Set #5

14.

Work out the reflection coefficient R for an electron reflecting off a potential (barrier) V, following the same steps as done in class for the transmission coefficient T.

a) Give a concise expression for incidence below barrier (E<V)
b) Give the value of R and T when E=V.
c) Give a concise expression for incidence above barrier (E>V)
Provide an estimate for E=5 μeV, V=4.9 μeV and a=1 μm.
d) What does it mean that electrons are reflected back when passing above the barrier?
e) Find the energies at which electrons passing above the barrier are NOT at all reflected.

15.

Compute the *reflection (R) & transmission (T)* coefficients for a single free electron impinging on a barrier V through the "*current probability density*":

$$\vec{j}(\vec{r},t) = \frac{i\hbar}{2m}\left[\Psi(\vec{r},t)\,\vec{\nabla}\Psi*(\vec{r},t) - \Psi*(\vec{r},t)\,\vec{\nabla}\Psi(\vec{r},t)\right]$$

16.

a. Use the appropriate numerics (Matlab, Mathematica, Python, etc) and "Check" that the polynomials $u_n(x)$ (in class) are solutions of the of the Hermite equation under the condition that the Hermite equation's coefficient be even integer "2n".

b. Use the appropriate numerics (Matlab, Mathematica, Python, etc) and "check" that the eigen-functions $\psi_n(x)$ are an orthogonal set of eigen-functions.

Extra.

For an asymmetric 1D barrier the continuity at the well boundary at x=a yields the following eigenvalue equation:

$$\cot\left[ka + \delta(k)\right] = -\sqrt{\frac{2mV_2}{\hbar^2 k^2} - 1}$$

Check that the the correct solution for the energy has the following form (- sign):

$$ka + \delta(k) = -sin^{-1}\frac{\hbar k}{\sqrt{2mV_2}} + \pi n_2$$

Work out the *reflection* coefficient R for electrons reflecting off a potential (barrier) V (follow the same steps as done in class for the transmission coefficient T).

a. Give a concise expression for incidence below barrier ($E<V$)

b. Give a concise expression for incidence above barrier ($E>V$). Provide an estimate for $E=5$ μeV, $V=4.9$ μeV and $a=1$ μm. What does it mean that electrons are reflected back when passing above the barrier?

c. Give the value of R and T when $E=V$.

e. Find the energies at which electrons passing above the barrier are NOT at all reflected.

Reflection Coefficient

a)
$$A e^{k_1 a}\left(1-\frac{k_1}{ik}\right)+B e^{-k_1 a}\left(1+\frac{k_1}{ik}\right)=0 \qquad \text{Sum } 3\,\&\,4$$

$$2A = A_1\left(1+\frac{ik}{k_1}\right)+B_1\left(1-\frac{ik}{k_1}\right) \qquad \text{Sum } 1\,\&\,2$$

$$2B = A_1\left(1-\frac{ik}{k_1}\right)+B_1\left(1+\frac{ik}{k_1}\right) \qquad \text{Diff. } 1\,\&\,2$$

$$2A e^{k_1 a}\left(1-\frac{k_1}{ik}\right)+2B e^{-k_1 a}\left(1+\frac{k_1}{ik}\right)=0$$

$$\left[A_1\left(1+\frac{ik}{k_1}\right)+B_1\left(1-\frac{ik}{k_1}\right)\right]e^{k_1 a}\left(1-\frac{k_1}{ik}\right)+\left[A_1\left(1-\frac{ik}{k_1}\right)+B_1\left(1+\frac{ik}{k_1}\right)\right]e^{-k_1 a}\left(1+\frac{k_1}{ik}\right)=0$$

$$B_1\left[\left(1-\frac{ik}{k_1}\right)\left(1-\frac{k_1}{ik}\right)e^{k_1 a}+\left(1+\frac{ik}{k_1}\right)\left(1+\frac{k_1}{ik}\right)e^{-k_1 a}\right]=$$

$$-A_1\left[\left(1+\frac{ik}{k_1}\right)\left(1-\frac{k_1}{ik}\right)e^{k_1 a}+\left(1-\frac{ik}{k_1}\right)\left(1+\frac{k_1}{ik}\right)e^{-k_1 a}\right].$$

$$B_1\left[-(k_1-ik)^2 e^{k_1 a}+(k_1+ik)^2 e^{-k_1 a}\right]=-A_1\left[-(k_1^2+k^2)e^{k_1 a}+(k_1^2+k^2)e^{-k_1 a}\right]$$

