1) Free particles – optional:

a) Write down, in the x-basis, the time-independent Schrödinger equation for a particle of mass m moving in one dimension in the presence of a potential $V(x)$?

b) Show that, when $V(x) = 0$, the wave function

$$\psi_{E,\alpha}(x) = N \exp(i\alpha\sqrt{2mE}x/\hbar)$$

describes a particle with energy eigenvalue E and momentum eigenvalue $\alpha\sqrt{2mE}$, where $E \geq 0$ and $\alpha = \pm 1$.

c) The wave function in part (a) is $\langle x|E,\alpha\rangle$ (*i.e.*, the projection on to the x-basis of the energy and momentum eigenket $|E,\alpha\rangle$). Derive the normalisation N such that the eigenkets $\{|E,\alpha\rangle\}$ are orthonormal (*i.e.*, $\langle E,\alpha|E',\alpha'\rangle = \delta(E-E')\,\delta_{\alpha,\alpha'}$).

d) A particle is in the state

$$\psi(x) = N^{+}\mathrm{e}^{ipx/\hbar} + N^{-}\mathrm{e}^{-ipx/\hbar}.$$

Give the possible outcome of the observation of the energy? What possible results follow from observation of the momentum? What is the probability of finding momentum p? What is the expectation value of the current operator at the position x (*i.e.*, the current density at x) in this state? Briefly discuss the major difference between this state and a classical state of the same energy.

2) Expansion of a box (after Shankar, 5.2.1): A particle is in the ground state of a one-dimensional box. Suddenly the box (symmetrically) doubles its length, leaving the state undisturbed. Determine the probability of finding the particle in the new ground state.

3) Expansion of a box (after Shankar, 5.2.4): A particle is in the n^{th} excited state $|n\rangle$ of a one-dimensional box of length L. Determine the force encountered as the walls are slowly pushed in. Assume *adiabaticity*, *i.e.*, that the quantum number(s) of the state do not vary as the properties (here, the length) of the system are adjusted. Compare your result for the force with that obtained for a classical particle of the same energy. [Hint: You may compute the latter via the frequency of collisions and the momentum transfer per collision.]

4) Delta function potential (after Shankar, 5.2.3): Consider the attractive potential $V(x) = -a\,\delta(x)$. Show that it admits a bound state, and determine the the corresponding energy eigenvalue. Sketch the wave function, indicating its essential features.

5) Potential step: The simplest change we can make to a free particle is to insert a potential step. We choose $V(x) = V_0\,\theta(x)$, with $V_0 > 0$ and $\theta(x)$ the usual Heaviside step function.

a) Sketch this potential.

Now there are two regions of space, $x < 0$ and $x > 0$; and two ranges of energy, $0 < E < V_0$ and $E > V_0$. In situations where the potential changes abruptly it is often a good strategy to solve the problem on either side and then match the solutions across the abrupt change.

b) For $E > V_0$, what is the nature of the solutions in regions to the left and to the right of the origin (*i.e.*, are they oscillatory, or exponentially decaying or growing)?

c) Show that the wave function

$$\psi(x) = \begin{cases} A\exp(ipx/\hbar) + B\exp(-ipx/\hbar), & \text{if } x < 0; \\ C\exp(iqx/\hbar), & \text{if } x > 0; \end{cases}$$

describes a particle with energy E, provided that certain conditions hold on p, q, A, B and C. State these conditions? Can E take on any value in the given range (*i.e.*, $E > V_0$)? Calculate the current for $x < 0$ and for $x > 0$? Briefly describe this state in terms of incident, reflected and transmitted waves. Are such states bound states?

Now consider the case $0 < E < V_0$. Classically, the region $x > 0$ is forbidden.

d) What is the nature of the solutions in regions $x < 0$ and $x > 0$? Show that the wave function

$$\psi(x) = \begin{cases} D\exp(ipx/\hbar) + F\exp(-ipx/\hbar), & \text{if } x < 0; \\ G\exp(-qx/\hbar), & \text{if } x > 0; \end{cases}$$

describes a particle with energy E, provided certain conditions on p, q, D, F and G are satisfied. State these conditions? Can E take on any values in the given range (*i.e.*, $0 < E < V_0$), or is it quantised? What is the current for $x < 0$ and for $x > 0$?

e) For the state $|\psi\rangle$ of part (d), are there incident and reflected waves? Is there a transmitted wave? How does the probability of finding a particle behave at large $|x|$? Are these states bound?

f) Is the classically forbidden region quantum mechanically forbidden? Why did we not include in the solution for $x > 0$ the term $H\exp(qx/\hbar)$ which also satisfies the Schrödinger equation?

6) Potential barrier – optional but recommended: As seen in the previous question, the potential step exemplifies two important quantum effects, namely

i) For $E > V_0$, incident particles can be reflected as well as transmitted; and

ii) For $0 < E < V_0$, there is an exponentially decaying probability of observing a particle in the classically forbidden region.

We can explore these effects further by changing the step into a barrier, *i.e.*, we now consider the potential

$$V(x) = V_0\{\theta(x) - \theta(x-a)\},$$

with $V_0 > 0$ and $a > 0$.

a) Sketch this potential.

In most physics problems it is a good idea to choose coordinates so that the barrier is symmetrically located. Although the physical results are independent of the choice of coordinates, the equations often turn out to be much simpler to solve. However, in this problem the algebra is simpler if the barrier runs from 0 to a.

