Columbia University
Department of Physics
QUALIFYING EXAMINATION

Wednesday, January 16, 2019
10:00AM to 12:00PM
Modern Physics
Section 3. Quantum Mechanics

Two hours are permitted for the completion of this section of the examination. Choose 4 problems out of the 5 included in this section. (You will not earn extra credit by doing an additional problem). Apportion your time carefully.

Use separate answer booklet(s) for each question. Clearly mark on the answer booklet(s) which question you are answering (e.g., Section 3 (Quantum Mechanics), Question 2, etc.).

Do **NOT** write your name on your answer booklets. Instead, clearly indicate your **Exam Letter Code**.

You may refer to the single handwritten note sheet on $8\frac{1}{2}$" × 11" paper (double-sided) you have prepared on Modern Physics. The note sheet cannot leave the exam room once the exam has begun. This note sheet must be handed in at the end of today's exam. Please include your Exam Letter Code on your note sheet. No other extraneous papers or books are permitted.

Simple calculators are permitted. However, the use of calculators for storing and/or recovering formulae or constants is NOT permitted.

Questions should be directed to the proctor.

Good Luck!

1. Consider a free particle in one dimension with mass m. At time $t = 0$ the expectation value of its position is $\langle x \rangle_0$, with a variance $(\Delta x)_0^2 = \langle x^2 \rangle_0 - \langle x \rangle_0^2$. Find the variance at some later time t. Express your answer in terms of t and expectation values of operators at $t = 0$, including the operators x, p, and combinations thereof.

2. Consider a particle in one dimension subject to a harmonic potential. The Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2} m\,\omega^2\,x^2.$$

Suppose that for $t < 0$ the particle is in the ground state of H. At $t = 0$, the particle is suddenly "liberated", in the sense that the potential is very quickly tuned to zero, and from that moment on the particle behaves as a free particle.

(a) What is the state of the particle right after being liberated?

(b) In order to tune the potential to zero, the experimenter had to do work on the particle. How much work? Which sign?

(c) Show that for very large positive times, $t >> 1/\omega$, the probability density to find the particle at a generic position x becomes flat, that is, x-independent.

3. Use trial wavefunctions of the form

$$\psi(x) = \left(\frac{a}{\pi}\right)^{1/4} e^{-a^2x^2/2}$$

(where a is an arbitrary constant) to estimate, and bound, the ground state energy of the one-dimensional Hamiltonian

$$H = \frac{p^2}{2m} - V_0\delta(x),$$

where V_0 is a constant and $V_0 > 0$.

4.

(a) Consider a free particle in one dimension with Hamiltonian $H = \frac{1}{2}p^2 = -\frac{1}{2}\partial_x^2$. Gaussian wave packets stay Gaussian wave packets under time evolution. Find the time evolution of the wave function

$$\psi(t,x) = e^{-\frac{x^2}{2A(t)} - C(t)}$$

with initial condition $A(0) = 0$, which is to say the particle is initially sharply localized at $x = 0$.

(b) Now consider a particle in a constant gravitational field, $H = \frac{1}{2}p^2 + g\,x$. This Hamiltonian still has the property that Gaussian wave packets evolve into Gaussian wave packets, but now the ansatz has to be generalized slightly to

$$\psi(t,x) = e^{-\frac{x^2}{2A(t)} - B(t)\,x - C(t)}.$$

Find the time evolution with initial conditions $A(0) = B(0) = 0$.

(c) Take the solution obtained in part (b) and replace t by $t - i$ (i as in $i = \sqrt{-1}$). The resulting wavefunction is still a perfectly good solution. Can you explain why? (i.e. What symmetry tells you a new solution can be obtained this way?) At what x does the resulting $|\psi|^2$ peak? (It would be some function of time).