$$\frac{B_1}{A_1}=\frac{(k_1^2+k^2)\,2\sinh k_1 a}{(k_1+ik)^2 e^{-k_1 a}-(k_1-ik)^2 e^{k_1 a}}=\frac{2(\;)\,\mathrm{sh}\,k_1 a}{2(k^2-k_1^2)\,\mathrm{sh}\,k_1 a+4ikk_1\cosh k_1 a}$$

$$R\equiv\left|\frac{B_1}{A_1}\right|^2=\frac{(k^2+k_1^2)^2\,\mathrm{sh}^2}{(k^2-k_1^2)^2\mathrm{sh}^2+4k^2k_1^2\underbrace{\mathrm{ch}^2}_{1+\mathrm{sh}^2}}=\frac{(k^2+k_1^2)\,\mathrm{sh}^2}{(k^2+k_1^2)\,\mathrm{sh}^2+4k^2k_1^2}$$

$$=\left[1+\frac{4E(V-E)}{V^2}\times\frac{1}{\sinh^2 k_1 a}\right]^{-1} \qquad \text{Reflectivity} \qquad (E<V)$$

b) $$R = \left[1 + \frac{4E(E-V)}{V^2} \frac{1}{\sin^2 \frac{\sqrt{2m(E-V)}}{\hbar} a} \right]^{-1} \qquad (E>V)$$

[$R \simeq 0.92$ for $E = 5\,\mu eV$
$V = 4.9\,\mu eV$
$a = 1\,\mu m$]

c) Argomento: $$\frac{4E(E-V)}{V^2} \times \frac{1}{\sin^2 \frac{\sqrt{2m(E-V)}}{\hbar} a} = \frac{4x(x-1)}{\sin^2 \frac{\sqrt{2mV}}{\hbar} a \sqrt{x-1}} \qquad (x \equiv E/V)$$

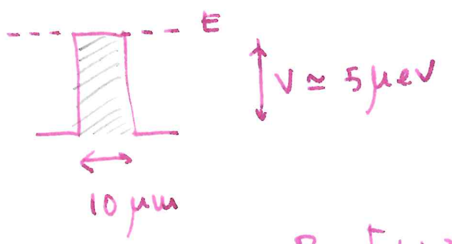
$$\lim_{x\to 1} \frac{4x(x-1)}{\sin^2 \frac{\sqrt{2mV}}{\hbar} a \sqrt{x-1}} = \frac{0}{0}$$ Indeterminato: $$\frac{8x-4}{\dfrac{2 \sin .. \cos .. \sqrt{\frac{2mV}{\hbar^2}}\, a}{2\sqrt{x-1}}} =$$

$$= \frac{8x-4}{\dfrac{\sin \frac{2\sqrt{2mV}}{\hbar} a \sqrt{x-1}}{2\sqrt{x-1}\; \frac{a\sqrt{2mV}}{\hbar}} \sqrt{\frac{2mV}{\hbar^2}}\, a \;\frac{a\sqrt{2mV}}{\hbar}} \xrightarrow[x\to 1]{} \frac{4}{\frac{2mV}{\hbar^2} a^2} = \frac{2\hbar^2}{mVa^2}$$

(N.B. $\sin x / x \xrightarrow[x\to 0]{} 1$)

$$R \xrightarrow[E\to V]{} \left[1 + \frac{2\hbar^2}{mVa^2} \right]^{-1}$$

Check: $\lim_{x\to 1^+}$ / $\lim_{x\to 1^-}$



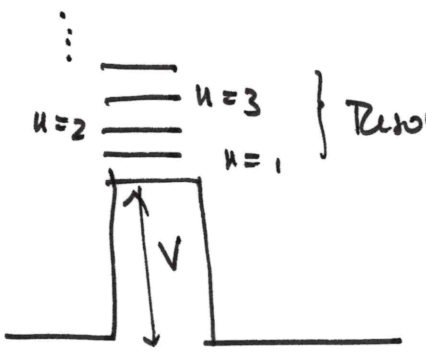
$$\frac{2\hbar^2}{mVa^2} = \frac{2(\hbar c)^2}{mc^2 Va^2} = \frac{2 \times (1973\, eV \times 10^{-10} m)^2}{0.5\, eV\, 10^{6}\; 5\times 10^{-6} eV\; (10\times 10^{-6} m)^2} \simeq 3\times 10^{-4}$$

$$R = [1 + 3\times 10^{-4}]^{-1} = 0.999....$$

) No Refl. occurs when : $\frac{\sqrt{2m(E-V)}}{\hbar}\, a = \pi n$

n integer

$$\frac{\hbar^2}{a^2}\pi^2 n^2 = 2m(E-V) \quad \text{or} \quad E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2 + V$$



