Warm-up: Bound and Scattering States of One Dimensional Quantum Mechanical Systems

- A "system" refers to an electron in a potential energy well, e.g., an electron in a one-dimensional infinite square well. The system is specified by a given Hamiltonian.
- Assume all systems are isolated.
- TISE and TDSE are abbreviations for the Time Independent Schrödinger Equation and Time Dependent Schrödinger Equation, respectively.
- $\hat{x}$, $\hat{p}$, $\hat{H}$ etc. refer to position, momentum and Hamiltonian **operators**, respectively. That is, the symbol ^ denotes an operator.
- The symbol $\sum$ in all questions denotes a sum over a complete set of states.
- Ψ refers to a general state, ψ_n refers to a stationary state wave function for the system, where $n = 1,2,3...$
- In $E_n\psi_n$ no summation is implied, unless explicitly written as $\sum E_n\psi_n$.
- Bound and scattering states refer to energy eigenstates (stationary states).
- The zero of the energy is chosen such that the potential energy is zero very far away from the region where the particle is interacting.
- In potential energy diagrams a piece of the potential energy is drawn. The slopes do not change after the last point drawn on either side. They are monotonic from thereon.

Comparison of Classical and Quantum Mechanical Systems

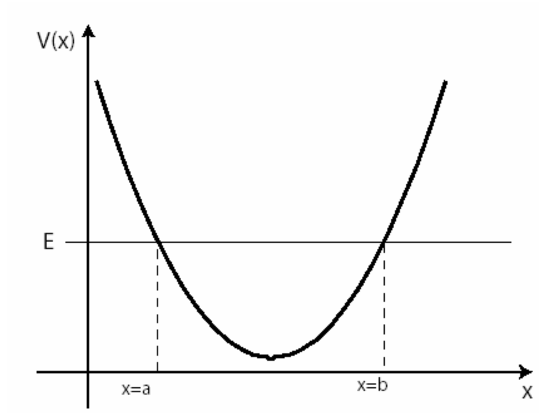


Figure 1: Simple Harmonic Oscillator Potential Energy

1. A toy car with total energy E is moving without friction in the simple harmonic oscillator potential energy shown in Fig.1. Choose all of the following statements that are correct about the system.

(I) The car is in a classical bound state.

(II) The car is bound between $x=a$ and $x=b$, it cannot be found anywhere outside that region.

(III) $x=a$ and $x=b$ are called classical turning points. When the car reaches one of them it turns back and moves until it reaches the other.

(a) (I) only
(b) (I) and (II) only
(c) (I) and (III) only
(d) (II) and (III) only
(e) All of the above

2. An electron with total energy E is initially localized in the region between $x=a$ and $x=b$ in the harmonic oscillator potential shown in Fig. 1. Choose all of the following statements that are correct about this quantum mechanical system.

(I) The electron is in a quantum mechanical bound state.

(II) The electron is bound between $x=a$ and $x=b$, it cannot be found anywhere outside that region.

(III) There is a finite probability that the electron will be found outside the region between $x=a$ and $x=b$.

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (II) only
(e) (I) and (III) only

3. A toy car with energy E is initially between x=a and x=b in the potential shown in Figure 2. Choose the statement that is correct about the toy car.

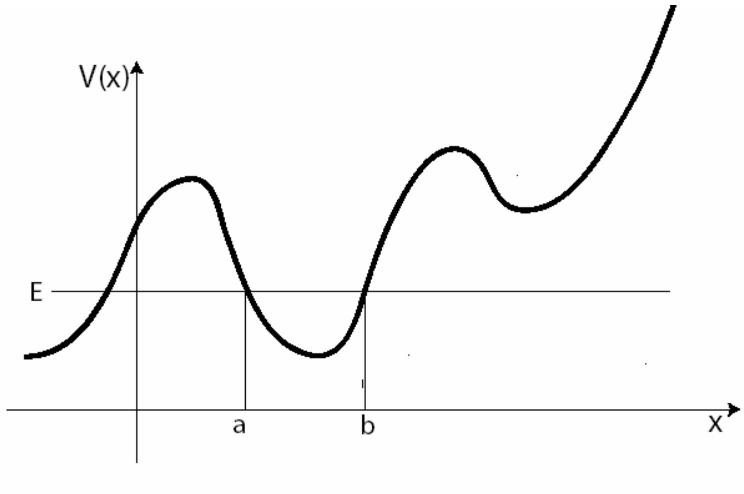


Figure 2

(a) It is in a bound state and it will remain between x=a and x=b.
(b) It is in a scattering state and there is a finite probability of finding it at $x = -\infty$.
(c) Nothing can be said without knowing the mass and speed explicitly.
(d) Nothing can be said without knowing the exact initial position of the car between x=a and x=b.
(e) This is not a reasonable system; one cannot have a potential energy that looks like this.

