,dk = \pi\left(\frac{2}{c}\right)\nu^2\,d\nu = n(\nu)\,d\nu$$

$$\ln(z!) \approx \left(z + \frac{1}{2}\right)\ln(z) - z + \frac{1}{2}\ln(2\pi) + \frac{1}{12z} - \frac{1}{360z^3} + \frac{1}{1260z^5} - \ldots$$

$$\ln(N!) \approx N\ln(N) - N$$

$$\rho(E)\,dE = \frac{e^{-E/(kT)}}{kT}\,dE \qquad P(n) = (1 - e^{-\alpha})e^{-n\alpha} \qquad \alpha = \frac{h\nu}{kT}$$

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2} \qquad f(x - vt) \qquad f(kx - \omega t)$$

---

4 Photons

$$KE = h\nu - w \qquad \Delta\lambda = \lambda_{\mathrm{scat}} - \lambda_{\mathrm{inc}} = \lambda_{\mathrm{C}}(1 - \cos\theta)$$

$$\lambda_{\mathrm{C}} = \frac{h}{m_e c} = 2.426310238(16) \times 10^{-12}\,\mathrm{m} \qquad e = 1.602176487(40) \times 10^{-19}\,\mathrm{C}$$

$$m_e = 9.1093826(16) \times 10^{-31}\,\mathrm{kg} = 0.510998918(44)\,\mathrm{MeV}$$

$$m_p = 1.67262171(29) \times 10^{-27}\,\mathrm{kg} = 938.272029(80)\,\mathrm{MeV}$$

$$\ell = \frac{1}{n\sigma} \qquad \rho = \frac{e^{-s/\ell}}{\ell} \qquad \langle s^m \rangle = \ell^m m!$$

---

5 Matter Waves

$$\lambda = \frac{h}{p} \qquad p = \hbar k \qquad \Delta x \Delta p \geq \frac{\hbar}{2} \qquad \Delta E \Delta t \geq \frac{\hbar}{2}$$

$$\Psi(x,t) = \int_{-\infty}^{\infty} \phi(k)\Psi_k(x,t)\,dk \qquad \phi(k) = \int_{-\infty}^{\infty} \Psi(x,0)\frac{e^{-ikx}}{\sqrt{2\pi}}\,dk$$

$$v_{\rm g} = \left.\frac{d\omega}{dk}\right|_{k_0} = \frac{\hbar k_0}{m} = \frac{p_0}{m} = v_{\rm clas,0}$$

---

6 Non-Relativistic Quantum Mechanics

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V \qquad T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \qquad H\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi = i\hbar\frac{\partial \Psi}{\partial t}$$

$$\rho = \Psi^*\Psi \qquad \rho\,dx = \Psi^*\Psi\,dx$$

$$A\phi_i = a_i\phi_i \qquad f(x) = \sum_i c_i\phi_i \qquad \int_a^b \phi_i^*\phi_j\,dx = \delta_{ij} \qquad c_j = \int_a^b \phi_j^* f(x)\,dx \qquad [A,B] = AB - BA$$

$$P_i = |c_i|^2 \qquad \langle A\rangle = \int_{-\infty}^{\infty} \Psi^* A\Psi\,dx = \sum_i |c_i|^2 a_i \qquad H\psi = E\psi \qquad \Psi(x,t) = \psi(x)e^{-i\omega t}$$

$$p_{\rm op}\phi = \frac{\hbar}{i}\frac{\partial\phi}{\partial x} = p\phi \qquad \phi = \frac{e^{ikx}}{\sqrt{2\pi}} \qquad \frac{\partial^2\psi}{\partial x^2} = \frac{2m}{\hbar^2}(V-E)\psi$$

$$|\Psi\rangle \qquad \langle\Psi| \qquad \langle x|\Psi\rangle = \Psi(x) \qquad \langle\vec{r}|\Psi\rangle = \Psi(\vec{r}) \qquad \langle k|\Psi\rangle = \Psi(k) \qquad \langle\Psi_i|\Psi_j\rangle = \langle\Psi_j|\Psi_i\rangle^*$$