} Resonant Transmission $(T=1 \quad R=0)$

- Express the *reflection (R) & transmission (T)* coefficients for an electron impinging on a potential (barrier) V in terms of the *"current probability density"* for a single electron:

$$\vec{j}(\vec{r},t) = \frac{i\hbar}{2m}\left[\Psi(\vec{r},t)\,\vec{\nabla}\,\Psi^*(\vec{r},t) - \Psi^*(\vec{r},t)\,\vec{\nabla}\,\Psi(\vec{r},t)\right]$$

From what we have done in class:

OUT: $\psi(x) = A_1 e^{ikx} + B_1 e^{-ikx}$ $k = \sqrt{2mE}/\hbar$

$\psi(x) = A_2 e^{ikx}$

For a single electron the charge current density are: $(\vec{k} = k\hat{i})$

Incident $\vec{j}_{INC}(x,t) = \frac{i\hbar}{2m}\left[|A_1|^2(-ik)\,2\right]\hat{i} = \frac{\hbar\vec{k}}{m}\,|A_1|^2$; $\vec{J}_{e,INC} = \frac{\hbar\vec{k}}{m}\,|A_1|^2$

Reflected $\vec{j}_{REFL.}(x,t) = \frac{i\hbar}{2m}\left[|B_1|^2(+ik)\,2\right]\hat{i} = -\frac{\hbar\vec{k}}{m}\,|B_1|^2$; $\vec{J}_{e,REFL} = -\frac{\hbar\vec{k}}{m}\,|B_1|^2$

Transmitted $\vec{j}_{TRANS}(x,t) = \frac{i\hbar}{2m}\left[|A_2|^2(-2ik)\right]\hat{i} = \frac{\hbar\vec{k}}{m}\,|A_2|^2$; $\vec{J}_{e,TRANS} = \frac{\hbar\vec{k}}{m}\,|A_2|^2$

Trans. coeff. defined in class:

$$T = \frac{|A_2|^2}{|A_1|^2} = \left(\frac{\hbar\vec{k}}{m}\right)^{-1}\cdot\vec{J}_{e,TRANS}\cdot\left(\frac{\hbar\vec{k}}{m}\right)\cdot\vec{J}_{e,INC}^{\,-1} = \frac{\vec{J}_{e,TRANS}}{\vec{J}_{e,INC}}$$

Also $\boxed{\vec{J}_{e,TRANS} = T \times \vec{J}_{e,INC}}$

Similarly:

$$R = \frac{|B_1|^2}{|A_1|^2} = \ldots = -\frac{\vec{J}_{e,REFL.}}{\vec{J}_{e,INC.}}$$

$$\boxed{\vec{J}_{e,REFL} = -R \times \vec{J}_{e,INC}}$$

From what we have done in class:

OUT: $\psi(x) = A_1 e^{ikx} + B_1 e^{-ikx}$ $\qquad k = \sqrt{2mE}/\hbar$

$\psi(x) = A_2 e^{ikx}$

For a single electron the charge current density are: $(\vec{k} \equiv k\hat{i})$

Incident $\quad \vec{J}_{INC}(x,t) = \frac{i\hbar}{2m}\left[|A_1|^2(-ik)\,2\right]\hat{i} = \frac{\hbar\vec{k}}{m}\,|A_1|^2$; $\quad \vec{J}_{e,INC} = \frac{\hbar\vec{k}}{m}\,|A_1|^2$

Reflected $\quad \vec{J}_{REFL}(x,t) = \frac{i\hbar}{2m}\left[|B_1|^2(+ik)\,2\right]\hat{i} = -\frac{\hbar\vec{k}}{m}\,|B_1|^2$; $\quad \vec{J}_{e,REFL} = -\frac{\hbar\vec{k}}{m}\,|B_1|^2$

Transmitted $\quad \vec{J}_{TRANS}(x,t) = \frac{i\hbar}{2m}\left[|A_2|(-ik)\right]\hat{i} = \frac{\hbar\vec{k}}{m}\,|A_2|^2$; $\quad \vec{J}_{e,TRANS} = \frac{\hbar\vec{k}}{m}\,|A_2|^2$