4. Consider the following quantum mechanical system: An electron with energy E is initially localized in the well between x=a and x=b in the potential shown in Figure 2. Choose the statement that is correct about the electron.

(a) It is in a bound state and it will remain between x=a and x=b.
(b) It is in a scattering state and there is a finite probability of finding it at $x \to -\infty$.
(c) Nothing can be said without knowing the Hamiltonian $\hat{H}$ explicitly.
(d) Nothing can be said without knowing the initial state of the electron (i.e., $\Psi(x.0)$) exactly.
(e) This is not a reasonable quantum mechanical system; one cannot have a potential energy that looks like this.

5. Consider the following quantum mechanical system: An electron with energy E is in the potential shown in Figure 3. Choose the statement that is correct about the electron.

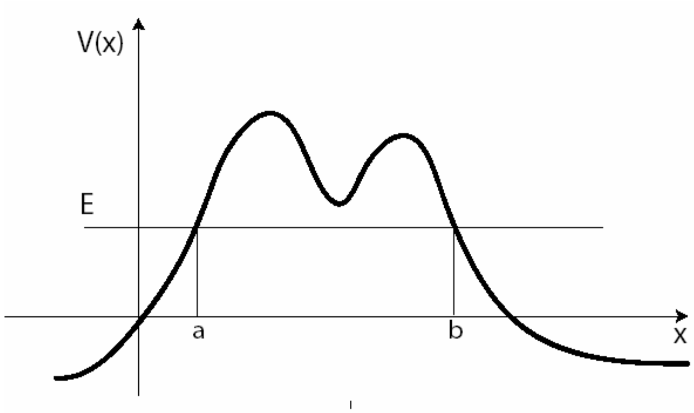


Figure 3

(a) It is in a bound state because the electron is confined between $x=a$ and $x=b$.
(b) It is in a bound state because the electron is confined outside the region between $x=a$ and $x=b$.
(c) It is in a scattering state and the electron can be found at $x = \pm\infty$.
(d) Whether it is a bound state or a scattering state depends on the electron's initial position.
(e) Nothing can be said without knowing the Hamiltonian $\hat{H}$ explicitly.

6. An electron with energy E is in the potential shown in Fig 3. It is at $x<a$ at time $t=0$. Choose all of the following statements that are correct about the electron at time t.

(I) It will be found at $x<a$ with 100% certainty because it doesn't have enough energy to pass to the other side.
(II) There is a finite probability that it will be found between $x=a$ and $x=b$.
(III) There is a finite probability that it will be found at $x>b$.

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (II) only
(e) (II) and (III) only

7. Choose all of the following statements that are correct.

(I) A quantum mechanical bound state is the same as a classical bound state.

(II) In a quantum mechanical bound state the particle cannot be found in the classically forbidden region.

(III) In a quantum mechanical bound state the particle can be found in the classically forbidden region, but its wave function will decay rapidly in that region.

(IV) In a quantum mechanical bound state the particle can be found in the classically forbidden region and it can have a oscillatory wave function in that region.

(a) (II) only
(b) (III) only
(c) (IV) only
(d) (I) and (II) only
(e) (III) and (IV) only

8. An electron is in a one dimensional potential energy well. The solution of the TISE is called a bound state solution,

(I) When the wave function decays to zero both as $x \to +\infty$ and $x \to -\infty$.

(II) When the energy E of the system is less than the potential energy both as $x \to +\infty$ and $x \to -\infty$.

(III) When the energy E of the system is less than the potential energy either as $x \to +\infty$ or $x \to -\infty$.

Choose all of the above statements that are correct.