$$\langle\phi_i|\Psi\rangle = c_i \qquad 1_{\rm op} = \sum_i |\phi_i\rangle\langle\phi_i| \qquad |\Psi\rangle = \sum_i |\phi_i\rangle\langle\phi_i|\Psi\rangle = \sum_i c_i|\phi_i\rangle$$

$$1_{\rm op} = \int_{-\infty}^{\infty} dx\,|x\rangle\langle x| \qquad \langle\Psi_i|\Psi_j\rangle = \int_{-\infty}^{\infty} dx\,\langle\Psi|x\rangle\langle x|\Psi\rangle \qquad A_{ij} = \langle\phi_i|A|\phi_j\rangle$$

$$Pf(x) = f(-x) \qquad P\frac{df(x)}{dx} = \frac{df(-x)}{d(-x)} = -\frac{df(-x)}{dx} \qquad Pf_{\rm e/o}(x) = \pm f_{\rm e/o}(x) \qquad P\frac{df_{\rm e/o}(x)}{dx} = \mp\frac{df_{\rm e/o}(x)}{dx}$$

---

7 Special Relativity

$$c = 2.99792458 \times 10^8\,\text{m/s} \approx 2.998 \times 10^8\,\text{m/s} \approx 3 \times 10^8\,\text{m/s} \approx 1\,\text{lyr/yr} \approx 1\,\text{ft/ns}$$

$$\beta = \frac{v}{c} \qquad \gamma = \frac{1}{\sqrt{1-\beta^2}} \qquad \gamma(\beta << 1) = 1 + \frac{1}{2}\beta^2 \qquad \tau = ct$$

Galilean Transformations	Lorentz Transformations
$x' = x - \beta\tau$	$x' = \gamma(x - \beta\tau)$
$y' = y$	$y' = y$
$z' = z$	$z' = z$
$\tau' = \tau$	$\tau' = \gamma(\tau - \beta x)$
$\beta'_{\text{obj}} = \beta_{\text{obj}} - \beta$	$\beta'_{\text{obj}} = \dfrac{\beta_{\text{obj}} - \beta}{1 - \beta\beta_{\text{obj}}}$

$$\ell = \ell_{\text{proper}}\sqrt{1-\beta^2} \qquad \Delta\tau_{\text{proper}} = \Delta\tau\sqrt{1-\beta^2}$$

$$m = \gamma m_0 \qquad p = mv = \gamma m_0 c\beta \qquad E_0 = m_0 c^2 \qquad E = \gamma E_0 = \gamma m_0 c^2 = mc^2$$

$$E = mc^2 \qquad E = \sqrt{(pc)^2 + (m_0c^2)^2}$$

$$KE = E - E_0 = \sqrt{(pc)^2 + (m_0c^2)^2} - m_0c^2 = (\gamma - 1)m_0c^2$$

$$f = f_{\text{proper}}\sqrt{\frac{1-\beta}{1+\beta}} \quad \text{for source and detector separating}$$

$$f(\beta << 1) = f_{\text{proper}}\left(1 - \beta + \frac{1}{2}\beta^2\right)$$

$$f_{\text{trans}} = f_{\text{proper}}\sqrt{1-\beta^2} \qquad f_{\text{trans}}(\beta << 1) = f_{\text{proper}}\left(1 - \frac{1}{2}\beta^2\right)$$

$$\tau = \beta x + \gamma^{-1}\tau' \quad \text{for lines of constant } \tau'$$

$$\tau = \frac{x - \gamma^{-1}x'}{\beta} \quad \text{for lines of constant } x'$$

$$x' = \frac{x_{\text{intersection}}}{\gamma} = x'_{x\text{ scale}}\sqrt{\frac{1-\beta^2}{1+\beta^2}} \qquad \tau' = \frac{\tau_{\text{intersection}}}{\gamma} = \tau'_{\tau\text{ scale}}\sqrt{\frac{1-\beta^2}{1+\beta^2}}$$

$$\theta_{\text{Mink}} = \tan^{-1}(\beta)$$