5. Consider a particle of mass m moving in one spatial dimension (x) with a potential of the form of a square barrier, i.e. the potential equals V for $0 < x < L$, but is zero everywhere else.Here $V > 0$. The Hamiltonian is the usual kinetic energy $p^2/(2m)$ plus the potential. Suppose the particle is coming in from $x = -\infty$ as a plane wave, i.e. the incoming wave-function takes the form $e^{-iEt+ikx}$, with $E = k^2/(2m)$. For $E < V$, it can be shown that the probability of reflection by the barrier is

$$P_{\text{reflection}} = \frac{1}{1 + \frac{4E(V-E)}{V^2}\frac{1}{[\sinh\alpha]^2}}.$$

What is α in terms of the quantities given in the problem?

Note: This problem can be solved exactly, but α can be found much more easily by matching with an approximation for $P_{\text{reflection}}$ that is valid when $V >> E$.

Question 1 Solution

We must use

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\langle [A,H]\rangle + \left\langle \frac{\partial A}{\partial t}\right\rangle .$$

We note that since $H = \dfrac{p^2}{2m}$, $\langle p\rangle$ and $\langle p^2\rangle$ are independent of time. We then compute

$$\begin{aligned}
\frac{d\langle x\rangle}{dt} &= \frac{1}{i\hbar}\left\langle \left[x, \frac{p^2}{2m}\right]\right\rangle \\
&= \frac{1}{i\hbar}\cdot\frac{1}{2m}\langle 2i\hbar p\rangle \\
&= \frac{\langle p\rangle}{m} \\
\frac{d\langle x^2\rangle}{dt} &= \frac{1}{i\hbar}\cdot\frac{1}{2m}\langle 2i\hbar\,(xp+px)\rangle \\
&= \frac{1}{m}\langle xp+px\rangle \\
\frac{d}{dt}(\Delta x)^2 &= \frac{d\langle x^2\rangle}{dt} - \frac{d\langle x\rangle^2}{dt} \\
&= \frac{1}{m}\langle xp+px\rangle - \frac{2}{m}\langle x\rangle\langle p\rangle \\
\frac{d^2}{dt^2}(\Delta x)^2 &= \frac{1}{i\hbar}\cdot\frac{1}{m}\langle [xp+px, H]\rangle - \frac{2}{m^2}\langle p\rangle^2 \\
&= \frac{1}{i\hbar}\cdot\frac{1}{2m^2}\left\langle \left[x,p^2\right]p + p\left[x,p^2\right]\right\rangle - \frac{2}{m^2}\langle p\rangle^2 \\
&= \frac{1}{i\hbar}\cdot\frac{1}{2m^2}\left\langle 4i\hbar p^2\right\rangle - \frac{2}{m^2}\langle p\rangle^2 \\
&= \frac{2}{m^2}\left\langle p^2\right\rangle - \frac{2}{m^2}\langle p\rangle^2 \\
&= \frac{2}{m^2}(\Delta p)^2 \\
\frac{d^3}{dt^3}(\Delta x)^2 &= 0.
\end{aligned}$$

Thus we find that the variance at time t is

$$(\Delta x)^2 = \frac{1}{m^2}(\Delta p)^2 t^2 + \frac{1}{m}\left(\langle xp+px\rangle_0 - 2\langle x\rangle_0\langle p\rangle\right)t + (\Delta x)_0^2 ,$$

where the 0 subscripts indicate evaluation at time $t = 0$.

Question 2 Solution

(a) Soon after $t = 0$, the particle is still in the same state as it was before, because for an instantaneous but finite change in the Hamiltonian, the wavefunction is a continuous function of time (this can be seen directly from the Schrödinger equation.) So, the state at $t = 0^+$ is the ground state of the original harmonic oscillator,

$$\psi(x, t = 0^+) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} .$$

(b) With the original harmonic oscillator Hamiltonian, the energy of our particle was the ground state energy, $E(t < 0) = \frac{1}{2}\hbar\omega$. However, with the new free particle Hamiltonian, the expectation value of the energy is *half* of that. This is a consequence of the virial theorem (for a harmonic oscillator, the energy is equally split between kinetic and potential). Alternatively, the explicit computation is

$$E(t > 0) = \int dx\, \psi^*(x) \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) \psi(x) = \frac{\hbar^2}{2m} \int dx \left|\frac{d}{dx}\psi(x)\right|^2 = \frac{1}{4}\hbar\omega .$$

So, overall the energy of our particle has changed by $\Delta E = -\frac{1}{4}\hbar\omega$. This is the work done by the experimenter, and it is negative.

