PHY 303, I-Semester 2023/24, Assignment 5 solution

(1) Wave function discontinuities [8 pts tot]: Consider the normalised wavefunction

$$\Psi(x) = \begin{cases} \frac{1}{\sqrt{L}} & \text{for } -\frac{L}{2} \leq x \leq \frac{L}{2} \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

for $L > 0$, describing a particle with free Hamiltonian $\hat{H} = \hat{p}^2/(2m)$.

(a) Show formally that the function has two discontinuities, then find the corresponding momentum space wavefunction $\Psi(p)$ and draw both probability densities, for position and for momentum measurements [5pts].
Solution: From the function it becomes apparent that the discontinuity check has to be performed at the points $-\frac{L}{2}$, $\frac{L}{2}$

$$for \ -\frac{L}{2}$$

$$\lim_{x\to(-\frac{L}{2})^-} \Psi(x) = 0 \neq \lim_{x\to(-\frac{L}{2})^+} \Psi(x) = \frac{1}{\sqrt{L}} \tag{2}$$

$$for \ \frac{L}{2}$$

$$\lim_{x\to(\frac{L}{2})^+} \Psi(x) = 0 \neq \lim_{x\to(\frac{L}{2})^-} \Psi(x) = \frac{1}{\sqrt{L}} \tag{3}$$

Thus the function is discontinuous at both $\frac{L}{2}, -\frac{L}{2}$. *To find the momentum space wavefunction* $\Psi(p)$, *we take the Fourier Transform of* $\Psi(x)$

$$\begin{aligned}\Psi(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \Psi(x) e^{-i\frac{p}{\hbar}x} \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\frac{L}{2}}^{\frac{L}{2}} dx \frac{1}{\sqrt{L}} e^{-i\frac{p}{\hbar}x} = \frac{1}{\sqrt{2\pi\hbar}} \sqrt{L} \frac{sin(\frac{Lp}{2\hbar})}{\frac{pL}{2\hbar}} \\ &= \frac{\sqrt{L}}{\sqrt{2\pi\hbar}} sinc(\frac{Lp}{2\hbar}) \quad where \ \ sinc(x) = \frac{sin(x)}{x}\end{aligned} \tag{4}$$

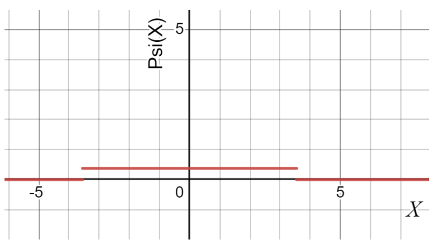

Figure 1: Discontinuous wavefunction $\Psi(x)$.

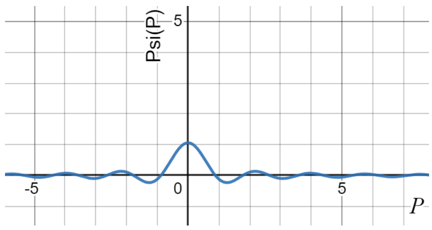

Figure 2: The momentum space wavefunction $\Psi(p)$ of a step function is a *sinc* function.

(b) Show that the expectation value of the kinetic (=total) energy in the state is infinite regardless of L, and discuss the implications of this for discontinuities in wavefunctions [3pts].
Solution: The total energy can calculated by $\int_{-\infty}^{\infty} \frac{p^2}{2m}\frac{L}{2\pi\hbar} sin(\frac{Lp}{2\hbar})^2 \frac{1}{(\frac{Lp}{2\hbar})^2} dp$. *Which boils down to* $K\int_{-\infty}^{\infty} sin(wp)^2\, dp$, *where* K *and* w *are constants. This integral clearly diverges and thus the Kinetic energy and consequently the total energy diverges regardless of L. Thus, in order to have a meaningful finite energy, we require continuous wavefunctions.*

(2) Bound states on two delta-function potentials [10pts tot]: Consider a double delta-function potential

$$V(x) = -\alpha[\delta(x-a) + \delta(x+a)]. \tag{5}$$

(a) Show that a wavefunction solving the TISE for the potential above must satisfy the condition

$$\lim_{\epsilon\to 0}\left[\phi(a+\epsilon)' - \phi(a-\epsilon)'\right] = -\frac{2m}{\hbar^2}\alpha\phi(a). \tag{6}$$

and a similar one involving location $x = -a$ [2pts].
Solution: See lecture section 2.8.

