PHY 303, I-Semester 2023/24, Assignment 3

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Due-date: 10. Sept 2023

Note the asymmetric distribution of marks (and expected effort) between Q1-Q4 in this assignment.

(1) Solutions of the TISE [6 pts]: We want to explore some important properties of all solutions of the TISE.

(a) Show that for all solution of Eq. (1.62), we require $E_n > V_{min}$, where $V_{min} = \min_x V(x)$, i.e. the minimal value taken by the potential energy [2pts].

(b) Show, that for a potential energy that is symmetric, $V(x) = V(-x)$, you can always choose all solutions of the TISE to be either symmetric or anti-symmetric [2pts].

(c) Show that all solutions of the TISE must be continuously differentiable at all x where the potential does not make an infinite jump [2pts].

Solution: 1(a)- The TISE is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\phi_n(x) = \hat{H}\phi_n(x) = E_n\phi_n(x) \tag{1}$$

$$\frac{d^2}{dx^2}\phi_n(x) = \frac{2m}{\hbar^2}\underbrace{[V(x) - E_n]}_{\equiv\Delta}\phi_n(x) = 0 \tag{2}$$

For $[E_n - V(x)] < 0$ the solution is oscillatory and for $[E_n - V(x)] > 0$ is is exponential. If $E < V_{min}$, then Δ defined above is positive for all x and hence $\frac{d^2}{dx^2}\phi(x)$ and $\phi(x)$ have the same sign for all x. Hence $\phi(x)$ always curves away from the x-axis (you can try this with any random drawing). This implies that $|\phi(x)|$ becomes larger as x increases. So $\phi(x) \not\to 0$ as $x \to \pm\infty$, hence for $E < V_{min}$ the solution $\phi_n(x)$ cannot be normalizable. Therefore we always require $E > V_{min}$.

1(b) - The TISE is

$$\frac{d^2}{dx^2}\phi_n(x) + \frac{2m}{\hbar}[E_n - V(x)]\phi_n(x) = 0 \tag{3}$$

Let us substitute $-x$ everywhere for x:

$$\frac{d^2}{dx^2}\phi_n(-x) + \frac{2m}{\hbar}\left[E_n - \underbrace{V(-x)}_{=V(x)}\right]\phi_n(-x) = 0. \tag{4}$$

This shows that $\phi(-x)$ is also a solution of the same TISE with the same energy as $\phi(x)$.

However we can show that if two solutions of the TISE in one dimension have the same energy, they must be linearly dependent. Assume we have two different solutions with eigenvalue E, then

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\phi_1(x)=E\phi_1(x),$$
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\phi_2(x)=E\phi_2(x). \tag{5}$$

Multiplying the first equation by ϕ_2 and the second by ϕ_1 and subtracting one from the other, we get:

$$\phi_1(x)\frac{d^2}{dx^2}\phi_2(x)-\phi_2(x)\frac{d^2}{dx^2}\phi_1(x)=0 \Leftrightarrow$$
$$\frac{d}{dx}\left[\phi_1(x)\frac{d}{dx}\phi_2(x)-\phi_2(x)\frac{d}{dx}\phi_1(x)\right]=0 \tag{6}$$

Integrating the latter over all x gives

$$\phi_1(x)\frac{d}{dx}\phi_2(x)-\phi_2(x)\frac{d}{dx}\phi_1(x)=const \tag{7}$$

Since $\phi_k \to 0$ at $|x|\to\infty$, in order to be normalizable, we know that $const=0$. Then we can write

$$\phi_1(x)\frac{d}{dx}\phi_2(x)=\phi_2(x)\frac{d}{dx}\phi_1(x) \Leftrightarrow$$
$$\frac{\phi_2'(x)}{\phi_2(x)}=\frac{\phi_1'(x)}{\phi_1(x)} \tag{8}$$

which we can integrate on both sides to give $\log\phi_2(x)=\log\phi_1(x)+const$ or $\phi_2(x)=c\phi_1(x)$.

Applied to the earlier two solutions $\phi(x)$ and $\phi(-x)$, this means $\phi(x)=c\phi(-x)$. Since $\phi(x)=\phi(--x)=c^2\phi(x)$, we require $c=\pm1$, so we have now shown that the solution must be either symmetric or anti-symmetric.