(c) For $t > 0$, the wave function obeys the free Schrödinger equation, which is easily solved in Fourier space. One has the initial condition

$$\tilde{\psi}(k, t = 0^+) \propto e^{-\frac{\hbar}{2m\omega}k^2} ,$$

where we are not displaying the constant normalization factor because it does not matter for what follows, and each Fourier mode evolves in time as $e^{-i\hbar\frac{k^2}{2m}t}$, so that

$$\tilde{\psi}(k, t > 0) \propto e^{-\frac{\hbar}{2m\omega}(1+i\omega t)k^2} .$$

For $t \gg 1/\omega$, this is

$$\tilde{\psi}(k, t \gg 1/\omega) \propto e^{-i\frac{\hbar t}{2m}k^2} .$$

Going back to position space, we have

$$\psi(x, t \gg 1/\omega) = \int \frac{dk}{2\pi}\, \tilde{\psi}(k, t \gg 1/\omega)\, e^{ikx} \propto \int \frac{dk}{2\pi} e^{-i(\frac{\hbar t}{2m}k^2 - kx)} \propto e^{+i\frac{m}{2\hbar t}x^2} ,$$

where we are keeping track of the x-dependence only. The probability density to find the particle at position x is

$$|\psi(x, t \gg 1/\omega)|^2 \propto 1 ,$$

that is, it is x-independent.

Question 3 Solution

Note: The question has a typo. The wavefunction should be

$$\psi(x) = \left(\frac{a}{\pi}\right)^{1/4} e^{-ax^2/2}$$

with $a > 0$. We compute

$$\begin{aligned}
\langle\psi|H|\psi\rangle &= \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} dx\, e^{-a^2x^2/2} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - V_0\delta(x)\right) e^{-a^2x^2/2} \\
&= \sqrt{\frac{a}{\pi}} \left(-V_0 - \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx\, \left(-a + a^2x^2\right) e^{-ax^2}\right).
\end{aligned}$$

Let $y = ax^2$, which implies

$$2ax\, dx = dy \implies dx = \frac{1}{2a}\frac{dy}{x} = \frac{1}{2\sqrt{a}}\frac{dy}{\sqrt{y}}.$$

We then find

$$\begin{aligned}
\langle\psi|H|\psi\rangle &= \sqrt{\frac{a}{\pi}} \left(-V_0 - \frac{\hbar^2}{2m}\frac{1}{2\sqrt{a}} \cdot 2a \int_0^{\infty} \frac{dy}{\sqrt{y}}\, (-1+y)\, e^{-y}\right) \\
&= \sqrt{\frac{a}{\pi}} \left(-V_0 - \frac{\hbar^2}{2m}\sqrt{a} \int_0^{\infty} \frac{dy}{\sqrt{y}}\, (-1+y)\, e^{-y}\right).
\end{aligned}$$

Recalling the definition of the gamma function:

$$\Gamma(x) = \int_0^{\infty} dy\, y^{x-1} e^{-y},$$

we find

$$\begin{aligned}
\int_0^{\infty} \frac{dy}{\sqrt{y}}\, (-1+y)\, e^{-y} &= -\Gamma\left(\frac{1}{2}\right) + \Gamma\left(\frac{3}{2}\right) \\
&= -\frac{1}{2}\Gamma\left(\frac{1}{2}\right) \\
&= -\frac{\sqrt{\pi}}{2}.
\end{aligned}$$

Thus

$$\begin{aligned}
E_a &= \sqrt{\frac{a}{\pi}} \left(-V_0 + \frac{\hbar^2\sqrt{\pi a}}{4m}\right) \\
&= -V_0\sqrt{\frac{a}{\pi}} + \frac{\hbar^2 a}{4m}
\end{aligned}$$

We must find the value of a that minimizes the energy. Computing $\frac{dE_a}{da}$ and setting this to zero yields

$$\begin{aligned} 0 &= -\frac{V_0}{2\sqrt{\pi a}} + \frac{\hbar^2}{4m} \\ a &= \frac{4m^2}{\pi \hbar^4} V_0^2. \end{aligned}$$

Thus

$$E_{\text{variational}} = -\frac{mV_0^2}{\pi \hbar^2}.$$

It turns out that the exact energy is $E_{\text{exact}} = -\frac{mV_0^2}{2\hbar^2}$.