(b) With that, show that the Ansatz

$$\phi(x) = \begin{cases} Ae^{-\kappa x} & \text{for } x \le -a, \\ B(e^{\kappa x} \pm e^{-\kappa x}) & \text{for } -a < x \le a, \\ Ae^{\kappa x} & \text{for } x > a, \end{cases} \tag{7}$$

can solve the TISE. Why can we choose this Ansatz?. Find the parameter κ required for this separately for $\pm$ and the equation linking it and the energy E. Solve that equation, numerically if need be [6pts].

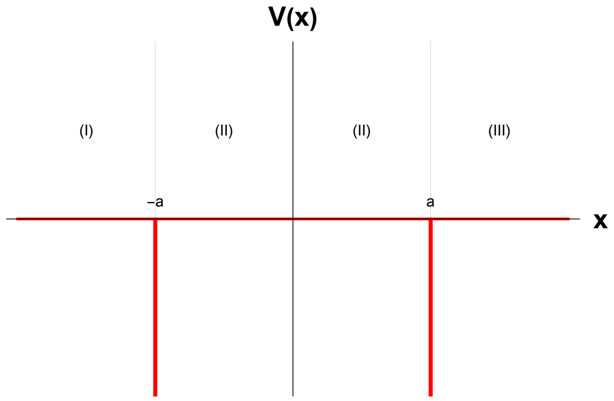

Figure 3: Plot of potential in Eq. (5)

(c) Discuss all solutions to this equation graphically. How many bound states are there? Is there always a bound state? [2 pts]

Solution: The argumentation why we can choose this Ansatz follows arguments we have seen many times before. For $E < 0$ there can be at most bound states since a particle at $x \to \pm\infty$ would have a negative kinetic energy. The solution everywhere except on the delta function spikes will be a superposition of exponentially decaying and increasing solutions (as in Eq. (7) for $-a < x \leq a$. However to the left of the leftmost delta function, we cannot have the term $\sim e^{-\kappa x}$ since it blows up at $x \to -\infty$ and similarly we can't have a term $\sim e^{\kappa x}$ to the right of the rightmost delta function. Finally we know from Assignment 3 Q1(b), that all solutions can be taken as either symmetric or anti-symmetric, since the potential Eq. (5) is symmetric ($V(x) = V(-x)$).

From the TISE we have $\kappa = \frac{\sqrt{2mE}}{\hbar}$.

***first for even solutions**:*

$$\phi(x) = \begin{cases} Ae^{-\kappa x} & (x < a), \\ B\left(e^{\kappa x} + e^{-\kappa x}\right) & (-a < x < a), \\ Ae^{\kappa x} & (x < -a). \end{cases}$$

The remaining boundary (connection) conditions are:

Continuity at a:

$$Ae^{-\kappa a} = B\left(e^{\kappa a} + e^{-\kappa a}\right)$$
$$\Rightarrow A = B\left(e^{2\kappa a} + 1\right) \qquad (8)$$

Discontinuous derivative at a:

$$lim_{\epsilon \to 0}\left[\phi(a+\epsilon)' - \phi(a-\epsilon)'\right] = -\frac{2m}{\hbar^2}\alpha\phi(a).$$
$$\Rightarrow -\kappa Ae^{-\kappa a} - B\left(\kappa e^{\kappa a} - \kappa e^{-\kappa a}\right) = -\frac{2m\alpha}{\hbar^2}Ae^{-\kappa a}$$

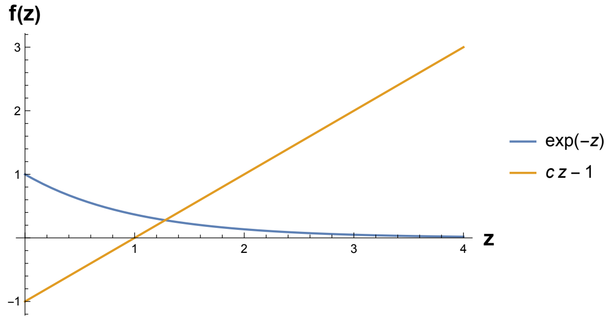

Figure 4: RHS and LHS of the transcendental equation (10).

$$\Rightarrow A + B\left(e^{2\kappa a} - 1\right) = \frac{2m\alpha}{\hbar^2\kappa}A$$
$$\Rightarrow B\left(e^{2\kappa a} - 1\right) = A\left(\frac{2m\alpha}{\hbar^2\kappa} - 1\right) \tag{9}$$