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (III) only
(e) (II) and (III) only

Hydrogen Atom

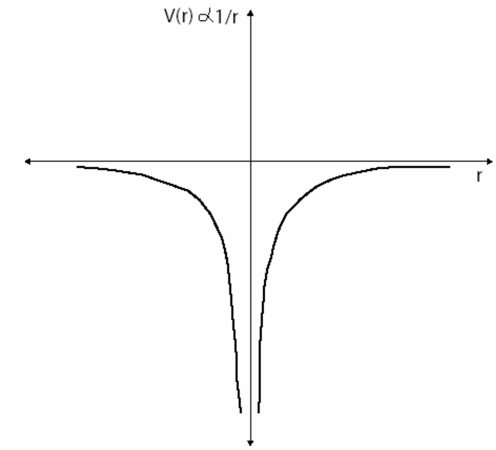


Figure 4: Hydrogen Atom Potential Energy $V \propto 1/r$.

9. Choose all of the following that are correct about an electron in a bound state in a hydrogen atom.

(I) It feels an average attractive force $\langle \vec{F} \rangle = \langle -\vec{\nabla} V \rangle \propto \left\langle \frac{1}{r^2} \right\rangle$ due to the presence of the proton.

(II) It has a discrete energy spectrum, it can have energy $\frac{-13.6eV}{n^2}$ where n=1,2,3…

(III) It has a continuous energy spectrum, all energies are allowed.

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (II) only
(e) (II) and (III) only

10. Choose all of the following that are correct about an electron that is in the vicinity of a proton, feeling the $1/r$ potential energy due to the proton, but that is not in a bound state as in a hydrogen atom.

(I) It feels an average attractive force $\langle \vec{F} \rangle = \langle -\vec{\nabla} V \rangle \propto \left\langle \frac{1}{r^2} \right\rangle$ due to the presence of the proton.

(II) It has a discrete energy spectrum, it can have energy $\frac{-13.6eV}{n^2}$ where n=1,2,3…

(III) It has a continuous energy spectrum, all energies are allowed.

(a) (I) only
(b) (II) only
(c) (I) and (II) only
(d) (I) and (III) only
(e) (II) and (III) only

<u>Note:</u> An electron such as the one in question 10, that is not bound to the proton but that interacts with the proton with a corresponding potential energy, is said to be in a scattering state

11. Choose all of the following that are correct about the Hydrogen atom.

(I) Bound states have energy $\frac{-13.6eV}{n^2}$, where n=1,2,3…

(II) An electron in the vicinity of the hydrogen atom that has energy E>0 will be in a scattering state.

(III) Scattering states have a discrete energy spectrum $E = \frac{+13.6eV}{n^2}$.

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (II) only
(e) (II) and (III) only

Pretest: Bound and Scattering States

1. What is a major difference between a classical bound state and a quantum mechanical bound state? Draw figures to illustrate your answer if necessary.

2. Draw a rough sketch of a potential energy that allows for only bound states, in quantum mechanics.

3. Draw a rough sketch of a potential energy that allows for only scattering states, in quantum mechanics.

4. Draw a rough sketch of a potential energy that allows for both bound and scattering states, in quantum mechanics.

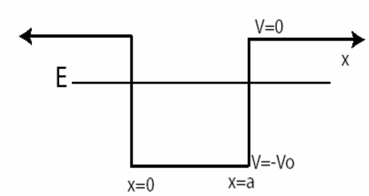
5. Briefly explain the difference between a bound state and a scattering state in quantum mechanics, including what conditions determine whether a particle will be in a bound state or a scattering state.

Tutorial: Bound and Scattering States of One Dimensional Quantum Mechanical Systems

Finite Square Well

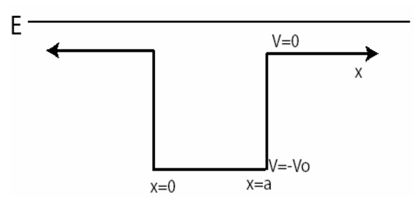
Since the Hydrogen atom is a three dimensional problem and $1/r$ is a complicated potential energy, a good understanding of the bound and scattering states can be obtained by considering a finite square well in one dimension.

1. Choose all of the following that are correct about an electron in a finite square well with energy E as shown in the figure below.



