ECE 5390 / MSE 5472, Fall Semester 2017

Quantum Transport in Electron Devices and Novel Materials

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Assignment 1, Solutions

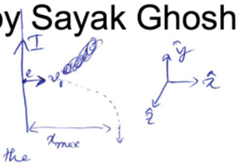
Problem 1.1: The electron that escaped

Problem 1.1) The electron that escaped

From the surface of a round wire of radius a carrying a dc current I an electron escapes with a velocity v_0 perpendicular to the surface. Find the maximum distance the electron travels from the axis of the wire before it turns back towards the wire.

Problems 1.1 & 1.2
Solns by Sayak Ghosh

1.1) Let electron escape with velocity $v_0 \hat{x}$, charge of electron is $e = 1.6\times10^{-19}$ C.



Magnetic field will only rotate velocity of electron in the x-y plane, so $v_z = 0$ always.

At any instant, velocity of electron

$\vec{v} = v_x \hat{x} + v_y \hat{y}$, such that $v_x^2 + v_y^2 = v_0^2$, since $\vec{B}$ field doesn't change magnitude of velocity.

Since electron confined to x-y plane, field affecting the electron $\vec{B} = \frac{\mu_0 I}{2\pi x}(-\hat{z})$

$$\vec{F} = -e(\vec{v}\times\vec{B})$$

$$\Rightarrow m\frac{d\vec{v}}{dt} = -e\frac{\mu_0 I}{2\pi x}(v_x\hat{y} - v_y\hat{x})$$

$$\Rightarrow \frac{dv_x}{dt} = \frac{e\mu_0 I}{2\pi m x}v_y \;;\; \frac{dv_y}{dt} = \frac{-e\mu_0 I}{2\pi m x}v_x$$

Electron will turn when $v_x = 0$, so $v_y = -v_0$

$$dv_y = -\frac{e\mu_0 I}{2\pi m x}v_x dt = -\frac{e\mu_0 I}{2\pi m x}dx$$

$$\Rightarrow \int_0^{-v_0} dv_y = \frac{-e\mu_0 I}{2\pi m}\int_a^{x_{max}}\frac{dx}{x}$$

$$\Rightarrow v_0 = \frac{e\mu_0 I}{2\pi m}\ln\left(\frac{x_{max}}{a}\right)$$

$$\Rightarrow \boxed{x_{max} = a\exp\left(\frac{2\pi m v_0}{e\mu_0 I}\right)}$$

Problem 1.2: Electron Transport in Crossed E and B Fields

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An electron of charge q and mass m at $t = 0$ is at rest at the origin of a region that has a $y-$directed electric field $\mathbf{E} = E\hat{\mathbf{y}}$ and a $z-$directed magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$. Neglect relativistic effects to find:

(a) the trajectory $x(t)$ and $y(t)$ the electron traverses due to the fields and sketch/plot it,

(b) the lengths the electron travels between successive moments of rest,

(c) the mean particle velocity projected along the $x-$axis, which is also called the *drift* velocity. How does the drift velocity depend on the charge and mass of the electron?

Solution in the next page.

1.2) Similar to (1.1), electron will have velocity confined to a plane, x-y plane, here.

$\vec{E} = E\hat{y}$
$\vec{B} = B\hat{z}$

a) $\vec{v} = v_x \hat{x} + v_y \hat{y}$

$\vec{F} = q(\vec{E} + \vec{v} \times \vec{B})$

$$\Rightarrow m \frac{d\vec{v}}{dt} = q\left(E\hat{y} + v_x B(-\hat{y}) + v_y B \hat{x}\right)$$

$$\Rightarrow \frac{dv_x}{dt} = \frac{qB}{m} v_y \quad ; \quad \frac{dv_y}{dt} = \frac{q}{m}(E - v_x B)$$

$$\frac{d^2 v_x}{dt^2} = \frac{q^2 B}{m^2}(E - v_x B) \quad -(1) \qquad \frac{d^2 v_y}{dt^2} = -\frac{q^2 B^2}{m^2} v_y \quad -(2)$$