Combining both equations

$$B\left(e^{2\kappa a} - 1\right) = B\left(e^{2\kappa a} + 1\right)\left(\frac{2m\alpha}{\hbar^2\kappa} - 1\right)$$
$$\Rightarrow e^{2\kappa a} - 1 = e^{2\kappa a}\left(\frac{2m\alpha}{\hbar^2\kappa} - 1\right) + \frac{2m\alpha}{\hbar^2\kappa} - 1$$
$$\Rightarrow 1 = \frac{2m\alpha}{\hbar^2\kappa} - 1 + \frac{2m\alpha}{\hbar^2\kappa}e^{-2\kappa a}$$
$$\Rightarrow \frac{\hbar^2\kappa}{m\alpha} = 1 + e^{-2\kappa a}$$
$$\Rightarrow e^{-2\kappa a} = \frac{\hbar^2\kappa}{m\alpha} - 1. \tag{10}$$

Eq.(10) is a transcendental equation for κ (and hence for E). we will solve it graphically: Let $z \equiv 2\kappa a, c \equiv \frac{\hbar^2}{2am\alpha}$, so $e^{-z} = cz - 1$, we then show the left hand side and right hand side of Eq. (10) separetely in Fig. 4, as a function of z.

From the graph, noting that c and z are both positive, we see that there is one (and only one) solution (for even ψ). If $\alpha = \frac{\hbar^2}{2ma}$, so $c = 1$, the calculator gives $z = 1.278$, so $\kappa^2 = -\frac{2mE}{\hbar^2} = \frac{z^2}{(2a)^2} \Rightarrow E = -\frac{(1.278)^2}{8}\left(\frac{\hbar^2}{ma^2}\right) = -0.204\left(\frac{\hbar^2}{ma^2}\right)$.

Now we look separately at odd solutions:

$$\phi(x) = \begin{cases} Ae^{-\kappa x} & (x < a), \\ B\left(e^{\kappa x} - e^{-\kappa x}\right) & (-a < x < a), \\ Ae^{\kappa x} & (x < -a). \end{cases}$$

The boundary condition:

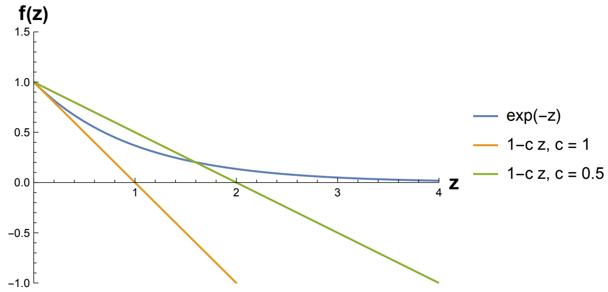

Figure 5: Plot for Eq. (13)

Continuity at a:

$$
\begin{aligned}
&Ae^{-\kappa a} = B\left(e^{\kappa a} - e^{-\kappa a}\right) \\
\Rightarrow &A = B\left(e^{2\kappa a} - 1\right)
\end{aligned} \tag{11}
$$

Discontinuous derivative at a:

$$
\begin{aligned}
&lim_{\epsilon\to 0}\left[\phi(a+\epsilon)' - \phi(a-\epsilon)'\right] = -\frac{2m}{\hbar^2}\alpha\phi(a). \\
\Rightarrow &-\kappa Ae^{-\kappa a} - B\left(\kappa e^{\kappa a} + \kappa e^{-\kappa a}\right) = -\frac{2m\alpha}{\hbar^2}Ae^{-\kappa a} \\
\Rightarrow &A + B\left(e^{2\kappa a} + 1\right) = \frac{2m\alpha}{\hbar^2\kappa}A \\
\Rightarrow &B\left(e^{2\kappa a} + 1\right) = A\left(\frac{2m\alpha}{\hbar^2\kappa} - 1\right)
\end{aligned} \tag{12}
$$

