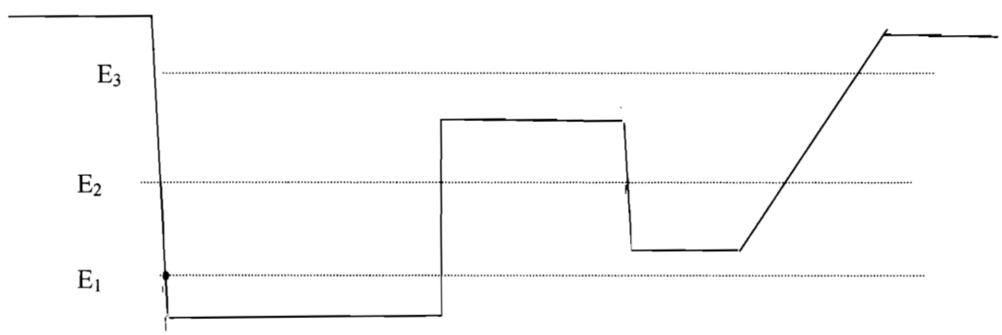
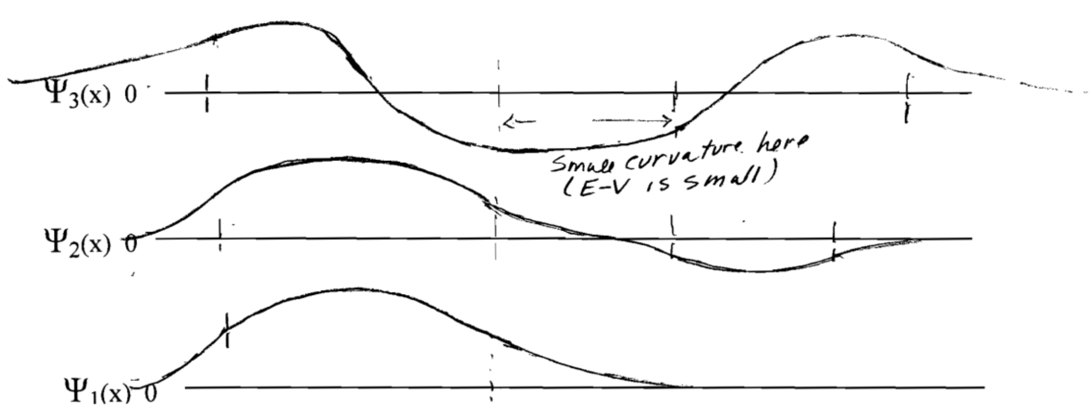
Homework #2 Solutions

CHMY 564
22jan17

1. *For the one-dimensional potential for a certain particle below, draw qualitatively the 3 lowest energy well-behaved energy eigenfunctions separately on the abscissas provided below. For full credit, the sign of the curvature must be correct at all points, as prescribed by the respective energy eigenvalues of these states shown by the dotted lines. In addition, other general aspects associated with the lowest 3 energy eigenfunctions of any system should be apparent in your drawing.*

10 pts





2. *For the 1s electron in the Li^{++} ion, $V(r) = -3/r$ in atomic units, and $\Psi = N\exp(-3r/a_0)$, where a_0 = bohr radius =1 a.u. . Does a significant amount of tunneling occur for the electron? If your answer is yes, in what region of space is the electron tunneling?*

The idea here is simply to note that that if V > E then the fractional minus the curvature of Ψ, i.e., T, will be negative (assuming Ψ is positive), meaning T will be curiously negative, which is the signature of tunneling.

For Li^{+2} ,$T = E - V = -4.5 - (3/r)$ in atomic units. This becomes negative if $r > 0.66667a_0$ for Li^{2+} in 1s. (but for H atom, tunneling sets is when $r > 2\ a_0$.

Electrons in the outer regions of ALL atoms are tunneling.

3. (a) *Does tunneling generally occur for all quantum states of any harmonic oscillator?*

(b) *Depictions shown on figures below taken from some textbooks may be criticized. Are all the harmonic oscillator wavefunctions on the figures on this page correctly drawn in terms of curvature? If not, point out which ones are bad, and explain what is incorrect, why it is correct.*

(c) *Provide correctly drawn functions for the lowest 3 levels of a harmonic oscillator.*

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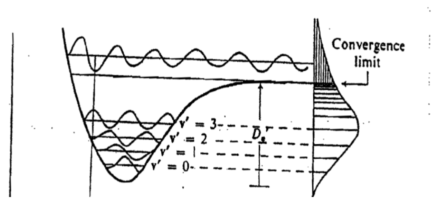
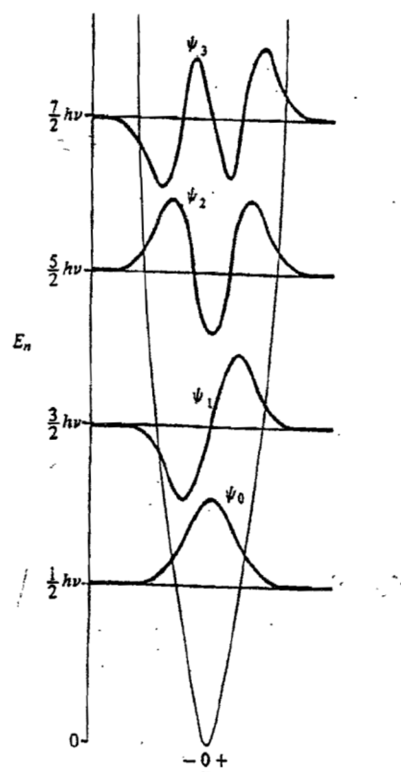


gure 4-4 Energy levels, wave functions and probability densities for the one-mensional harmonic oscillator. The zero of each ψ and $|\psi|^2$ is placed at the cor-sponding energy level. The dashed curves show probability densities for a classical cillator having the same energies as the quantum-mechanical oscillator. From ff C. Davis, Jr., *Advanced Physical Chemistry*. Copyright © 1965 (New York: onald Press). (With permission.)



3. (a) Yes, for any particle bound in a finite potential.

(b) On the right, they are all nearly correct, but technically all have some positive fractional curvature in the non-tunneling region.

On the left, all are bad, most in multiple ways:

1. None are tunneling, but should be.
2. v'=0 has 2 node but should have 0.
3. v'=2 has 4 nodes but should have 2.

Highest level is not tunneling on left end, and fractional curvature is constant but should be varying with E-V. Should be many more nodes, because E-V is so high.

The others often do not have the inflection point at the turning point. v=0 has 2 nodes but should have none. v= 2 has 4 nodes, but should have 2, etc.

(c) Those in the 2nd figure of https://en.wikipedia.org/wiki/Quantum_harmonic_oscillator#/ are precisely correct.