Now we have three spatial regions and two energy ranges, $E > V_0$, and $V_0 > E > 0$. As with the potential step, when particles are incident from the left with $E > V_0$, there is a non-zero probability that they will be reflected. We will concentrate on the phenomenon of tunnelling, which occurs for $0 < E < V_0$. Classically, particles with these energies are confined either to the left or to the right of the barrier. Quantum mechanically this is not so: because the particles can be found in the barrier, there is a finite probability that they will emerge beyond it.

b) Show that, for $0 < E < V_0$, the wave function

$$\psi(x) = \begin{cases} A\exp(ipx/\hbar) + B\exp(-ipx/\hbar), & \text{if } x < 0; \\ C\exp(kx/\hbar) + D\exp(-kx/\hbar), & \text{if } 0 < x < a; \\ A\,S(E)\,\exp(ip(x-a)/\hbar), & \text{if } a < x; \end{cases}$$

satisfies the Schrödinger equation. Why can we now include the term $D\exp(-kx/\hbar)$? What state does this wave function describe (incident, transmitted, reflected,. . . , from where)? Give p and k in terms of M, E, $\hbar$ and V_0?

c) By matching the wave function and its derivative across $x = 0$ and across $x = a$, show that

$$S(E) = \frac{2ikp}{2ikp\cosh(ka/\hbar) + (p^2 - k^2)\sinh(ka/\hbar)}.$$

It is useful to write the transmitted wave in part (b) having extracted the coefficient $A\,S(E)\exp(-ipa/\hbar)$. This is because the incident current is proportional to $|A|^2$ and the transmitted current is proportional to $|A|^2|S(E)|^2$. The ratio of these two currents, $|S(E)|^2$, is defined to be the transmissivity $T(E)$.

d) Calculate $T(E)$ in terms of E, V_0, a, $\hbar$ and m.

7) Potential well: We now turn to bound states. These are states that can be normalised to unity and correspond to proper kets in the Hilbert space.

Consider the potential

$$V(x) = -V_0\{\theta(x + a/2) - \theta(x - a/2)\},$$

with $V_0 > 0$ and $a > 0$. There are three regions of space and two regions of energy.

a) Sketch the potential.

Again, the solution procedes by matching. In this case, the following quantum mechanical effects emerge:

i) There are bound (or localised) states, with quantised (or discrete) energy levels;

ii) There are extended (or non-localised, or scattering) states with a continuum of energies;

iii) Particles incident from the left with energy $E > 0$ can be transmitted or reflected with uniquely determined probabilities.

Let us explore these phenomena in the case of our simplified model potential. First consider states with $E < 0$, the bound states.

b) Show that the two wave functions

$$\psi_+(x) = \begin{cases} C\exp(kx/\hbar), & \text{if } x < -a/2; \\ A\cos(px/\hbar), & \text{if } -a/2 < x < a/2; \\ C\exp(-kx/\hbar), & \text{if } a/2 < x; \end{cases}$$

$$\psi_-(x) = \begin{cases} D\exp(kx/\hbar), & \text{if } x < -a/2; \\ B\sin(px/\hbar), & \text{if } -a/2 < x < a/2; \\ -D\exp(-kx/\hbar), & \text{if } a/2 < x; \end{cases}$$

are solutions of the time-independent Schrödinger equation.

c) Give the conditions that p, k, A, C, B and D must satisfy?

d) Why are the solutions $\exp(k|x|/\hbar)$ not included?

e) Discuss, briefly, how quantisation arises through the requirement that $\psi(x)$ be normalisable either to unity or to the Dirac delta function.

f) The parity operator, P, acts as follows

$$P|x\rangle = |-x\rangle.$$

Give its matrix elements in the x-basis? How does P act on an arbitrary ket $|\phi\rangle$? Describe, in words, the action of P on wave functions? What are the eigenvalues of P? Does the hamiltonian for this problem commute with P? Are the functions $\psi_\pm(x)$ eigenfunctions of P? What are their eigenvalues?

g) Show that the possible values of E for even (*i.e.*, +1) parity eigenfunctions satisfy $k/p = \tan(pa/2\hbar)$.

h) Show that the possible values of E for odd (*i.e.*, -1) parity eigenfunctions satisfy $k/p = -\cot(pa/2\hbar)$.

i) Briefly discuss how these transcendental equations may be solved graphically. Using a graphical argument, show that for *sufficiently small* V_0 there are no odd parity solutions. How small is *sufficiently small*?

We now turn to scattering states. Consider particles with $E > 0$, incident from the left. It can be shown, using the matching conditions at $x = \pm a/2$, that if

$$\psi(x) = A\exp(ipx/\hbar) + B\exp(-ipx/\hbar) \quad \text{for} \quad x < -a/2,$$

then

$$\psi(x) = A\,S(E)\exp(ip(x-a)/\hbar) \quad \text{for} \quad x > a/2,$$

where

$$S(E) = \left\{\cos(\overline{p}a/\hbar) - i\left(\frac{p^2+\overline{p}^2}{2p\overline{p}}\right)\sin(\overline{p}a/\hbar)\right\}^{-1}$$

and $\overline{p}^2 = 2m(E+V_0)$.

j) Show that the transmissivity is given by

$$T(E) = \left\{1 + \frac{\sin^2(\overline{p}a/\hbar)}{4\frac{E}{V_0}(1+\frac{E}{V_0})}\right\}^{-1}.$$

k) Is $T(E)$ oscillatory or monotonic?

l) Are there maxima of T as a function of E?

m) What value does T take at these maxima?

n) What is the amplitude of the reflected wave at a maximum of $T(E)$? Note that perfect transmission [*i.e.*, $T(E) = 1$] can be accompanied by a phase shift $\delta(E)$, not to be confused with a Dirac δ-function, such that

$$S(E) = |S(E)|\,\exp(i\delta(E)).$$

Briefly discuss why this is called a phase shift.

o) At what values of $\overline{p}$ do the maxima (also known as resonances) occur?

p) (**optional**) Show that $S(E)$ has poles at those (negative) energies E at which the potential has a bound state. Discuss why this is physically reasonable?