Combining both equations

$$
\begin{aligned}
&B\left(e^{2\kappa a} + 1\right) = B\left(e^{2\kappa a} - 1\right)\left(\frac{2m\alpha}{\hbar^2\kappa} - 1\right) \\
\Rightarrow &e^{2\kappa a} + 1 = e^{2\kappa a}\left(\frac{2m\alpha}{\hbar^2\kappa} - 1\right) - \frac{2m\alpha}{\hbar^2\kappa} + 1 \\
\Rightarrow &1 = \frac{2m\alpha}{\hbar^2\kappa} - 1 - \frac{2m\alpha}{\hbar^2\kappa}e^{-2\kappa a} \\
\Rightarrow &\frac{\hbar^2\kappa}{m\alpha} = 1 - e^{-2\kappa a} \\
\Rightarrow &e^{-2\kappa a} = 1 - \frac{\hbar^2\kappa}{m\alpha}.
\end{aligned} \tag{13}
$$

We again inspect the transcendental equation $e^{-z} = 1 - cz$ graphically in Fig. 5). This time there may or may not be a solution. Both graphs have their y-intercepts at 1 , but if c is too large (α too small), there may be no intersection (orange line), whereas if c is smaller (green line) there will be. (Note that $z = 0 \Rightarrow \kappa = 0$ is not a *solution, since ψ is then non-normalizable.) The slope of e^{-z} (at $z = 0$) is -1 ; the slope of $(1 - cz)$ is $-c$. So there is an odd solution $\Leftrightarrow c < 1$, or $\alpha > \hbar^2/2ma$.*

Conclusion: One bound state if $\alpha \leq \hbar^2/2ma$; two if $\alpha > \hbar^2/2ma$.

For $c < 1$

$$\alpha = \frac{\hbar^2}{ma} \Rightarrow c = \frac{1}{2} \cdot \begin{cases} \text{Even: } e^{-z} = \frac{1}{2}z - 1 \Rightarrow z = 2.21772 \\ \text{Odd: } e^{-z} = 1 - \frac{1}{2}z \Rightarrow z = 1.59362 \end{cases} \tag{14}$$

Two bound state energy are given by

$$E = -0.615 \left(\hbar^2/ma^2\right); E = -0.317 \left(\hbar^2/ma^2\right). \tag{15}$$

For $c > 1$

$$\alpha = \frac{\hbar^2}{4ma} \Rightarrow c = 2. \text{ Only even: } e^{-z} = 2z - 1 \Rightarrow z = 0.738835; \quad E = -0.0682 \left(\hbar^2/ma^2\right). \tag{16}$$

(3) Measurements: [12 pts] Consider a Hilbertspace with three basis vectors $|\,a\,\rangle$, $|\,b\,\rangle$, $|\,c\,\rangle$, and three operators:

$$\hat{O}_1 = \kappa\left(|\,a\,\rangle\langle\,a\,| - |\,c\,\rangle\langle\,c\,|\right), \tag{17}$$

$$\hat{O}_2 = \frac{\kappa}{\sqrt{2}}\left(|\,a\,\rangle\langle\,b\,| + |\,b\,\rangle\langle\,a\,| + |\,b\,\rangle\langle\,c\,| + |\,c\,\rangle\langle\,b\,|\right), \tag{18}$$

$$\hat{O}_3 = \frac{\kappa}{\sqrt{2}}\left(-i|\,a\,\rangle\langle\,b\,| + i|\,b\,\rangle\langle\,a\,| + -i|\,b\,\rangle\langle\,c\,| + i|\,c\,\rangle\langle\,b\,|\right). \tag{19}$$

$$\tag{20}$$

(a) Find the matrix representation of these operators in the basis $\{|\,a\,\rangle, |\,b\,\rangle, |\,c\,\rangle\}$, all eigenvectors and eigenvalues for each and all commutators among those three operators.

The matrix conversion can be done by representing each three different kets along the rows and the bras along the columns. Thus, element i, j would correspond to the co-efficient of $|\,i\,\rangle\langle\,j\,|$.

$$\hat{O}_1 = \begin{matrix} & \langle\,a\,| & \langle\,b\,| & \langle\,c\,| \\ |\,a\,\rangle & \kappa & 0 & 0 \\ |\,b\,\rangle & 0 & 0 & 0 \\ |\,c\,\rangle & 0 & 0 & -\kappa \end{matrix} \tag{21}$$

$$\hat{O}_2 = \frac{\kappa}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{22}$$

$$\hat{O}_3 = \frac{\kappa}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \tag{23}$$

The normalised eigenvectors and eigenvalues for the respective matrices are:

For $\hat{O}_1$

$$v_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \lambda_1 = \kappa \ ; \ v_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \lambda_2 = 0 \ ; \ v_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \lambda_2 = -\kappa$$