Solving (1),

$$\frac{d^2 v_x}{dt^2} = \frac{q^2 B}{m^2}(E - v_x B)$$

Let $v_x B - E = u \Rightarrow \frac{d^2 u}{dt^2} = B \frac{d^2 v_x}{dt^2}$

$$\frac{d^2 u}{dt^2} = -\frac{q^2 B^2}{m^2} u \Rightarrow u = u_0 \cos\left(\frac{qB}{m}t + \phi\right)$$

$$\Rightarrow v_x = \frac{E}{B} + \frac{u_0}{B}\cos\left(\frac{qB}{m}t + \phi_1\right) \quad -(3).$$

Solving (2),

$$\frac{d^2 v_y}{dt^2} = -\frac{q^2 B^2}{m^2} v_y \Rightarrow v_y = v_2 \sin\left(\frac{qB}{m}t + \phi_2\right) \quad -(4)$$

Initial condition, $v_x = v_y = 0$, $x = y = 0$.
using this in (3) & (4) gives,

$$v_x = \frac{E}{B}\left(1 - \cos\left(\frac{qB}{m}t\right)\right)$$

$$= \frac{E}{B}\left(1 - \cos(\omega_c t)\right) \qquad \omega_c = \frac{qB}{m}, \text{ cyclotron frequency.}$$

$$v_y = \frac{E}{B}\sin(\omega_c t)$$

$$x(t) = x(t=0) + \int_0^t v_x dt$$

$$\Rightarrow \boxed{x(t) = \frac{E}{B}\left(t - \frac{\sin(\omega_c t)}{\omega_c}\right)}$$

$$y(t) = y(t=0) + \int_0^t v_y \, dt$$

$$\Rightarrow \boxed{y(t) = \frac{E}{\omega_c B}\left(1 - \cos(\omega_c t)\right)}$$

b) Electron is at rest when $\vec{v} = 0$.

$v_x = 0 \Rightarrow \cos(\omega_c t) = 1 \Rightarrow t = \frac{2n\pi}{\omega_c}$ (n integer, $n \geq 0$)

$v_y = 0 \Rightarrow \sin(\omega_c t) = 0 \Rightarrow t = \frac{2n\pi}{\omega_c}$.

$\therefore$ Time between successive rests,

$$\Delta t = \frac{2\pi}{\omega_c}$$

Length travelled between successive stops

$$= \int_0^{2\pi/\omega_c} \sqrt{v_x^2 + v_y^2}\, dt$$

$$= \int_0^{2\pi/\omega_c} E/B \sqrt{1 + \cos^2(\omega_c t) - 2\cos(\omega_c t) + \sin^2(\omega_c t)}\, dt$$

$$= \frac{E}{B}\int_0^{2\pi/\omega_c} \sqrt{2(1 - \cos(\omega_c t))}\, dt$$

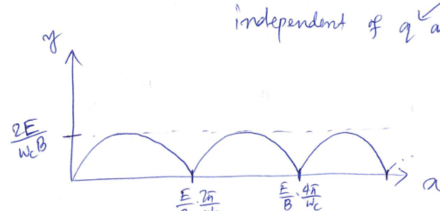
$$= E/B \int_0^{2\pi/\omega_c} 2\sin\left(\frac{\omega_c t}{2}\right) dt$$

$$= \frac{E}{B} \cdot \frac{4}{\omega_c} \cdot 2 = \boxed{\frac{8E}{\omega_c B}}$$

(c) In $x(t) = \frac{E}{B}\left(t - \frac{\sin(\omega_c t)}{\omega_c}\right)$, the x distance increases due to linear term in t, and $\sin(\omega_c t)$ is periodic in time, so it doesn't affect mean distance travelled.

$\therefore$ Mean x-velocity $= \frac{E/B\, t}{t} = \boxed{\frac{E}{B}}$

independent of q and m.