Trans. coeff. defined in class:

$$T \equiv \frac{|A_2|^2}{|A_1|^2} = \left(\frac{\hbar\vec{k}}{m}\right)^{-1} \cdot \vec{J}_{e,TRANS} \cdot \left(\frac{\hbar\vec{k}}{m}\right) \cdot \vec{J}_{e,INC}^{\,-1} = \frac{\vec{J}_{e,TRANS}}{\vec{J}_{e,INC}}$$

Also $\boxed{\vec{J}_{e,TRANS} = T \times \vec{J}_{e,INC}}$

Similarly:

$$R \equiv \frac{|B_1|^2}{|A_1|^2} = \dots = -\frac{\vec{J}_{e,REFL}}{\vec{J}_{e,INC}}$$

$$\boxed{\vec{J}_{e,REFL} = -R \times \vec{J}_{e,INC}}$$

Use the appropriate numerics (Matlab, Mathematica, Python, etc) to "check" that eigen-energies E_n and eigen-functions $\psi_n(x)$ are an orthogonal set of eigen-functions.

"Check" that the polynomials $u_n(x)$ (given in class) are solutions of the of the Hermite equation under the condition that the equation coefficient be an even integer "$2n$".

```
(*GROUND & FIRST EXCITED STATE EIGENFUNCTION*)
```

In[•]:= `TableForm[ Table[HermiteH[n, x], {n, 0, 3}]]`

Out[•]//TableForm=

$$1$$
$$2\,x$$
$$-2+4\,x^2$$
$$-12\,x+8\,x^3$$

```
(*HERMITE EQUATION*)
```

In[•]:= `u = HermiteH[0, x];`

$\partial_{x,x}u - 2\,x\,\partial_x u + (2\times 0)\,u$

`u = HermiteH[1, x];`

$\partial_{x,x}u - 2\,x\,\partial_x u + (2\times 1)\,u$

`u = HermiteH[2, x];`

$\mathtt{FullSimplify}\left[\partial_{x,x}u - 2\,x\,\partial_x u + (2\times 2)\,u\right]$

Out[•]= 0

Out[•]= 0

Out[•]= 0

```
(*EIGENFUNCTIONS NORMALIZATION PROPERTIES*)
```

In[•]:= $\mathtt{psi0} = \frac{1}{\pi^{1/4}\sqrt{x0}}\,\mathtt{Exp}\left[-\frac{x^2}{2\,x0^2}\right]\,\mathtt{HermiteH}\left[0, \frac{x}{x0}\right];$

$\mathtt{Integrate}\left[\mathtt{psi0}^2, \{x, -\infty, +\infty\}, \mathtt{Assumptions} \to \mathtt{Re}\left[x0^2\right] > 0\right]$

$\mathtt{psi1} = \frac{1}{\pi^{1/4}\sqrt{2\,x0}}\,\mathtt{Exp}\left[-\frac{x^2}{2\,x0^2}\right]\,\mathtt{HermiteH}\left[1, \frac{x}{x0}\right];$

$\mathtt{Integrate}\left[\mathtt{psi1}^2, \{x, -\infty, +\infty\}, \mathtt{Assumptions} \to \mathtt{Re}\left[x0^2\right] > 0\right]$

$\mathtt{psi2} = \frac{1}{\pi^{1/4}\sqrt{2^3\,x0}}\,\mathtt{Exp}\left[-\frac{x^2}{2\,x0^2}\right]\,\mathtt{HermiteH}\left[2, \frac{x}{x0}\right];$

$\mathtt{Integrate}\left[\mathtt{psi2}^2, \{x, -\infty, +\infty\}, \mathtt{Assumptions} \to \mathtt{Re}\left[x0^2\right] > 0\right]$