(a) It is in a bound state.
(b) It is in a scattering state.
(c) It is in a bound state between $x=0$ and $x=a$ and in a scattering state everywhere else.
(d) Such an energy is not possible because energy should be higher outside the well.
(e) It cannot be determined without knowing the wave function Ψ .

2. Choose all of the following that are correct about an electron in a finite square well with energy E as shown in the figure below.



(a) It is in a bound state.
(b) It is in a scattering state.
(c) Such an energy is not possible because energy should be lower inside the well.
(d) It cannot be determined without knowing the wave function Ψ .
(e) None of the above.

3. Choose all of the following that are true about an electron in the finite square well shown in Figure 5, coming from $x = -\infty$ with energy E>0.

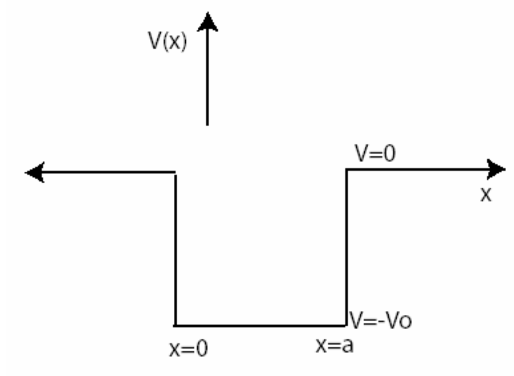


Figure 5:Finite Square Well of width *a*

(I) It will keep moving in a straight line with 100% certainty.
(II) It can bounce off of the potential well and be found at $x = -\infty$ at a later time.
(III) Its wave function will decay rapidly inside the well.

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (II) only
(e) None of the above.

4. Choose all of the following statements that are correct about an electron in a finite square well potential as shown in Fig 5

(a) It is always in a bound state.
(b) It is always in a scattering state.
(c) It is in a bound state between x=0 and x=a and a scattering state elsewhere.
(d) It can be in a scattering state or a bound state depending on its initial position.
(e) It can be in a scattering state or a bound state depending on its energy.

5. Choose all of the following that are correct about an electron in a linear superposition of bound states in the finite square well shown in Fig 5.

(I) It cannot be found in the classically forbidden region.
(II) It cannot be found infinitely far away from the potential energy well at $x \to \pm\infty$.
(III) It cannot be more localized than the width of the well, i.e., Ψ cannot go to zero before x=0 and x=a.

(a) (II) only
(b) (I) and (II) only
(c) (I) and (III) only
(d) (II) and (III) only
(e) All of the above.

6. Choose all of the following that are correct about an electron in a bound state in the finite square well shown in Fig 5.

(I) Its wave function decays rapidly outside the boundaries of the well (in the classically forbidden region).
(II) Its wave function is normalizable.
(III) The probability of finding it ia zero as $x \to \pm\infty$.

(a) (II) only
(b) (I) and (II) only
(c) (I) and (III) only
(d) (II) and (III) only
(e) All of the above.

7. Choose all of the following that are correct about an electron in a bound state in the finite square well shown in Fig 5.

(I) Its wave function is nonzero only in the well.
(II) Its energy must be negative.
(III) It can only have discrete energies.

(a) (I) only
(b) (II) only
(c) (I) and (II) only
(d) (I) and (III) only
(e) (II) and (III) only

8. Choose all of the following statements that are correct about an electron with energy $-V_0 < E < 0$ in the finite square well shown in Fig 5.

- (I) It is in a bound state between $x = 0$ and $x = a$, and a scattering state outside the well.
- (II) It is in a bound state and the wave function will be rapidly decaying outside the well (in the classically forbidden region).
- (III) It is in a scattering state because the finite square well doesn't allow bound state solutions.

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (III) only
(e) None of the above.

9. Choose all of the following statements that are correct for an electron, whether it is in a bound state or a scattering state, in a finite square well.

- (I) It is attracted to the potential well.
- (II) Its energy levels are discrete.
- (III) Its wave function is normalizable.

