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 $V_{min} = \text{min}_x V(x)$, 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].

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

(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 distribrutions in this case? What is the fundamental difference to the classical oscillator? What quantum mechanical theorem enforces this difference? [6 pts]

(3) Schrödinger's equation in momentum space: [6 pts] Suppose a particle of mass m can move in one dimension under the influence of the potential $V(x)$. In Eq. (2.93) of the lecture, we introduced the momentum space representation $\tilde{\phi(k)}$ of the wavefunction.

(a) Find also a momentum space representation of the TISE which a momentum space wavefunction has to fulfill.[1] *Hint: Your calculation should lead you towards the definition of the Fourier transformed potential:*

$$\tilde{V}(p - p') = \frac{1}{\sqrt{2\pi\hbar}} \int dx V(x) e^{-i\frac{(p-p')}{\hbar}x} \tag{1}$$

which should appear in your final equation. [3pts]

[1]The TISE 1(.62) that we have considered so far is said to be in the "position space representation". Its momentum space variant should only have $i\hbar\frac{\partial}{\partial t}\phi(\tilde{k}, t) = \cdots$ as the left hand side.

(b) Discuss the physical meaning of each term. Discuss what happens to the momentum probability distribution for the case $V(x) = 0$, or $V(x) \neq 0$. You may want to consider the change of the momentum space wavefunction during an infinitesimal time element dt [3pts].

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

$$V(x) = \begin{cases} \infty & x < -a, \\ 0 & -a \leq x < 0, \\ V_0 > 0 & 0 \leq x < b, \\ \infty & x > b \end{cases} \tag{2}$$

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]

(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]

(4c) Suppose a wavefunction at time $t = 0$ is given by $\Psi(x, t = 0) = e^{-(x-\frac{b}{3})^2/(2\sigma^2)}/(\pi\sigma^2)^{1/4}$, with $0 < \sigma = b/8$ 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 $V(x)$. For that, make sure you do not go to times so large that there is a chance for the particle to leave your discretised x range between $L_{\min} = -16$, $L_{\max} = 16$, hence e.g. $t < 8$. [6 pts]