For $\hat{O}_2$

$$v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \quad \lambda_1 = 0 \ ; \ v_2 = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} \quad \lambda_2 = \kappa \ ; \ v_3 = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} \quad \lambda_2 = -\kappa$$

For $\hat{O}_3$

$$v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \quad \lambda_1 = 0 \ ; \ v_2 = \frac{1}{2} \begin{pmatrix} -1 \\ -i\sqrt{2} \\ 1 \end{pmatrix} \quad \lambda_2 = \kappa \ ; \ v_3 = \frac{1}{2} \begin{pmatrix} -1 \\ i\sqrt{2} \\ 1 \end{pmatrix} \quad \lambda_2 = -\kappa$$

Since we already found the matrix representations above, the commutators can be calculated using matrix multiplications, yielding:

$$\left[\hat{O}_2, \hat{O}_3\right] = i\kappa\hat{O}_1 \ ; \ \left[\hat{O}_3, \hat{O}_1\right] = i\kappa\hat{O}_2 \ ; \ \left[\hat{O}_1, \hat{O}_2\right] = i\kappa\hat{O}_3 \tag{24}$$

(b) From that derive an uncertainty relation between the three observables described by $\hat{O}_j$. Also discuss uncertainties between $\hat{O}_2$ and $\hat{O}_\perp \equiv \hat{O}_1^2 + \hat{O}_3^2$.
Solution: For general operators, the uncertainty principle is $\sigma_A \sigma_B \geq \sqrt{\left(\frac{1}{2i}\langle[\hat{A}, \hat{B}]\rangle\right)^2}$. *We can insert the commutation relations of operators* $\hat{O}_j$, *and find for example* $\sigma_{\hat{O}_2}\sigma_{\hat{O}_3} \geq |\frac{1}{2}\langle\hat{O}_1\rangle| = 0$ *from the first equation in (24). This in general (in general* $\langle\hat{O}_1\rangle$ *will be nonzero), we cannot know the observables for* $\hat{O}_2$ *and* $\hat{O}_3$ *simultaneously to arbitrary precision. Similar relations arise from the other two commutators.*

Now to check the commutator of $\hat{O}_2$ *and* $\hat{O}_\perp$

$$\begin{aligned} \left[\hat{O}_2, \hat{O}_\perp\right] &= \left[\hat{O}_2, \hat{O}_1^2\right] + \left[\hat{O}_2, \hat{O}_1^2\right] = \left[\hat{O}_2, \hat{O}_1\right]\hat{O}_1 + \hat{O}_1\left[\hat{O}_2, \hat{O}_1\right] + \left[\hat{O}_2, \hat{O}_3\right]\hat{O}_3 + \hat{O}_3\left[\hat{O}_2, \hat{O}_3\right] \\ &= -i\hat{O}_3\hat{O}_1 - i\hat{O}_1\hat{O}_3 + i\hat{O}_1\hat{O}_3 + i\hat{O}_3\hat{O}_1 = 0 \end{aligned} \tag{25}$$

Thus the uncertainty relation is $\sigma_{\hat{O}_2}\sigma_{\hat{O}_\perp} \geq 0$, and observables corresponding to these operators <u>*can*</u> *be known simultaneously perfectly.*

(c) Suppose the system is initially in the state $|\,\Psi\,\rangle = (|\,a\,\rangle - |\,b\,\rangle + i|\,c\,\rangle)/\sqrt{3}$. From this discuss the following sequence:

(i) What is the probability to find $o_2 = 0, \pm\kappa$ upon measuring $\hat{O}_2$?

(ii) Suppose we measured $o_2 = \kappa$, what is the probability to measure $o_2 = \kappa$ if the measurement is repeated immediately after the first?

(iii) Immediately following that, we measure $\hat{O}_1$ and suppose we find $o_1 = \kappa$. Immediately after this step, we measure $\hat{O}_2$ again, which answers can we find, and with which probabilty?