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (II) only
(e) None of the above

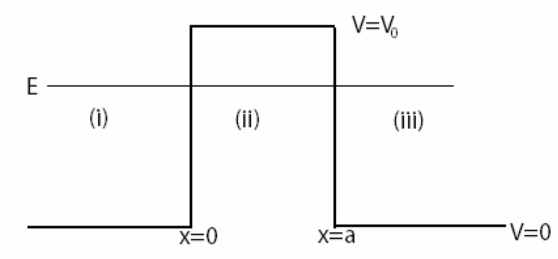
10. Consider the following conversation between Leyla and Reyna.

Leyla: Why are scattering states not normalizable?
Reyna: Because the probability of finding the particle at $x \to \pm\infty$ is non zero.
Leyla: But we learned that allowed wave functions must be normalizable. Scattering state wave functions are also allowed. Isn't that a contradiction?
Reyna: It isn't. Scattering states themselves are not normalizable, but a normalizable wave packet can be obtained from their linear superposition.

Do you agree with Reyna's explanation? Draw a diagram of a normalizable wave packet for a finite square well.

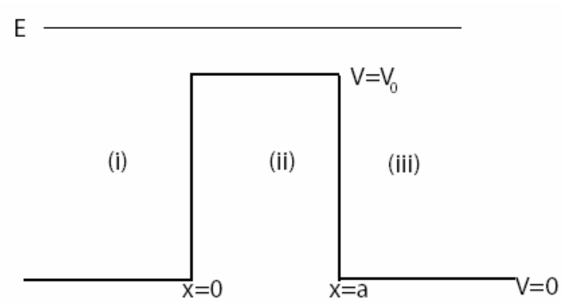
Potential Barrier

11. Choose all of the following statements that are correct about an electron with energy E in the vicinity of an potential barrier, as shown in the figure below.



(a) It is in a bound state.
(b) It is in a scattering state.
(c) Such an energy is not possible because energy should be higher inside the barrier.
(d) It cannot be determined without knowing the wave function Ψ .
(e) None of the above.

12. Choose all of the following statements that are correct about an electron with energy E in the vicinity of an potential barrier, as shown in the figure below.



(a) It is in a bound state.
(b) It is in a scattering state.
(c) Such an energy is not possible because energy should be lower outside the well.
(d) It cannot be determined without knowing the wave function Ψ .
(e) None of the above.

13. Which of the following statements is correct about the potential barrier shown in Figure 6?

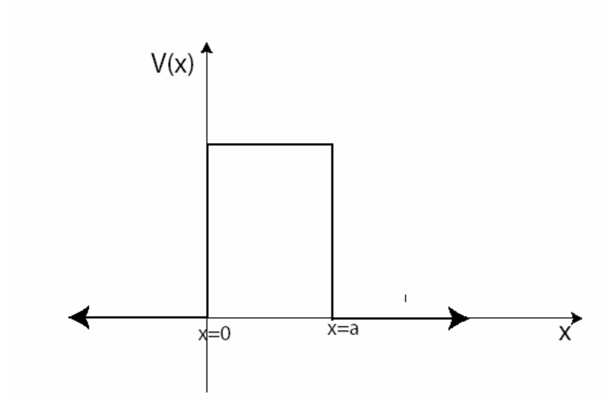


Figure 6

(a) It only allows bound states.
(b) It only allows scattering states.
(c) It allows both bound states and scattering states.
(d) It allows neither because it is not a possible potential energy in quantum mechanics.
(e) Nothing can be said without knowing the Hamiltonian $\hat{H}$.

14. Consider the conversation below between Fred and Barney:

Fred: Why does the potential barrier only allow for scattering states even when the energy is lower than the potential energy., but no bound states?
Barney: It doesn't make sense at first, but think of a physical example. A potential energy barrier, that is, potential energy $V(x)>0$ means it is a repulsive potential. Similarly, a well means it is an attractive potential. Imagine a proton, moving towards and feeling the repulsive force of a stationary proton. The potential energy diagram will look like the one in Figure 6. The incoming proton can scatter off of the stationary proton, but it won't ever be bound.

Do you agree with Barney? Explain.

15. Choose all of the following that are correct about the infinite square well.

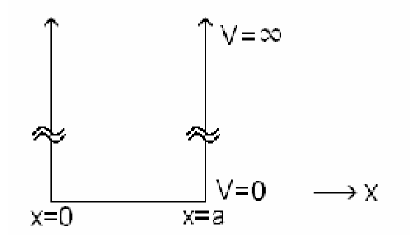


Figure 7: Infinite Square Well

(I) It only allows for bound states, because the potential energy $V(x) \to \infty$ at $x \to \pm\infty$.