Question 4 Solution

(a) Substituting $\psi = e^{-\frac{x^2}{2A(t)} - C(t)}$ into the time-dependent Schrödinger equation $i\partial_t \psi = H\psi$ yields a closed system of ODEs for A and C:

$$\dot{A} = i\,, \qquad \dot{C} = \frac{i}{2A}\,.$$

The first ODE with initial condition $A(0) = 0$ is solved by $A = it$. The second ODE is then solved by by $C(t) = \frac{1}{2}\log t$ plus a constant. We conclude that up to an overall normalization constant

$$\psi(t,x) = \boxed{\frac{1}{\sqrt{t}}\, e^{i\,x^2/2t}}\,.$$

(Alternatively this can be solved by Fourier transforming, time evolving, and Fourier transforming back.)

(b) The solution method detailed in part (a) is applicable to this case as well. Again the Gaussian ansatz gives a closed system of ODEs:

$$\dot{A} = i\,, \qquad \dot{B} = ig - \frac{B}{t}\,, \qquad \dot{C} = \frac{i}{2}\left(\frac{1}{A} - B^2\right)\,.$$

The first ODE with $A(0) = 0$ is solved by $A(t) = it$. The second ODE is solved by writing it as $\frac{d}{dt}(tB) = igt$, which for initial condition $B(0) = 0$ integrates to $B(t) = igt/2$. Using the solutions for A and B, the third ODE becomes $\dot{C} = \frac{1}{2t} + \frac{i}{8}g^2t^2$, which integrates to $C(t) = \frac{1}{2}\log t + \frac{i}{24}g^2t^3$ plus a constant. We conclude that up to an overall normalization constant

$$\psi(t,x) = \boxed{\frac{1}{\sqrt{t}}\,\exp i\left(\frac{x^2}{2t} - \frac{gtx}{2} - \frac{g^2t^3}{24}\right)}\,.$$

(c) The new wavefunction is still a solution because of the time translation invariance of the Schrödinger equation. The find the peak of $|\psi(x)|^2$, it suffices to consider the x-dependent part of $|\psi(t-i,x)|^2$:

$$|\psi_i(t,x)|^2 \,\propto\, \exp \mathrm{Re}\, i\left(\frac{x^2}{t-i} - g(t-i)x\right) = \exp\left(-\frac{x^2}{t^2+1} - gx\right)\,.$$

The maximum lies at $\boxed{x = -\frac{1}{2}g(t^2+1)}$, following a downward parabolic trajectory as expected from classical mechanics.

Question 5 Solution

The easiest way to answer this question is to recall the WKB result that the probability of transmission in the limit of a tall barrier is

$$P_{\text{transmission}} \approx e^{-2\gamma},$$

where

$$\gamma = \int_0^L dx \sqrt{2m(V-E)} = L\sqrt{2m(V-E)}.$$

Here we have set $\hbar$ to 1. Since $P_{\text{reflection}} = 1 - P_{\text{transmission}}$ and the hyperbolic sine in the expression for $P_{\text{reflection}}$ can be the only source of an exponential dependence, it must be that $\alpha = L\sqrt{2m(V-E)}$.