Out[•]= $\sqrt{\frac{1}{x0^2}}\,x0$

Out[•]= $\sqrt{\frac{1}{x0^2}}\,x0$

Out[•]= $\sqrt{\frac{1}{x0^2}}\,x0$

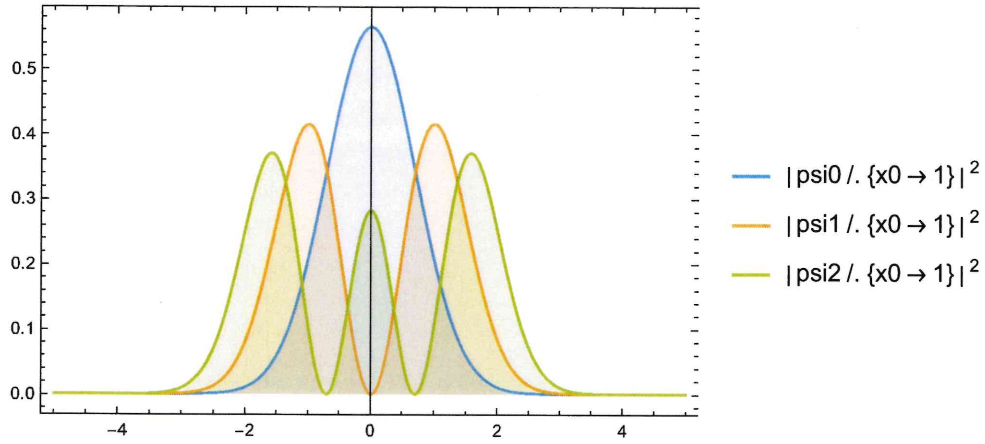
(*GROUND STATE VARIANCE $\sigma_0 = \sqrt{2}\,x0$*)

$x0 \to \sqrt{\frac{\hbar}{m\,\omega}};$

```
(*TAKE x0→1*)
```

In[ ]:=
```
Plot[{Abs[psi0 /. {x0 → 1}]^2, Abs[psi1 /. {x0 → 1}]^2, Abs[psi2 /. {x0 → 1}]^2},
 {x, -5, 5}, PlotRange → All, Frame → True,
 PlotLegends → "Expressions", Filling → Axis]
```

Out[ ]=



In[ ]:=
```
FullSimplify[{psi0, psi1, psi2} // TraditionalForm,
 Assumptions → {m > 0, ℏ > 0, ω > 0}]
```

Out[ ]//TraditionalForm=

$$\left\{\frac{e^{-\frac{x^2}{2\,x0^2}}}{\sqrt[4]{\pi}\,\sqrt{x0}}, \frac{\sqrt{2}\,x\,e^{-\frac{x^2}{2\,x0^2}}}{\sqrt[4]{\pi}\,x0^{3/2}}, -\frac{e^{-\frac{x^2}{2\,x0^2}}\left(x0^2-2\,x^2\right)}{\sqrt{2}\,\sqrt[4]{\pi}\,x0^{5/2}}\right\}$$

```
(*EIGENFUNCTIONS ORTHOGONALITY PROPERTIES*)
```

In[ ]:=
```
Integrate[psi0 * psi1, {x, -∞, +∞}, Assumptions → Re[x0^2] > 0]
Integrate[psi0 * psi2, {x, -∞, +∞}, Assumptions → Re[x0^2] > 0]
Integrate[psi1 * psi2, {x, -∞, +∞}, Assumptions → Re[x0^2] > 0]
```

Out[ ]= 0

Out[ ]= 0

Out[ ]= 0

✦ For an asymmetric 1D barrier the continuity at the well boundary at x=a yields the following eigenvalue equation:

$$\cot\left[ka + \delta(k)\right] = -\sqrt{\frac{2mV_2}{\hbar^2 k^2} - 1}$$

Check that the correct solution for the energy has the following form (- sign):

$$ka + \delta(k) = -sin^{-1}\frac{\hbar k}{\sqrt{2mV_2}} + \pi n_2$$

$\cos[\sin^{-1}x] = \sqrt{1-x^2}$

$$\cot(ka+\delta) = \frac{\cos[\;]}{\sin[\;]} = \frac{\cos[-\sin^{-1}\frac{\hbar k}{\sqrt{\ }} + \pi n_2]}{\sin[-\sin^{-1}\frac{\hbar k}{\sqrt{\ }} + \pi n_2]} = \frac{(-)^{n_2}[\cos(\sin^{-1}\frac{\hbar k}{\sqrt{\ }})]}{(-)^{n_2+1}\sin[\sin^{-1}\frac{\hbar k}{\sqrt{\ }}]}$$

$\sin[\sin^{-1}x] = x$

$$= -\sqrt{1-\frac{\hbar^2 k^2}{2mV_2}} \Big/ \frac{\hbar k}{\sqrt{2mV_2}} = -\sqrt{\frac{1}{\frac{\hbar^2 k^2}{2mV_2}} - 1} = -\sqrt{\frac{2mV_2}{\hbar^2 k^2} - 1} \quad \underline{\underline{\text{Ok}}}$$