(II) The wave function of a bound particle will decay rapidly outside the well, but there is a finite probability that it will be found outside the well.

(III) The wave function of a bound particle will discontinuously go to zero at the boundaries. The probability of finding it outside is exactly zero.

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (II) only
(e) (I) and (III) only

16. Choose all of the following that are correct about the simple harmonic oscillator.

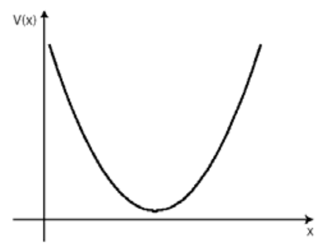


Figure 8: Harmonic Oscillator Potential Energy

(I) It only allows for bound states, because the potential energy $V(x) \to \infty$ as $x \to \pm\infty$.

(II) The wave function of a bound particle with a given energy will decay rapidly in the classically forbidden region, but there is a finite probability that it will be found in that region.

(III) The wave function of a bound particle will discontinuously go to zero at the boundaries. The probability of finding it outside is exactly zero.

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (II) only
(e) (I) and (III) only

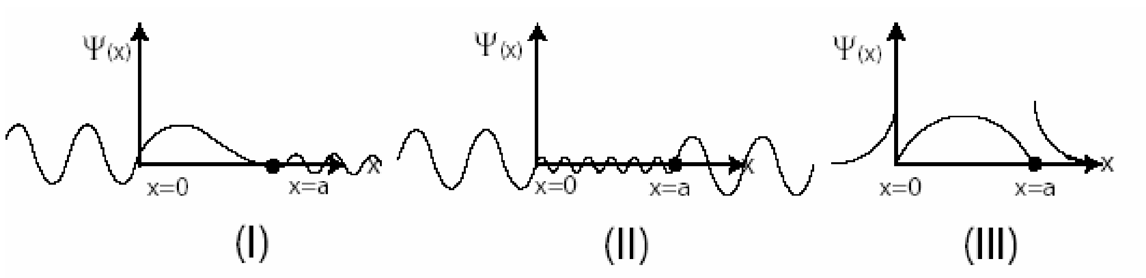
17. Consider an electron confined in one of the following one dimensional potential energy wells:

(I) Infinite square well
(II) Finite square well
(III) Simple harmonic oscillator

Choose all of the above systems that allow both the bound and scattering state solutions for the TISE:

(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (II) only
(e) (II) and (III) only

18. Choose all of the following wave functions that are possible scattering state wave functions (solutions to TISE with energy $E>0$) for an electron in a one dimensional <u>finite</u> square well of depth $-V_o$ and width a (boundaries between $x=0$ and $x=a$):



(a) (I) only
(b) (II) only
(c) (III) only
(d) (I) and (II) only
(e) (II) and (III) only

19. Sally makes a concatenated chain of 100 gold atoms in vacuum. Ignore the interaction of the electrons with the each other and with the gold nuclei. Assume that all electrons inside the chain are free to move along the chain in one dimension. Assume that the probability of electrons leaking from the gold chain into air is <u>zero</u>.
The model that most appropriately describes this system of 100 atoms is,

(a) Hydrogen atom.
(b) A single 1-D finite square well.
(c) A single 1-D simple harmonic oscillator.
(d) A single 1-D delta function potential well.
(e) None of the above.

Note: *In reality, the best model to describe the above system is a finite square well, because one cannot have an infinitely deep potential well. However, when the finite well is as deep as it is in this question, we can often approximate it to an infinite square well.*

20. Sally makes a concatenated chain of 300 gold atoms. All assumptions in question 19 hold. Choose all of the following statements that correctly compare or contrast the model for this system with the one on question 19.

(I) The depth of the well is the same because the same type of atom is used.

(II) The width of the well is larger because there are more atoms in the chain.

(III) The energy levels are given by $E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$, so the energy levels will be closer together, since the well is wider.

(a) (I) only
(b) (II) only
(c) (I) and (II) only
(d) (II) and (III) only
(e) All of the above.