A more elaborate answer would be to solve this problem exactly. Divide up space into 3 regions: I (to the left of potential barrier), II (under the barrier), III (to the right of the barrier). The wavefunction takes the form:

$$\begin{aligned}
&\text{Region I:} \quad e^{-iEt+ikx} + Re^{-iEt-ikx} \\
&\text{Region II:} \quad (1+R-D)e^{-iEt+i\widetilde{k}x} + De^{-iEt-i\widetilde{k}x} \\
&\text{Region III:} \quad Te^{-iEt+ik(x-L)},
\end{aligned}$$

where we have enforced continuity of the wavefunction at $x = 0$ and ignored the normalization factor. Here $\widetilde{k}$ satisfies

$$\frac{k^2}{2m} = E = \frac{\widetilde{k}^2}{2m} + V,$$

i.e., $\widetilde{k} = ib$, where $b = \sqrt{2m(V-E)}$. Enforcing continuity of the wavefunction at $x = L$ and continuity of its spatial derivative at $x = 0$ and $x = L$ gives

$$\begin{aligned}
T &= (1+R-D)e^{i\widetilde{k}L} + De^{-i\widetilde{k}L}, \\
k(1-R) &= \widetilde{k}(1+R) - 2\widetilde{k}D, \\
kT &= \widetilde{k}(1+R-D)e^{i\widetilde{k}L} - \widetilde{k}De^{-i\widetilde{k}L}.
\end{aligned}$$

From the second equation, we see that

$$D = \frac{1}{2}\left[\left(1 - \frac{k}{\widetilde{k}}\right) + \left(1 + \frac{k}{\widetilde{k}}\right)R\right].$$

Substituting this into the first equation gives an expression for T:

$$2T = \left[\left(1 + \frac{k}{\widetilde{k}}\right) + \left(1 - \frac{k}{\widetilde{k}}\right)R\right]e^{i\widetilde{k}L} + \left[\left(1 - \frac{k}{\widetilde{k}}\right) + \left(1 + \frac{k}{\widetilde{k}}\right)R\right]e^{-i\widetilde{k}L},$$

whereas doing the same in the third equation gives:

$$2T = \frac{\widetilde{k}}{k}\left[\left(1+\frac{k}{\widetilde{k}}\right)+\left(1-\frac{k}{\widetilde{k}}\right)R\right]e^{i\widetilde{k}L} - \frac{\widetilde{k}}{k}\left[\left(1-\frac{k}{\widetilde{k}}\right)+\left(1+\frac{k}{\widetilde{k}}\right)R\right]e^{-i\widetilde{k}L}$$

Combining gives

$$R = -\frac{\left(1+\frac{k}{ib}\right)\left(1-\frac{ib}{k}\right)e^{-bL}+\left(1-\frac{k}{ib}\right)\left(1+\frac{ib}{k}\right)e^{bL}}{\left(1-\frac{k}{ib}\right)\left(1-\frac{ib}{k}\right)e^{-bL}+\left(1+\frac{k}{ib}\right)\left(1+\frac{ib}{k}\right)e^{bL}}.$$

The probability of reflection is

$$|R|^2 = \left(1+\frac{4}{\left(1+\frac{k^2}{b^2}\right)\left(1+\frac{b^2}{k^2}\right)}\frac{1}{\left[\sinh(bL)\right]^2}\right)^{-1}.$$

It is useful to note that

$$\left(1+\frac{k}{ib}\right)^2\left(1-\frac{ib}{k}\right)^2+\left(1-\frac{k}{ib}\right)^2\left(1+\frac{ib}{k}\right)^2 = -2\left(1+\frac{b^2}{k^2}\right)\left(1+\frac{k^2}{b^2}\right),$$

and

$$\left(1-\frac{k}{ib}\right)^2\left(1-\frac{ib}{k}\right)^2+\left(1+\frac{k}{ib}\right)^2\left(1+\frac{ib}{k}\right)^2 = -2\left(1+\frac{b^2}{k^2}\right)\left(1+\frac{k^2}{b^2}\right)+16,$$

Lastly, substituting in expressions for k and b, we have

$$|R|^2 = \left(1+\frac{4E(V-E)}{V^2}\frac{1}{\left[\sinh\left(L\sqrt{2m(V-E)}\right)\right]^2}\right)^{-1}.$$