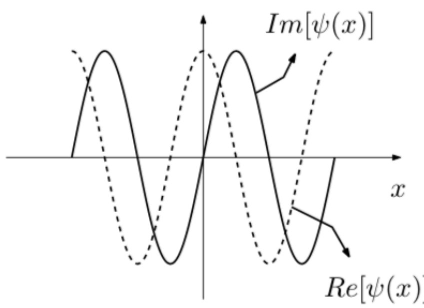
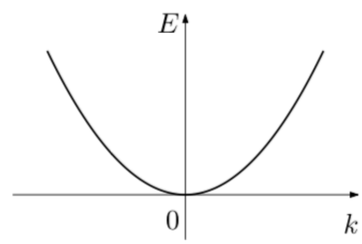
Trajectory is a cycloid.

Problem 1.3) Exactly solved problems of quantum mechanics

Quantum mechanical states of *definite energy* for electrons are of central importance in this class. Make a table where your columns are a) the electric potential $V(r)$, b) the definite energy wavefunctions in real space $\psi_E(x)$, c) The corresponding energy eigenvalues E_n, and d) a sketch of the potential, eigenfunctions, and eigenvalues for

1) The completely free electron in 1D $V(x) = 0$ in $-\infty \leq x \leq +\infty$,
2) The 'quasi'-free electron in 1D $V(x) = 0$ in a 'circle' of length L,
3) The electron in a box with $V(x) = 0$ for $0 \leq x \leq L$ and $V(x) = \infty$ for $x < 0$ and $x > L$,
4) The harmonic oscillator $V(x) = \frac{1}{2}kx^2$, and
5) The hydrogen atom with $V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$.

We will refer to this table frequently in the course.

<table>
<tr><th>Potential $V(r)$</th><th>Wavefunctions $\psi_E(r)$</th><th>Eigenvalues E_n</th></tr>
<tr>
<td>(1) Free particle
$V(x) = 0, -\infty < x < \infty$</td>
<td>$\psi_E(x) = Ae^{\iota kx}$

</td>
<td>$E = \hbar^2k^2/2m$

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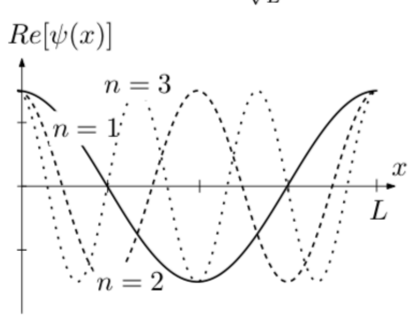
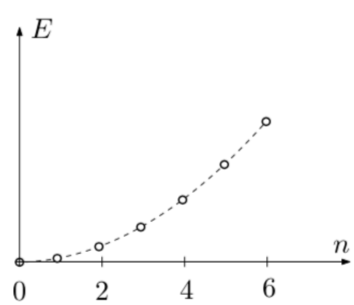
</tr>
<tr>
<td>(2) 'Quasi-Free' particle
$V(x) = 0, x \in [0, L]$</td>
<td>$\psi_E(x) = \frac{1}{\sqrt{L}}e^{\iota 2\pi nx/L}$

</td>
<td>$E = n^2h^2/2mL^2, n = 0, 1, \ldots$

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</table>

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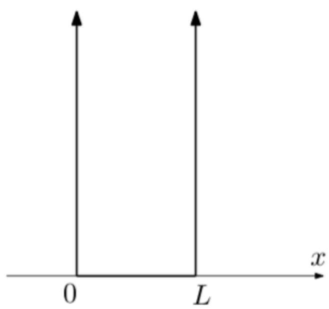
<tr><th>Potential $V(r)$</th><th>Wavefunctions $\psi(r)$</th><th>Eigenvalues E_n</th></tr>
<tr><td>

(3) Particle in a box

$$V(x) = \begin{cases} 0, & x \in [0, L] \\ \infty, & \text{otherwise.} \end{cases}$$