1(c)- We know that the solution of a TISE which is a second-order (in x) differential equation $\phi_n(x)$ has to be a continuous function. The TISE is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\phi_n(x)=E_n\phi_n(x)$$

Observe that the RHS of the equation is continuous as established previously. Thus the LHS and consequently the double-derivative should also yield a continuous function. For the double-derivate $\phi_n''(x)$ to be defined at all x and also to yield a continuous function, $\phi'(x)$ has to be continuous at all x.
Thus $\phi_n(x)$ and $\phi_n'(x)$ are both continuous at all $x \implies \forall n,\quad \phi_n(x)$ is continuously

differentiable at all x.

(2) Zero point motion [8pts]: Consider a particle of mass m moving in one dimension in a harmonic oscillator potential $V(x) = \frac{1}{2}m\omega^2 x^2$.

(a) Treating the particle classically, with phase space coordinates $[x(t), p(t)]$, what is its state of lowest possible energy, and what dynamics $x(t)$, $p(t)$ does this correspond to? [2 pts]

(b) Now changing to quantum mechanics, what is the state of lowest possible energy? What can you say about position and momentum probability distributions in this case? What is the fundamental difference to the classical oscillator? What quantum mechanical theorem enforces this difference? [6 pts]

Solution : 2(a)- The energy of the harmonic oscillator is given as $E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$. *Drawing the energy in phase space would yield a parabola with Energy along Z-axis and [x(t)] along X-axis and [p(t)] along Y-axis. Thus, one can conclude that the lowest possible energy in the phase space would correspond to [x(t)]=0 and [p(t)]=0, thus the particle is at the origin without moving, and remains like that.*

2(b) - The lowest energy state is at the energy $E = \frac{\hbar\omega}{2}$ *with the wavefunction* $\phi_0(x) = \mathcal{N}e^{-\frac{1}{2}\frac{x^2}{\sigma^2}} = \frac{1}{(\sigma^2\pi)^{1/4}}e^{-\frac{1}{2}\frac{x^2}{\sigma^2}}$. *Thus the position probability distribution is a gaussian* $|\phi|^2 = \frac{e^{-x^2/\sigma^2}}{(\sigma^2\pi)^{1/2}}$. *The momentum distribution can be calculated by taking the Fourier transform of* $\phi(x)$.

$$
\begin{aligned}
\tilde{\phi}(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\phi(x)e^{-ipx/\hbar} \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\frac{1}{(\sigma^2\pi)^{1/4}}e^{-\frac{1}{2}\frac{x^2}{\sigma^2}}e^{-ipx/\hbar} \\
&= \frac{\sigma^{1/2}}{(\pi^2\hbar)^{1/2}}e^{\frac{-p^2\sigma^2}{2\hbar^2}}
\end{aligned}
$$

The fundamental difference between these results and the classical one, is that most likely the particle will NOT be at the origin with momentum zero. We say that momentum and position suffer "zero point fluctuations" hence the probability distributions have nonzero width centred on $x = 0$ *and* $p = 0$. *The quantum mechanical theorem that enforces this is Heisenberg's uncertainty relation, which would prohibit a state with* $x \equiv 0$ *and* $p \equiv 0$ *and no uncertainty, since then* $\sigma_x = \sigma_p = 0$. *The fact that* $x = 0$ *and* $p = 0$ *are not allowed, now also is the reason for the lowest accessible energy to be* $E = \frac{\hbar\omega}{2} > 0$.

(3) Schrödinger's equation in momentum space: [6 pts] → see solution of assignment 4

(4) Infinite square well potential with step: [**20pts**] Consider the Infinite square well potential with a potential step given by

$$V(x) = \begin{cases} \infty & x < -a, \\ 0 & -a \le x < 0, \\ V_0 > 0 & 0 \le x < b, \\ \infty & x > b \end{cases} \tag{9}$$

for $0 < a < b$.