Solution: (i)
Take the projections of the state onto the three eigenvectors of $\hat{O}_2$

$$\begin{aligned} P(o_2 = 0) &= |\langle\, v_1\,|\,\Psi\,\rangle|^2 = \left(|-\frac{1}{\sqrt{6}} + \frac{i}{\sqrt{6}}|\right)^2 = \frac{1}{3} \\ P(o_2 = \kappa) &= |\langle\, v_2\,|\,\Psi\,\rangle|^2 = |\frac{1}{2\sqrt{3}} - \frac{1\sqrt{2}}{2\sqrt{3}} + i\frac{1}{2\sqrt{6}}|^2 = \frac{1}{6}(2-\sqrt{2}) \\ P(o_2 = -\kappa) &= |\langle\, v_3\,|\,\Psi\,\rangle|^2 = |\frac{1}{2\sqrt{3}} + \frac{\sqrt{2}}{2\sqrt{3}} + i\frac{1}{2\sqrt{3}}|^2 = \frac{1}{6}(2+\sqrt{2}) \end{aligned} \tag{26}$$

(ii) Immediately after the measurement of $o_2 = \kappa$ the state has collapsed onto the eigenvector v_2. Thus the probability to measure $o_2 = \kappa$ in an immediate repetition of this measurement is 1.
(iii) If we have found $o_1 = \kappa$ in this latest measurement, the state has collapsed again this time into $|\,\Psi_{inst}\,\rangle = |\,a\,\rangle$ with column vector representation $\begin{pmatrix}1\\0\\0\end{pmatrix}$. Now to find the probabilities of outcomes of measurements of $\hat{O}_2$, we newly take the projection of this stage onto the eigenvectors of $\hat{O}_2$, which are:

$$\begin{aligned} P(o_2 = 0) &= \langle\, v_1\,|\,\Psi_{inst}\,\rangle = \frac{1}{2}, \\ P(o_2 = \kappa) &= \langle\, v_2\,|\,\Psi_{inst}\,\rangle = \frac{1}{4}, \\ P(o_2 = -\kappa) &= \langle\, v_3\,|\,\Psi_{inst}\,\rangle = \frac{1}{4}. \end{aligned} \tag{27}$$

Importantly, measuring $\hat{O}_1$ in between the first and second measurement of $\hat{O}_2$ as changed the probability to find $o_2 = \kappa$ from 100% (directly after the first measurement) to only 25 % now.

(d) What changes if you swap the final measurement of $\hat{O}_1$ in the list above with a measurement of $\hat{O}_\perp$? Discuss all similarities and differences, and relate whatever you find to the uncertainty relations you have derived earlier.
Solution: Observe from 4(b) that $\hat{O}_2$ *commutes with* $\hat{O}_\perp$ *and thus the uncertainty between their measurements is* $\sigma_{o_2}\sigma_{o_\perp} \geq 0$. *Thus, the observables are compatible a.k.a both can be measured at the same time without affecting each other. Hence, measurement of* $o_\perp$ *does not affect the probabilities of measuring the value of* o_2 *which was given as 100% for* $o_2 = \kappa$ *after the first measurement, and remains 100% also after measuring* $\hat{O}_\perp$ *in between. You can verify explicitly that the eigenvector* $|\, v_2 \,\rangle$ *of* $\hat{O}_2$ *is* <u>*also*</u> *an eigenvector of* $\hat{O}_\perp$.

(4) Box inside a box: [10pts] Consider the infinite square well potential, with an additional step potential inside:

$$\bar{V}(x) = \begin{cases} \infty & x \leq 0, \\ 0 & 0 < x \leq \frac{a}{2} - \frac{L}{2}, \\ V_0 > 0 & \frac{a}{2} - \frac{L}{2} < x \leq \frac{a}{2} + \frac{L}{2} \\ 0 & \frac{a}{2} + \frac{L}{2} < x \leq a \\ \infty & x > a. \end{cases} \tag{28}$$

Let us assume that $V_0 < \frac{\hbar^2\pi^2}{2ma^2}$. Let us denote the usual infinite square well potential without that step (as in lecture notes Eq. (2.10)) by $V(x)$, and define two Hamiltonians $\hat{\bar{H}} = \hat{T} + \bar{V}(x)$ and $\hat{H} = \hat{T} + V(x)$, where $\hat{T}$ is the kinetic energy operator of a particle of mass m in one dimension.

(a) Make a drawing of this potential. Argue why all eigenstates $\bar{\phi}_n(x)$ of the present Hamiltonian $\hat{\bar{H}}$ can be expressed in terms of eigenstates $\phi_n(x)$ of the usual Hamiltonian $\hat{H}$. Then find an argument, why it might be justified, for the above low value of V_0, to attempt to express the new lowest energy eigenstates of $\hat{\bar{H}}$ only using the M lowest energy eigenstates of $\hat{H}$, for small M, let's say $M = 3$.
Solution: The drawing of the potential is shown in Fig. 6.