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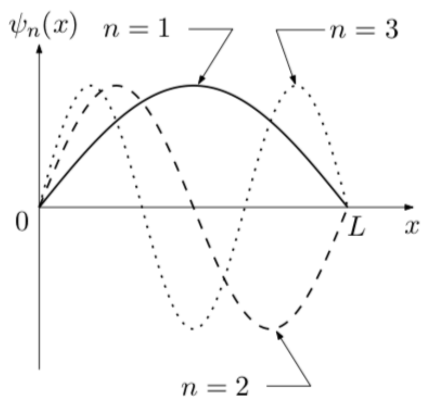
$$\psi_n(x) = \sqrt{\frac{2}{L}} sin\left(\frac{n\pi x}{L}\right)$$
$$n = 1, 2, \ldots$$



</td><td>

$$E_n = \frac{n^2 h^2}{8mL^2}$$

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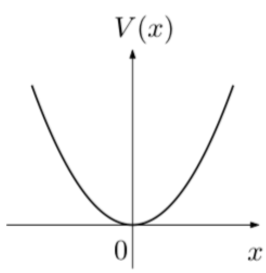
<tr><td>

(4) Harmonic oscillator

$$V(x) = \frac{1}{2} m\omega^2 x^2$$
$$x \in (-\infty, \infty)$$



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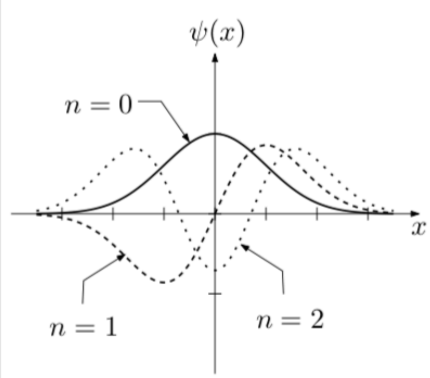
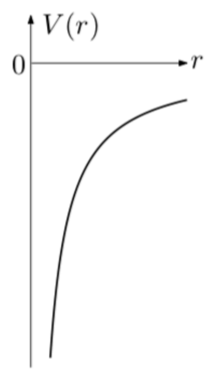
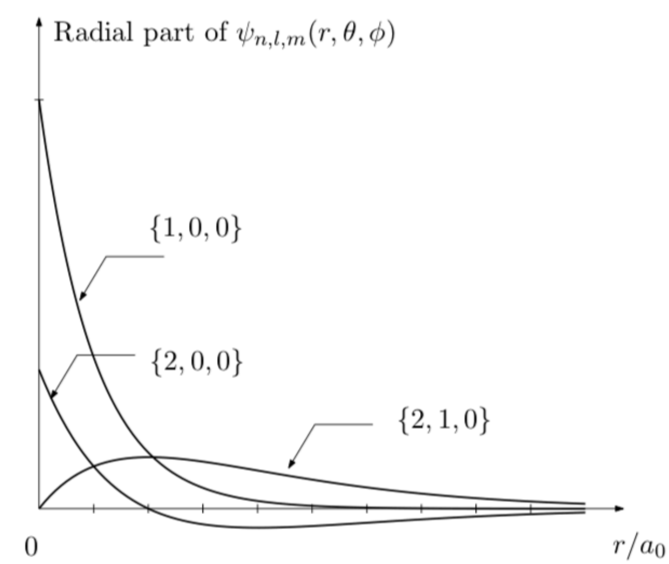
$$\psi_n(x) = \frac{1}{\sqrt{2^n\, n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \times e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right),$$
$$n = 0, 1, 2, \ldots$$
$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right)$$



</td><td>

$$E = \left(n + \tfrac{1}{2}\right)\hbar\omega, n = 0, 1, \ldots$$

</td></tr>
</table>

Potential $V(r)$	Wavefunctions $\psi(r)$ and eigenvalues E_n
(5) Hydrogen atom $V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$ $r \in [0, \infty)$ 	$\psi_{n,l,m}(r,\theta,\phi)$ with $n = 1, \ldots,$ $l = 0, 1, \ldots, n-1,$ $m = -l, \ldots, 0, \ldots, l.$ $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$ $E_n = -\frac{\hbar^2}{2ma_0^2}\frac{1}{n^2}$ $\psi_{1,0,0}(r) = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$ $\psi_{2,0,0}(r) = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$ $\psi_{2,1,0}(r) = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0}\cos\theta$ $\psi_{2,1,\pm 1}(r) = \frac{1}{8}\sqrt{\frac{1}{\pi}}\left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0}\sin\theta e^{\pm i\phi}$ 