(4a) Make a drawing of this potential and then find all allowed eigenstates ϕ_n and energies $E_n > 0$. *Hints: You may use mathematica where possible, in particular for solving any transcendental equations you might encounter numerically (and! graphically), for a few cases. Also best work with a real Ansatz, and phase shift your trigonometric functions so that the boundary conditions at $x = -a, b$ can be easily build in. Just describe how you can normalise your functions in the end, you can do this numerically in part (c).* [8 pts]

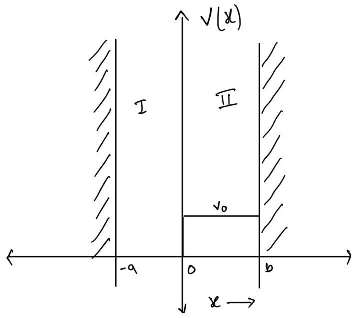

Figure 1: potential given in equation (9).

Solution: The potential given in equation (9) *is shown in Figure 1. To find the allowed eigenstates and energies $E_n > 0$, we divide the whole region into two region as shown in figure. Here we will treat region I and II separately and then enforce boundary condition at $x = -a, 0, b$.*

In each region we have the time independent Schrödinger equation as given in lecture notes equation (2.21)

$$\frac{\partial^2}{\partial x^2}\phi_n^{(r)}(x) = -\left(k_n^{(r)}\right)^2 \phi_n^{(r)}(x) \tag{10}$$

here $r \in \{I, II\}$ each region with wavenumber $k_n^{(r)} = \sqrt{2m\left[E_n - V(x)\right]}/\hbar$

$$\phi_n^{(I)}(x) = A\sin\left[k_n^{(I)}x\right] + B\cos\left[k_n^{(I)}x\right], \textit{ for } -a \le x < 0 \tag{11}$$

$$\phi_n^{(II)}(x) = C\sin\left[k_n^{(II)}x\right] + D\cos\left[k_n^{(II)}x\right], \textit{ for } 0 \le x < b \tag{12}$$

With $E_n > 0$ we have two case, $E_n < V_0$ and $E_n > V_0$.
***Case - 1** ($0 < E_n < V_0$)*
For this case, $k_n^{(I)} = \sqrt{2mE_n}/\hbar = k_n$. In second region $k_n^{(II)} = \sqrt{2m\left[E_n - V_0\right]}/\hbar = i\kappa_n$

with $\kappa_n = \sqrt{2m\left[V_0 - E_n\right]}/\hbar$*. for second region it is better to write solution in terms of exponential function. We also shift*[1] *the functions to better accommodate the boundary conditions. Combining all this we have the wavefunction*

$$\begin{aligned}\phi_n^{(I)}(x) &= A\sin k(x+a) + B\cos k(x+a),\ for\ -a \le x < 0\\ \phi_n^{(II)}(x) &= Ce^{-\kappa(x-b)} + De^{\kappa(x-b)},\ for\ 0 \le x < b\end{aligned}$$

Demanding the boundary condition $\phi_n^{(I)}(x) = 0$ *at* $x = -a$ *we have* $B = 0$*. Similarly for* $\phi_n^{(II)}(x) = 0$ *at* $x = b$ *we have* $C = -D$*.*

$$\phi_n^{(I)}(x) = A\sin k(x+a),\ for\ -a \le x < 0 \tag{13}$$

$$\phi_n^{(II)}(x) = D(e^{\kappa(x-b)} - e^{\kappa(x-b)}) = D\sinh\left(\kappa(x-b)\right),\ for\ 0 \le x < b \tag{14}$$

Finally the boundary condition at $x = 0$ *are* $\phi_n^{(I)}(x) = \phi_n^{(II)}(x)$ *and* $\partial\phi_n^{(I)}(x)/\partial x = \partial\phi_n^{(II)}(x)/\partial x$ *which give*

$$\begin{aligned}A\sin\left(ka\right) &= D\sinh\left(-\kappa b\right)\\ Ak\cos\left(ka\right) &= D\kappa\cosh\left(-\kappa b\right)\end{aligned}$$

From the above equation we have

$$\begin{aligned}\frac{1}{k}\tan\left(ka\right) &= \frac{1}{\kappa}\tanh\left(-\kappa b\right)\\ \Rightarrow\frac{\kappa}{k} &= \frac{\tanh\left(-\kappa b\right)}{\tan\left(ka\right)}\\ \Rightarrow\sqrt{\frac{V_0 - E}{E}} &= \frac{\tanh\left(-\kappa b\right)}{\tan\left(ka\right)}\end{aligned} \tag{15}$$

