Phys 115A HW 2

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> **Question 1.** *To build a little more experience with separation of variables, consider the heat equation in one spatial dimension:*
> $$\frac{1}{k}\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2}$$
> *where $u(x,t)$ corresponds to the temperature of an object with thermal conductivity k.*
> *1. Using separation of variables, $u(x,t) = u_x(x)u_t(t)$, and separation constant $-\alpha^2$, separate the heat equation into ordinary differential equations for u_t and u_x.*
> *2. Find the general solution to the differential equation satisfied by $u_x(x)$.*
> *3. Find the general solution to the differential equation satisfied by $u_t(t)$.*
> *4. Write down the general solution $u(x,t)$ to the heat equation.*

Proof.

1. Given the separation of variables $u(x,t) = u_x(x)u_t(t)$, plug into the formula we get the following:

$$\frac{1}{k}\frac{\partial}{\partial t}(u_x(x)u_t(t)) = \frac{\partial^2}{\partial x^2}(u_x(x)u_t(t)) \implies \frac{1}{k}\frac{du_t}{dt}u_x(x) = \frac{d^2u_x}{dx^2}u_t(t) \tag{1}$$

$$\implies \frac{1}{k}\cdot\frac{1}{u_t(t)}\frac{du_t}{dt} = \frac{1}{u_x(x)}\frac{d^2u_x}{dx^2} \tag{2}$$

Notice that the line aboe have the left side being dependent only on t, while the right side is solely dependent on x, hence the whole equation must be constant. With the separation constant given by $-\alpha^2$, we get the following two ordinary differential equations:

$$\frac{1}{k}\cdot\frac{1}{u_t(t)}\frac{du_t}{dt} = \frac{1}{u_x(x)}\frac{d^2u_x}{dx^2} = -\alpha^2 \tag{3}$$

$$\implies \begin{cases} \frac{du_t}{dt} = -k\alpha^2 u_t(t) \\ \frac{d^2u_x}{dx^2} = -\alpha^2 u_x(x) \end{cases} \tag{4}$$

2. For $u_x(x)$, since it satisfies $\frac{d^2u_x}{dx^2} + \alpha^2 u_x(x) = 0$ (or can rewrite as $\frac{d^2u_x}{dx^2} - (i\alpha)^2 u_x(x) = 0$), then the general solution of this is given by $Ae^{i\alpha x} + Be^{-i\alpha x}$, where $A, B \in \mathbb{C}$ are arbitrary constants (depending on the initial condition).

   (Note: If want real solution instead, it depends on the constant α, so here we'll provide the most general form).

3. For $u_t(t)$, since it satisfies $\frac{du_t}{dt} = -k\alpha^2 u_t(t)$, then the general solution $u_t(t) = Ke^{-k\alpha^2 t}$, where $K \in \mathbb{C}$ is an arbitrary constant (depending on the initial condition).

(Note: If want real solution just take the arbitrary constants in $\mathbb{R}$ instead).

4. If plug

$\square$

> **Question 2.** *Prove the following three theorems:*
>
> *1. For normalizable solutions, the separation constant E must be real. Hint: Write E (in Griffiths eq. 2.7, i.e. $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$) as $E_0 + i\Gamma$, with E_0 and Γ real, and show that Γ must be zero if Griffiths eq. 1.20 (i.e.*
>
> $$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$$
>
> *is to hold for all t.*
>
> *2. The time-independent wavefunction $\psi(x)$ can always be taken to be real (unlike $\Psi(x,t)$, which is necessarily complex). This doesn't mean that every solution to the time-independent Schrödinger equation is real; what it says is that if you've got one that is not, it can always be expressed as a linear combination of solutions (with the same energy) that are. So you might as well stick to ψ's that are real. Hint: if $\psi(x)$ satisfies Griffiths eq. 2.5 (i.e.*
>
> $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$
>
> *for a given E, so too does its complex conjugate, and hence also the real linear combinations $\psi + \psi^*$ and $i(\psi - \psi^*)$.*
>
> *3. If $V(x)$ is an even function (that is, $V(-x) = V(x)$) then $\psi(x)$ can also be taken to be either even or odd. Hint: If $\psi(x)$ satisfies Griffiths eq. 2.5, for a given E, then so too does $\psi(-x)$, and hence also the even and odd linear combinations $\psi(x) \pm \psi(-x)$.*

Proof.