Problem 1.4: A Quantum-Mechanical Anti-Reflection Coating

Problem 1.4) A Quantum Mechanical anti-reflection Coating

Solve this interesting problem shown in Fig 1 from Kroemer's QM text. One can implement the scheme in semiconductor heterostructure devices for electrons incident at energy $\mathcal{E}$ from the left as shown in the figure. Discuss how the design will work only for specific electron energies, and what happens if the electron energy is changed for a particular design. Provide sketches wherever appropriate.

#5•3-1: Zero-Reflection Conditions at a Double-Step Barrier

Devise a quantum-mechanical "antireflection coating"; that is, determine the proper width L and height V_1 of an intermediate potential step to suppress the reflection of a wave of a specific incident energy at a barrier of height $V_2 < \mathcal{E}$ (Fig. 5•3–3).

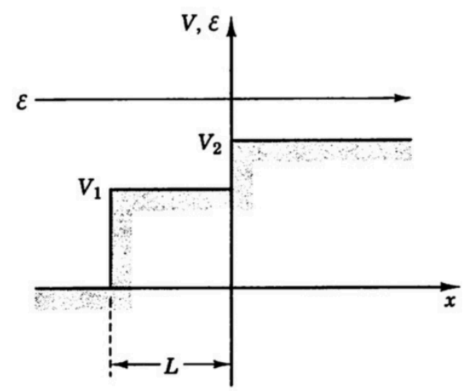
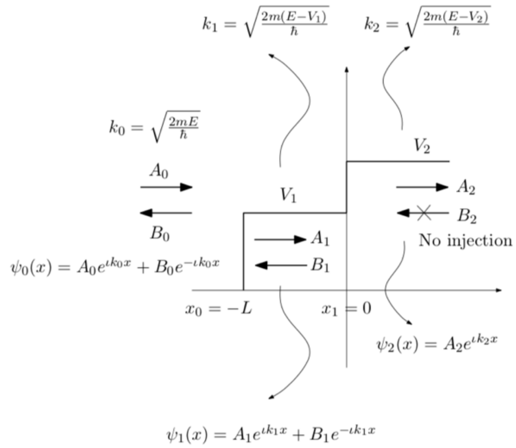


Figure 5•3–3. Zero-reflection barrier.

Figure 1: Designing an anti-reflection coating for an electron incident on a barrier.

Solution in the next page.



Solution:

From the continuity of the wavefunction and its derivative at $x_0 = -L$ and $x_2 = 0$, we get

$$A_1 + B_1 = A_2 \tag{31}$$
$$A_1 k_1 - B_1 k_1 = A_2 k_2 \tag{32}$$
$$A_0 e^{-\iota k_0 L} + B_0 e^{\iota k_0 L} = A_1 e^{-\iota k_1 L} + B_1 e^{\iota k_1 L} \tag{33}$$
$$A_0 k_0 e^{-\iota k_0 L} - B_0 k_0 e^{\iota k_0 L} = A_1 k_1 e^{-\iota k_1 L} - B_1 k_1 e^{\iota k_1 L} \tag{34}$$