We can solve the transcendental equation (15) *graphically as shown in figure 2 to find the eigenvalues and using that we could find the eigenstates.*

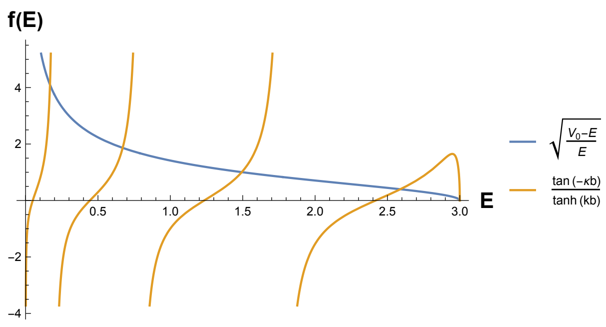

Figure 2: graphical solution to equation (15)

Case - 2 $(E_n > V_0)$
For this case, $k_n^{(I)} = \sqrt{2mE_n}/\hbar = k_n$*. In second region* $k_n^{(II)} = \sqrt{2m\left[E_n - V_0\right]}/\hbar =$

[1] Note that when e.g. $\sin(kx)$ was a solution of the TISE, also $\sin(kx + c)$ with constant c is one.

k'_n. Here also we shift the functions to better accommodate the boundary conditions. Combining all this we have the wavefunction

$$\phi_n^{(I)}(x) = A\sin k(x+a) + B\cos k(x+a),\ \textit{for}\ -a \leq x < 0$$
$$\phi_n^{(II)}(x) = C\sin k'(x-b) + D\cos k'(x-b),\ \textit{for}\ 0 \leq x < b$$

Putting the boundary conditions for the $\phi_n^{(I)}(x) = 0$ at $x = -a$ we have $B = 0$. Similarly for $\phi_n^{(II)}(x) = 0$ at $x = b$ we have $D = 0$.

$$\phi_n^{(I)}(x) = A\sin k(x+a),\ \textit{for}\ -a \leq x < 0 \tag{16}$$
$$\phi_n^{(II)}(x) = D\sin k'(x-b),\ \textit{for}\ 0 \leq x < b \tag{17}$$

Boundary condition at $x = 0$ i.e., $\phi_n^{(I)}(x) = \phi_n^{(II)}(x)$ and $\partial\phi_n^{(I)}(x)/\partial x = \partial\phi_n^{(II)}(x)/\partial x$ gives

$$A\sin(ka) = C\sin(-k'b)$$
$$Ak\cos(ka = Ck'\cos(-\kappa b)$$

From the above equation we have

$$\frac{1}{k}\tan(ka) = \frac{1}{k'}\tan(-k'b)$$
$$\Rightarrow \frac{k'}{k} = \frac{\tan(-k'b)}{\tan(ka)}$$
$$\Rightarrow \sqrt{\frac{E-V_0}{E}} = -\frac{\tan(k'b)}{\tan(ka)} \tag{18}$$

Similarly to Eq. (15), we can solve the transcendental equation (18) *graphically to find the eigenvalues as shown below and using those we could then find the eigenstates.*

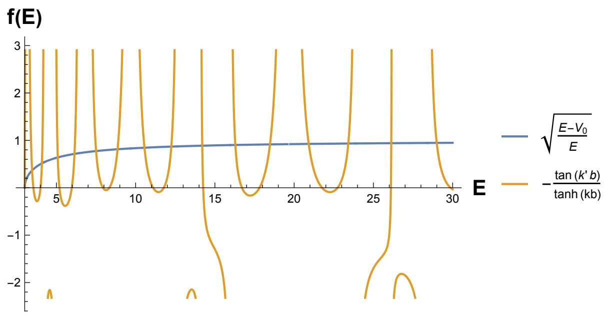

Figure 3: graphical solution to equation (18)

(4b) The code ***Assignment3_program_draft_v1.nb*** *is set up to discretise the TISE Eqn. (1.62) as discussed in example 10 of the lecture, and then find the eigenfunctions $\bar{\phi}_n$ and eigenvalues $\bar{E}_n > 0$ numerically directly. All you have to do is add the potential step at* `INSERT STEP HERE` *and add a missing piece in the derivative at* `MISSING PIECE`*.*