1. Suppose $\Psi(x,t)$ is a separable solution to the Schrödinger equation that is a scaled version of a wave function (so it's normalizable), then since $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$ for some constant $E \in \mathbb{C}$, then $E = E_0 + i\Gamma$ for some $E_0, \Gamma \in \mathbb{R}$. Now, suppose the solution Ψ itself is normalized, we have the following:

$$1 = \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{\infty} \left(\psi(x)e^{-i(E_0+i\Gamma)t/\hbar}\right)\left(\psi^*(x)\left(e^{-i(E_0+i\Gamma)t/\hbar}\right)^*\right) dx \tag{5}$$

$$= \int_{-\infty}^{\infty} |\psi(x)|^2 \cdot e^{2\Gamma t/\hbar} dx = e^{2\Gamma t/\hbar}\int_{-\infty}^{\infty} |\psi(x)|^2 dx \tag{6}$$

Since $\int_{-\infty}^{\infty} |\psi(x)|^2 dx$ must stay as constant for all $t \in \mathbb{R}$, for the whole expression to be 1 for all $t \in \mathbb{R}$, one must have $e^{2\Gamma t/\hbar}$ being a constant also. Hence we must have $\Gamma = 0$, showing that $E = E_0 + i\Gamma = E_0 \in \mathbb{R}$.

2. Suppose $\psi(x)$ satisfies the time independent Schrödinger equation, we have the following:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \tag{7}$$

Where both $V, E \in \mathbb{R}$. Hence, if taken the complex conjugation, we get:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\right)^* + (V\psi)^* = (E\psi)^* \implies -\frac{\hbar^2}{2m}\frac{d^2\psi^*}{dx^2} + V\psi^* = E\psi^* \tag{8}$$

Hence, ψ^* is also a solution to the Time-independent Schrödinger equation. As a result, since $\psi(x) = \text{Re}(\psi)(x) + i\text{Im}(\psi)(x)$, where $\text{Re}(\psi)(x) = \frac{1}{2}(\psi(x) + \psi^*(x))$, and $\text{Im}(\psi)(x) = \frac{1}{2i}(\psi(x) - \psi^*(x))$, then since

linear combinations of solutions to a differential equation is still a solution (and the fact that $\psi : \mathbb{R} \to \mathbb{C} \cong \mathbb{R}^2$ is differentiable, one must have both its real and imaginary parts being differentiable also), then $\mathrm{Re}(\psi)(x), \mathrm{Im}(\psi)(x)$ are both solutions to the Time-Independent Schrödinger equation. Hence, with these two components being real, $\psi(x)$ can be written as linear combinations of real solutions.

3. Given that $V(x)$ is even, then $V(x) = V(-x)$. Now, if we consider $\psi(-x)$ instead, then we have $\frac{d}{dx}\psi(-x) = -\psi'(-x)$, and $\frac{d^2}{dx^2}\psi(-x) = \frac{d}{dx}\left(-\psi'(-x)\right) = \psi''(-x)$. Hence, since $\psi(x)$ is a solution to the Time-Independent Schrödinger equation by assumption, we have $-\frac{\hbar^2}{2m}\psi''(x)+V(x)\psi(x) = E\psi(x)$, then plug in $u = -x$ instead, we get $-\frac{\hbar^2}{2m}\psi''(-x) + V(-x)\psi(-x) = E\psi(-x)$, which implies the following:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}(\psi(-x)) + V(x)\psi(-x) = E\psi(-x) \tag{9}$$

Hence, $\psi(-x)$ is also a solution.

Then, as a result $\frac{\psi(x)+\psi(-x)}{2}$ and $\frac{\psi(x)-\psi(-x)}{2}$ are both solutions to the time-independent Schrödinger equation, where the first one is even, the latter one is odd, and $\psi(x) = \frac{\psi(x)+\psi(-x)}{2} + \frac{\psi(x)-\psi(-x)}{2}$. Hence, any solution $\psi(x)$ can be expressed as linear combinations of odd and even functions.