from which, we have

$$A_1 = \frac{A_2}{2}\left(1 + \frac{k_2}{k_1}\right) \tag{35}$$
$$B_1 = \frac{A_2}{2}\left(1 - \frac{k_2}{k_1}\right) \tag{36}$$
$$\implies A_0 e^{-\iota k_0 L} + B_0 e^{\iota k_0 L} = \frac{A_2}{2}\left(\frac{k_1 + k_2}{k_1}\right) e^{-\iota k_1 L} + \frac{A_2}{2}\left(\frac{k_1 - k_2}{k_1}\right) e^{\iota k_1 L} \tag{37}$$
$$\text{and } A_0 e^{-\iota k_0 L} - B_0 e^{\iota k_0 L} = \frac{A_2}{2}\left(\frac{k_1 + k_2}{k_0}\right) e^{-\iota k_1 L} - \frac{A_2}{2}\left(\frac{k_1 - k_2}{k_0}\right) e^{\iota k_1 L} \tag{38}$$
$$\implies e^{-\iota k_0 L} + r e^{\iota k_0 L} = t\left(\frac{(k_1 + k_2) e^{-\iota k_1 L} + (k_1 - k_2) e^{\iota k_1 L}}{2k_1}\right) = t\alpha \text{ (say)} \tag{39}$$
$$\text{and } e^{-\iota k_0 L} - r e^{\iota k_0 L} = t\left(\frac{(k_1 + k_2) e^{-\iota k_1 L} - (k_1 - k_2) e^{\iota k_1 L}}{2k_0}\right) = t\beta \text{ (say)} \tag{40}$$
$$\implies r = \left(\frac{1 - \beta/\alpha}{1 + \beta/\alpha}\right) e^{-\iota 2 k_0 L} \tag{41}$$

where $r = B_0/A_0$ is the reflection amplitude and $t = A_2/A_0$ is the transmission amplitude.

In order to have an anti-reflection coating, we need $r = 0$. Setting $\alpha = \beta$ yields

$$e^{\iota 2 k_1 L} = \frac{(k_1 + k_2)(k_1 - k_0)}{(k_1 - k_2)(k_1 + k_0)}. \tag{42}$$

Since $|e^{\iota 2 k_1 L}| = 1$ and $k_0 > k_1 > k_2$ are real, the above equation is satisfied if and only if both sides equal -1. We hence get

$$(k_1 + k_2)(k_0 - k_1) = (k_1 + k_0)(k_1 - k_2) \tag{43}$$
$$\implies k_1^2 = k_0 k_2 \tag{44}$$
$$\implies V_1 = E - \sqrt{E(E - V_2)} \tag{45}$$

and

$$e^{\iota 2 k_1 L} = -1 \tag{46}$$
$$\implies L = \frac{n\pi}{2k_1}, n = 1, 3, \ldots \tag{47}$$
$$\text{with } k_1 = \frac{\sqrt{2m}}{\hbar}\left[E(E - V_2)\right]^{1/4} \tag{48}$$

Note that the quantum mechanical conditions $k_1^2 = k_0 k_2$ and $L = n\pi/2k_1 = n\frac{\lambda_1}{4}$ for *electron waves* are very similar to what we typically encounter in dielectric anti-reflection coatings for *electromagnetic waves* under the name of quarter wave transformers.

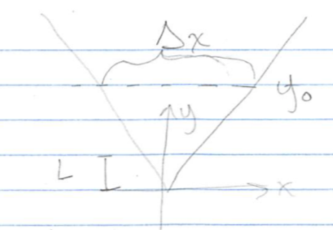
Problem 1.5: Electron ‘dripping’ through a cone

Problem 1.5) Electron ‘dripping’ through a cone

An electron “sits” in the ground state in a cone-shaped “bag” under the influence of gravity. The lower end of the plastic bag is cut with scissors. Find the time it takes for the electron to fall out of the bag.

Problem 1.5 (Ian Briggs)

1.5)



$\Delta x = ky$

cut cone at height L

energy conservation: $\frac{\Delta p_{x_0}^2}{2m} + mgy_0 = \frac{\Delta p_x^2}{2m} + mgy + \frac{1}{2}mv_y^2$