The old basis are eigenstate of the old Hamiltonian ($\hat{H}$) *which is a hermitian operator thus the eigenstates* ($\phi_n(x)$) *forms a basis for any integrable function between* $[0, a]$. *We expect eigenfunctions of the new Hamiltonian* ($\hat{\bar{H}}$) *to vanish outside the range* $[0, a]$ *for the same reasons that they vanish there for the old Hamiltonian* ($\hat{H}$)*, hence each eigenfunction of the new Hamiltonian can be expanded in terms of those of the old one.*

In the limit discussed above if we expand the new states in terms of old ones and take the (kinetic) energy expectation value of the new states, the ground-state cannot have a too large contribution of high energy old states, since this would give it a very high energy itself. For this reason we can write the new ground-state as linear combination of the lowest energy eigenstates of $\hat{H}$.

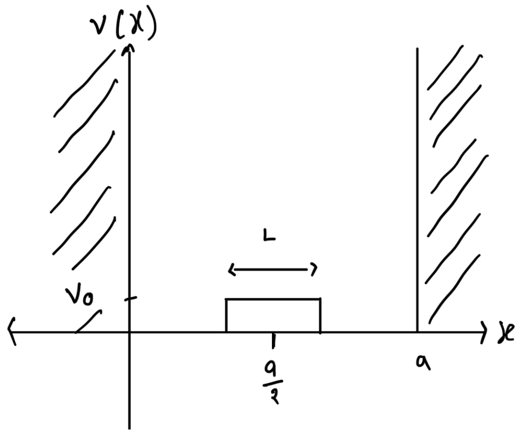

Figure 6: Potential given in Eq. (28), with a small steplike perturbation inside an infinite square well.

(b) Write the present Hamiltonian $\hat{\bar{H}}$ explicitly in matrix form, using only the $M = 3$ lowest energy eigenstates of $\hat{H}$ as a basis (i.e. Eq. (2.18) of lecture notes, for $n = 1, 2, 3$). Explicitly find a matrix in terms of parameters, solving any integrations that might be required.

Solution:

We want to find the Matrix form of $\hat{\bar{H}}$ in the basis of $\hat{H}$, effectively that requires to calculate $\bar{H}_{mn} = \langle\, \phi_m\, |\hat{\bar{H}}|\, \phi_n\, \rangle$ with $m, n = 1, 2, 3$. Let us separate $\hat{\bar{H}}$ as $\hat{H} + \hat{\bar{V}}$. Now the matrix form becomes $\bar{H}_{mn} = H_{mn} + \bar{V}_{mn}$. In $|\, \phi_n\, \rangle$ basis we know the H is diagonal with corresponding energy value i.e.

$$H_{mn} = \begin{cases} E_n & m = n, \\ 0 & m \neq n. \end{cases} \tag{29}$$

Now we need to find the other missing quantity $\bar{V}_{mn} = \langle\, \phi_m\, |\hat{\bar{V}}|\, \phi_n\, \rangle$. In terms of integration we will have

$$\bar{V}_{mn} = \int_{a/2-L/2}^{a/2+L/2} \phi_m^*(x) V_0 \phi_n(x) dx \tag{30}$$

Finding $\bar{V}_{mm}$

$$\begin{aligned} \bar{V}_{mm} &= \int_{a/2-L/2}^{a/2+L/2} \phi_1^*(x) V_0 \phi_1(x) dx \\ &= V_0 \frac{2}{a} \int_{a/2-L/2}^{a/2+L/2} \sin\left(\frac{m\pi x}{a}\right)^2 dx \end{aligned}$$

$$
\begin{aligned}
&= V_0\frac{1}{a}\int_{a/2-L/2}^{a/2+L/2}\left[1-\cos\left(\frac{2m\pi x}{a}\right)\right]dx \\
&= V_0\frac{L}{a} - V_0\frac{1}{a}\int_{a/2-L/2}^{a/2+L/2}\cos\left(\frac{2m\pi x}{a}\right)dx \\
&= V_0\frac{L}{a} - V_0\frac{1}{2m\pi}\left[\sin\left(\frac{2m\pi x}{a}\right)\right]_{a/2-L/2}^{a/2+L/2} \\
&= V_0\frac{L}{a} - V_0\frac{1}{2m\pi}\left[\sin\left(m\pi+\frac{m\pi L}{a}\right)-\sin\left(m\pi-\frac{m\pi L}{a}\right)\right] \\
&= V_0\left[\frac{L}{a}-\frac{(-1)^m}{m\pi}\sin\left(\frac{m\pi L}{a}\right)\right] \qquad (31)
\end{aligned}
$$