$\square$

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Question 3. *Show that E must exceed the minimum value of $V(x)$, for every normalizable solution to the time-independent Schrödinger equation. What is the classical analog to this statement?*

Hint: Rewrite Griffiths eq. 2.5 (i.e.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

in the form

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[V(x) - E]\psi;$$

if $E < V_{\min}$, then ψ and its second derivative always have the same sign – argue that such a function cannot be normalized.

Proof. Suppose the contrary that $E < V_{\min}$, then rewrite the Time-Independent Schrödinger equation, we get:

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V(x) - E)\psi \tag{10}$$

Where, since $E < V_{\min}$, then let $\epsilon = V_{min} - E > 0$, we have $\qquad\qquad\square$

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Question 4. *You prepare a particle in the infinite square well (with walls at $x = 0, a$) in an initial state described by a linear combination of two stationary states,*

$$\Psi(x, 0) = A[\psi_2(x) + \psi_3(x)]$$

where ψ_2, ψ_3 are given by Griffiths eq. 2.31 (i.e. $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$) with $n = 2, 3$ respectively.
(a) Normalize $\Psi(x, 0)$, i.e., find A.
(b) Find $\Psi(x, t)$ and $|\Psi(x, t)|^2$. Express the latter as a sinusoidal function of time in terms of the variable $\omega = \pi^2 \hbar / 2ma^2$.
(c) Compute $\langle x \rangle$. Is this an interesting function of time? Note: the integral is painful, but please work your way through it by hand and show your work. Integration by parts and trigonometric identities (including one that Griffiths uses while proving orthogonality of the stationary states) are both your friends!
(d) Compute $\langle p \rangle$.
(e) If you measured the energy of the particle, what values might you get, and what is the probability of getting them? What is the expectation value of H, and how does this relate to the energies E_2 and E_3 of ψ_2 and ψ_3?

Proof. □

Question 5. *We have emphasized that overall phases of the wave function are irrelevant, since they cancel out of physical quantities. But the relative phase matters! Imagine we change the phase in the previous problem so that our initial state is*

$$\Psi(x,0) = A[\psi_2(x) + e^{i\phi}\psi_3(x)]$$

for some real constant ϕ.
(a) Find $\Psi(x,t)$ and $|\Psi(x,t)|^2$.
(b) Find $\langle x \rangle$.
(c) Find $\langle p \rangle$.
(d) Discuss how these results differ from the case of $\phi = 0$. Consider especially the cases $\phi = \pi/2$ and $\phi = \pi$.

Proof. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

Question 6. *Solve the time-independent Schrödinger equation with appropriate boundary conditions for the "symmetric" infinite square well with*

$$V(x) = \begin{cases} 0 & -\frac{a}{2} \leq x \leq \frac{a}{2} \\ \infty & otherwise \end{cases}$$

Determine the wavefunctions ψ_n and their energies by computing the solutions in each region and matching at the boundaries. What coordinate change can you do to bring your solutions for the ψ_n into the same form as the ones we found in lecture for the infinite square well with walls at $x = 0, a$?

Proof. □

Question 7. *Consider again the "symmetric" infinite square well from the previous problem. Suppose we measure the energy of a particle in this box, and we find the ground-state energy*

$$E_1 = \frac{\hbar^2 \pi^2}{2ma^2}.$$

We then know the particle is in the ground state with wavefunction $\psi_1(x)$, which is the $n = 1$ wavefunction you found in the previous problem. Then we suddenly pull the walls of the well out rapidly so that they are at $x = \pm 2a$ instead of $x = \pm a/2$; we do it so rapidly that the state of the particle doesn't change at that moment. Now, of course, the particle is no longer in a state of definite energy in the new well; its wavefunction is no longer a single separable solution of the Schrödinger equation with the larger box.

(a) Find the solutions to the time-independent Schrödinger equation (the ψ_n and E_n) in the new well with walls at $x = \pm 2a$.

(b) We measure the energy of the particle right after pulling the walls out to $x = \pm 2a$. What is the most probable result of this measurement? What is the probability of this result?

(c) What is the next-most probable result, and the probability of this result?

(d) What is the expectation value of the energy? Why should you have expected this answer?

You probably think this is a crazy example, but it is a good analogy for what happens to the potential experienced by the electron in tritium (an isotope of hydrogen whose nucleus consists of one proton and two neutrons) when nuclear reactions convert the tritium into ^3He (whose nucleus consists of two protons and one neutron).

Proof. □