21. Sally makes a concatenated chain of 10^8 gold atoms so that the end effects are negligible and the chain can be considered infinitely long. The free electrons are still confined to one dimension.
The model that most appropriately describes this system is,

(a) Free particle in one dimension.
(b) A single 1-D delta function potential well.
(c) A single 1-D finite square well.
(d) A single 1-D simple harmonic oscillator.
(e) None of the above.

22. Sally makes a one dimensional concatenated chain consisting of metal atoms of types A and B, so that 100 atoms of type B are enclosed between 10^6 atoms of type A on each side. Assume that each electron in type B atom is free to move inside the chain of type B atoms, but encounters a finite constant potential barrier in the A region.

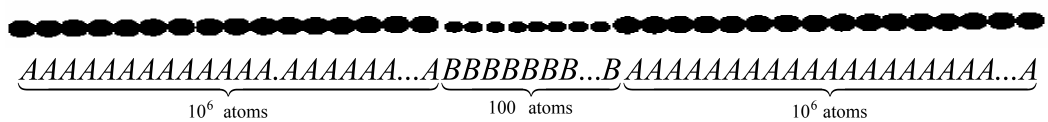


Figure 9: The ABA chain Sally made in question 23

The model that most appropriately describes this system is,

(a) A single 1-D infinite square well.
(b) A single 1-D finite square well.
(c) A single 1-D simple harmonic oscillator.
(d) A single 1-D delta function well.
(e) None of the above.

Summary:

Classical Bound and Scattering States

If the one dimensional potential energy $V(x)$ is higher than the particle's total energy E then the particle is confined in the potential energy well. It can only move between two *classical turning points.* This is called a **classical bound state**. See Fig. 1.

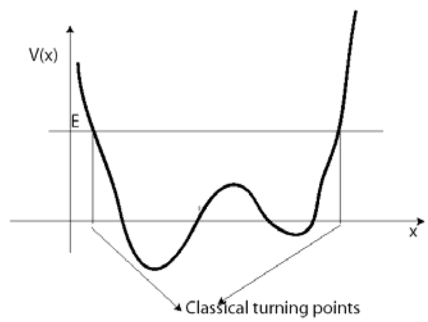


Fig 1: Bound State

If E is greater than $V(x)$ at all points on one side or on both sides of the particle, the particle can come from infinity, and go back to infinity. These are called **classical scattering states**. See Figure 2.

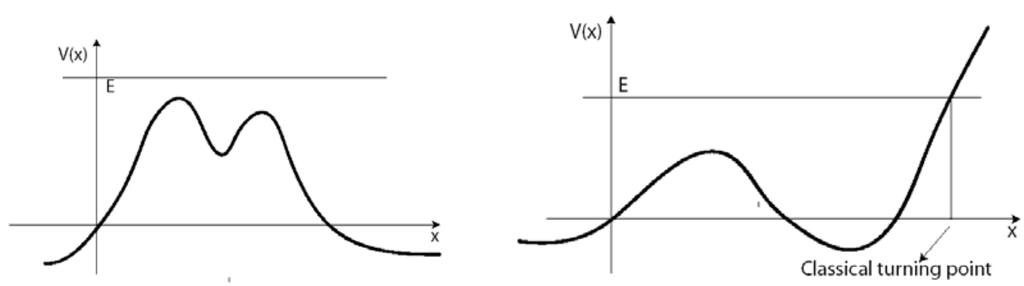


Fig 2: Scattering States

Quantum Mechanical Bound and Scattering States

Quantum Mechanical Bound State:

- The total energy of the particle is less than the potential energy at both plus and minus infinity. That is, $E < V(x \to +\infty)$ **AND** $E < V(x \to -\infty)$.
- Bound state wave functions are normalizable.
- Probability of finding the particle as $x \to \pm\infty$ is zero.
- The wave function can tunnel into the classically forbidden regions but it will rapidly decay in those regions.

Quantum Mechanical Scattering State:

- The total energy E of the particle is greater than the potential energy at either plus infinity or at minus infinity. That is, $E < V(x \to +\infty)$ **OR** $E < V(x \to -\infty)$.
- The scattering state wave functions are not normalizable, but one can make a normalizable linear superposition.
- Probability of finding the particle either as $x \to +\infty$ or $x \to -\infty$, or both, are non zero.
- The wave function is oscillatory either as $x \to +\infty$ or $x \to -\infty$, or at both.