$\Delta p_x \Delta x \approx \hbar \qquad \frac{\Delta p_x^2}{2m} = \frac{\hbar^2}{2m\Delta x^2} = \frac{\hbar^2}{2m(ky)^2}$

$$\frac{\hbar^2}{2m(ky_0)^2} + mgy_0 = \frac{\hbar^2}{2m(ky)^2} + mgy + \frac{1}{2}mv_y^2$$

$$\frac{\hbar^2}{2m(ky_0)^2} - \frac{\hbar^2}{2m(ky)^2} + mg(y_0 - y) = \frac{m}{2}v_y^2$$

$$\left[\frac{\hbar^2}{2mk^2}\left(\frac{1}{y_0^2} - \frac{1}{y^2}\right) + mg(y_0 - y) = \frac{m}{2}v_y^2\right] \cdot \frac{2}{m}$$

$$\left(\frac{\hbar}{mk}\right)^2\left(\frac{1}{y_0^2} - \frac{1}{y^2}\right) + 2g(y_0 - y) = v_y^2$$

$$v_y = \left[\left(\frac{\hbar}{mk}\right)^2\left(\frac{1}{y_0^2} - \frac{1}{y^2}\right) + 2g(y_0 - y)\right]^{1/2}$$

$$T = \int dt = \int \frac{dy}{v_y} = \int \frac{dy}{\left[\left(\frac{\hbar}{mk}\right)^2\left(\frac{1}{y_0^2} - \frac{1}{y^2}\right) + 2g(y_0 - y)\right]^{1/2}}$$

solving for y_0:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\Psi(x,y)+mgy\,\Psi(x,y)=E\,\Psi(x,y)$$

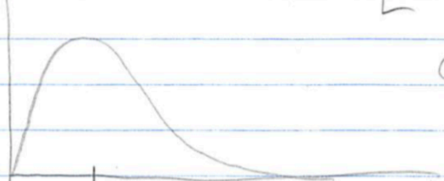
assuming $\Psi(x,y)=X(x)\,Y(y)$

$$-\frac{\hbar^2}{2m}\frac{1}{X(x)}\frac{\partial^2 X(x)}{\partial x^2}-\frac{\hbar^2}{2m}\frac{1}{Y(y)}\frac{\partial^2 Y}{\partial y^2}+mgy=E$$

$$-\frac{\hbar^2}{2m}\frac{1}{Y(y)}\frac{\partial^2 Y(y)}{\partial y^2}+mgy=c_y$$

$$\frac{\hbar^2}{2m}\frac{\partial^2 Y(y)}{\partial y^2}=(c_y-mgy)\,Y(y)$$

$$\Rightarrow Y(y)\sim \mathrm{AiryAi}\left[-C_1+\left(\frac{2gm^2}{\hbar^2}\right)^{1/3}y\right]$$



$C_1 = 2.338$

$\langle y\rangle$ ← expectation of y roughly occurs at peak of Airy function

$$-2.338+\left(\frac{2gm^2}{\hbar^2}\right)^{1/3}\langle y\rangle=-1.019$$

$$\left(\frac{2gm^2}{\hbar^2}\right)^{1/3}\langle y\rangle=1.319\ ;\quad y_0=\langle y\rangle=1.319\left(\frac{\hbar^2}{2gm^2}\right)^{1/3}$$

$$T=\int\frac{dy}{v_y}=\int_{y_0}^{L}\frac{dy}{\left[\left(\frac{\hbar}{mk}\right)^2\left(\frac{1}{y_0^2}-\frac{1}{y^2}\right)+2g(y_0-y)\right]^{1/2}}$$

another calculation of y_0

$$E = \frac{\hbar^2}{2m(ky)^2} + mgy$$ → find where energy is at a minimum

$$\frac{\partial E}{\partial y} = \frac{\partial}{\partial y}\left[\frac{\hbar^2}{2mk^2} y^{-2} + mgy\right] = -\frac{2\hbar^2}{2mk^2} y_0^{-3} + mg = 0$$

$$\frac{2\hbar^2}{2mk^2}\frac{1}{y_0^3} = mg \quad ; \quad y_0^3 = \left(\frac{\hbar^2}{mk^2}\right)\left(\frac{1}{mg}\right)$$

$$y_0 = \left(\frac{\hbar^2}{m^2 g k^2}\right)^{1/3}$$

↗ shares $\left(\frac{\hbar^2}{m^2 g}\right)^{1/3}$ dependence w/ other soln for y_0