For $m = n+1$ and $n = m+1$, from symmetry around $a/2$ we know that this integral will be zero. As around $a/2$ the eigenfuctions are either even or odd, making the integral vanishes when integrated around a even range. i.e. $\bar{V}_{12} = \bar{V}_{21} = \bar{V}_{32} = \bar{V}_{23} = 0$.

lastly

$$
\begin{aligned}
\bar{V}_{13} = \bar{V}_{31} &= \int_{a/2-L/2}^{a/2+L/2}\phi_1^*(x)V_0\phi_3(x)dx \\
&= V_0\frac{2}{a}\int_{a/2-L/2}^{a/2+L/2}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{3\pi x}{a}\right)dx \\
&= V_0\frac{1}{a}\int_{a/2-L/2}^{a/2+L/2}\cos\left(\frac{2\pi x}{a}\right)-\cos\left(\frac{4\pi x}{a}\right) \\
&= V_0\left[\frac{1}{2\pi}\sin\left(\frac{2\pi x}{a}\right)-\frac{1}{4\pi}\sin\left(\frac{4\pi x}{a}\right)\right]_{a/2-L/2}^{a/2+L/2} \\
&= -\frac{4V_0\sin\left(\frac{\pi L}{2a}\right)\cos^3\left(\frac{\pi L}{2a}\right)}{\pi} \qquad (32)
\end{aligned}
$$

Combining all We get $\bar{H}$.

$$
\bar{H} = \begin{pmatrix}
\frac{\pi^2\hbar^2}{2a^2m}+V_0\left(\frac{L}{a}+\frac{\sin\left(\frac{\pi L}{a}\right)}{\pi}\right) & 0 & -\frac{4V_0\sin\left(\frac{\pi L}{2a}\right)\cos^3\left(\frac{\pi L}{2a}\right)}{\pi} \\
0 & \frac{2\pi^2\hbar^2}{a^2m}+V_0\left(\frac{L}{a}-\frac{\sin\left(\frac{2\pi L}{a}\right)}{2\pi}\right) & 0 \\
-\frac{4V_0\sin\left(\frac{\pi L}{2a}\right)\cos^3\left(\frac{\pi L}{2a}\right)}{\pi} & 0 & \frac{9\pi^2\hbar^2}{2a^2m}+V_0\left(\frac{L}{a}+\frac{\sin\left(\frac{3\pi L}{a}\right)}{3\pi}\right)
\end{pmatrix} \qquad (33)
$$

(c) Using that matrix representation, find the new eigenstates and eigenenergies, make a drawing of the former, and compare the latter explicitly with the eigenenergies of $\hat{H}$.

Solution: See the Mathematica file **`Assignment5_program_solution_v1.nb`** *for solution. There we find for parameter $a = 6$, $L = 2$, $V_0 = 0.07$, $\hbar = 1$ and $m = 1$ the new ground state to be*

$$\bar{\phi_1}(x) = 0.99964\phi_1(x) + 0.0268382 * \phi_3(x) \tag{34}$$

From these coefficient it is clear that the ground state of $\bar{H}$ is almost equal to ground state of H with overlap of 0.99964.The important point to notice is that for new ground state the coupling to the state $n = 2$ is 0. From comparison in Table 1 note that the

Table 1: Comparing E and $\bar{E}$

	$n = 1$	$n = 2$	$n = 3$
E	0.137078	0.548311	1.2337
$\bar{E}$	0.178931	0.561996	1.25781

ground state energy has increased the most while higher state energies increases very little.

(d) Now adapt the code which was provided for Assignment 3 Q4, to numerically solve the TISE, to numerically find eigenstates and energies of $\hat{\bar{H}}$ under conditions as discussed above, and thus verify your calculations. Choose parameters for which at least some of the lowest three new eigenstates visibly differ from the old ones, and discuss physical reasons for the differences (or absence thereof).
Solution: See the Mathematica file **`Assignment5_program_solution_v1.nb`** *for full solution and discussion.*