Then use the tools at the bottom of the script to compare its results with your analytical calculation from (4a). Sometimes you might discover your solution to be $\phi_n = -\bar{\phi}_n$ (where $\bar{\phi}_n$ is the numerically found eigenfuction and ϕ_n is the analytical solution found in 4(a)). Discuss why this implies that your solution was correct. Discuss why wavefunctions take the form they do, with as much detail as possible. [6 pts]

Solution: Look at the mathematica file Assignment3_program_solution_v3.nb for the numerical part of the solution. For the second part, eigenstates up to a phase factor represent the same state so ϕ_n and $-\bar{\phi}_n$ both represent same state, and you cannot control which of these is randomly chosen by the eigenvector finder in mathematica.

(4c) Suppose a wavefunction at time $t = 0$ is given by $\Psi(x, t = 0) = e^{-(x-\frac{b}{2})^2/(2\sigma^2)}/(\pi\sigma^2)^{1/4}$, with $0 < \sigma = b/5$ for $0 < x < b$ and $\Psi = 0$ outside this range. Using the numerical solution from (4b), extend the script to allow the calculation of $\Psi(x, t)$. For this change the earlier parameters to $L_{min} = -16$, $L_{max} = 16$, $a = 10$, $b = 13$, $V_0 = 5$. Discuss the time evolution of the probability density that you find, and why it makes sense. In particular compare it with that in the absence of a potential $V(x)$. [6 pts]

Solution: Look at the mathematica file Assignment3_program_solution_v3.nb for the numerical part of the solution. We find that the Gaussian wavepacket that we have initialised on the step part of the potential (region II) initially just spreads, just as we would expect for a free particle (week 5). In this initial phase, the evolution is exactly the same for the case with and without potential. It becomes more interesting, once the outer edge of the wavepacket hits either $x = 0$ (sudden drop of the potential by $\Delta V = V_0$), or $x = b$ (outer wall with $V \to \infty$. This time, e.g. $t = 6$ is shown in Fig. 4. it elastically reflects of the infinite barrier at the right edge ($x = b = 13$), and also undergoes quantum reflection from the drop at $x = 0$ (see below Eq. (2.38). With some probability the particle can overcome the reflection and enter the deeper part of the well, between $x = -a = -10$ and $x = 0$. It quickly reaches the left edge and reflects back, leading to the pronounced interference features between left and right travelling waves. Bonus questions: How can you estimate the wavelength of this feature?

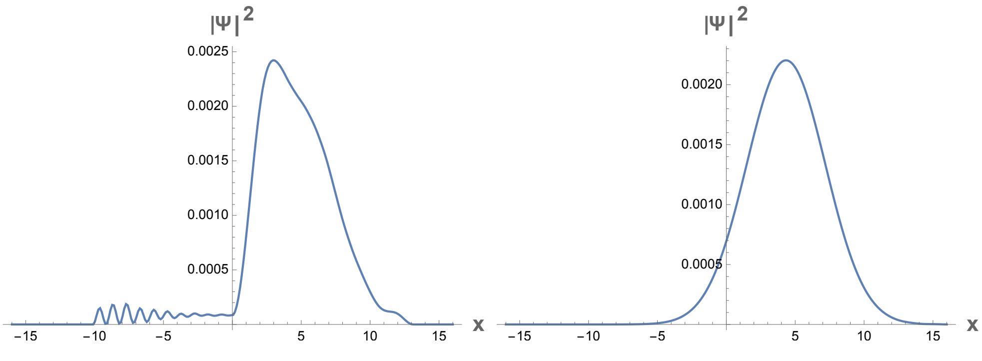

Figure 4: Gaussian wavepacket spreading inside of a potential with step, $t = 6$ after initialisation in the $\Psi(x, t = 0)$ given in (4c) (we are using $\hbar = m = 1$). (right) Without potentials, it spreads exactly as it would for a free particle (week 5). (left) Within potential, reflection and quantum reflection at $x = b$ and $x = a$ are seen, as discussed in the text.