Difference between Classical and Quantum Mechanical Bound and Scattering States:

A classical bound state can be a quantum mechanical scattering state because;

- Classically if there are turning points on both sides, the particle is bound, since there is no tunneling.
- In quantum mechanics however, instead of local considerations such as turning points, one must compare the energy of the particle to the potential energy at $x = \pm\infty$ to see if the particle is in a bound state or a scattering state.

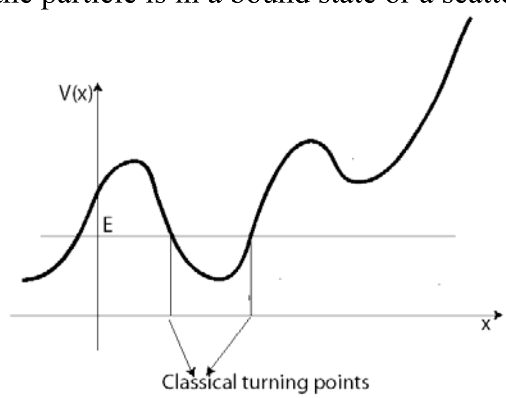
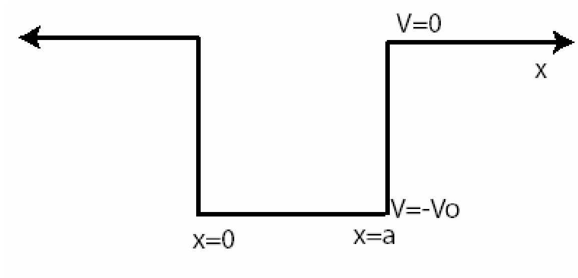


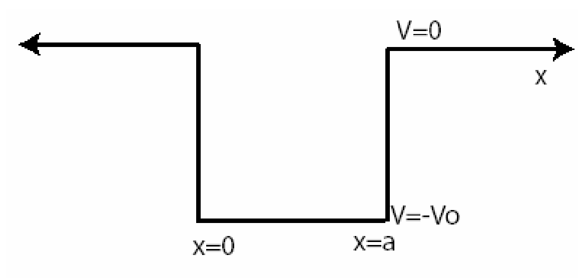
Fig 3: Classically bound Quantum Mechanically scattering state

Posttest: Bound and Scattering States

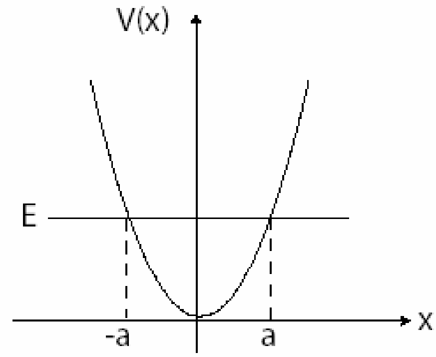
1. An electron is in the finite square well below. If the electron has energy E_b it is in a bound state, if it has energy E_s it is in a scattering state. Draw the energies E_b and E_s on the figure. Provide your reasoning. If it is not possible to have either bound or scattering states, explain why not.



2. An electron with energy E is in the finite square well below. Can the same electron be in a bound state and a scattering state depending on its position? If so, draw the energy E that allows for this on the figure, and explain. If not, explain why not.



3. An electron with a finite energy E is in a simple harmonic oscillator potential as shown in the figure below. It is initially localized between $x = -a$ and $x = a$.



(a) Is it in a bound state or a scattering state? Explain.

(b) Is there a finite nonzero probability that it will be found at $x = \pm\frac{3a}{2}$? Explain.

(c) Is there a finite nonzero probability that it will be found at $x = +\infty$ or at $x = -\infty$? Explain.

4. Draw a potential energy diagram and indicate the particle's total energy on the diagram such that it is classically in a bound but quantum mechanically in a scattering state. Explain. If such a potential energy is not possible, say so, and explain why not.

5. Draw a potential energy diagram and indicate the particle's total energy on the diagram such that it is in a quantum mechanically bound state but a classically scattering state. Explain. If such a potential energy is not possible, say so, and explain why not.