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HW 12 Quantum Mechanics II April 29, 2023

Collaborators

I worked with **Andrew Binder** to complete this homework.

Problem 1

Use the WKB approximation to find the allowed energies (E_n) of an infinite square well with a "shelf," of height V_0, extending half-way across (Figure 7.3):

$$V(x) = \begin{cases} V_0, & (0 < x < a/2), \\ 0, & (a/2 < x < a), \\ \infty, & \text{(otherwise)} \end{cases}$$

Express your answer in terms of V_0 and $E_n^0 \equiv (n\pi\hbar)^2/2ma^2$ (the nth allowed energy for the infinite square well with *no* shelf). Assume that $E_1^0 > V_0$, but do *not* assume that $E_n \gg V_0$. Compare your result with what we got in Section 7.1.2, using first-order perturbation theory. Note that they are in agreement if either V_0 is very small (the perturbation theory regime) or n is very large (the WKB–semi-classical–regime).

Solution: Here we use the WKB approach, which tells us that for an infinite well, we have

$$\int_0^a \sqrt{2m(E - V_0)}dx = n\pi\hbar$$

The integral on the left needs to be broken up into two integrals, from 0 to $a/2$ and then from $a/2$ to a:

$$\int_0^a p(x)dx = \int_0^{a/2} \sqrt{2m(E - V_0)}dx + \int_{a/2}^a \sqrt{2mE}dx$$
$$n\pi\hbar = \frac{a}{2}\left[\sqrt{2m(E_n - V_0)} + \sqrt{2mE_n}\right]$$

Solving this equation for E_n (I got lazy and threw this into mathematica), we get:

$$E_n = \frac{(2\hbar^2 n^2 \pi^2 + amV_0)^2}{8a^2\hbar^2 mn^2\pi^2} = E_n^0 + \frac{V_0}{2} + \frac{V_0^2}{16E_n^0}$$

From Section 7.1.2, we find that we got the energy levels to be

$$E_n = E_n^0 + \frac{V_0}{2}$$

This makes sense since for small perturbations (i.e. V_0 small), then the third term in the WKB equation $V_0^2/16E_n^0$ would be very small, so it makes sense that this term is neglected when considering perturbation theory. When n becomes large, we see that E_n grows large, so therefore this last term also goes to zero under large n. Therefore, we've confirmed that these two results agree for the two regimes we were asked to check. $\square$

Problem 2

use Equation 9.23 to calculate the approximate transmission probability for a particle of energy E that encounters a finite square barrier of height $V_0 > E$ and width $2a$. Compare your answer with the exact result (Problem 2.33), to which it should reduce in the WKB regime $T \ll 1$.

Solution: Let the left side of the barrier be at $x = 0$ and the right side be at $x = 2a$, for simplicity's sake with the integral. We know that for tunnelling, we have that

$$T \approx e^{-2\gamma}$$

where γ is defined as

$$\gamma = \int_{x_1}^{x_2} \sqrt{\frac{2m}{\hbar^2}(V(x) - E)}dx$$

So in our particular case, we can get:

$$\gamma = \int_0^{2a} \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}dx = 2a\sqrt{\frac{2m}{\hbar^2}(V_0 - E)} = \frac{2a}{\hbar}\sqrt{2m(V_0 - E)}$$

Therefore, our transmission coefficient is:

$$T \approx \exp\left(-\frac{4a}{\hbar}\sqrt{2m(V_0 - E)}\right)$$

From Problem 2.33, we get the exact transmission as:

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)}\sinh^2\gamma}$$

In the case where T is small, then from our WKB approximation we can see that γ must be large in order for T to be small. Thus, we can use an approximation for the sinh function:

$$\sinh^2\gamma \approx \left(\frac{e^\gamma}{2}\right)^2 = \frac{e^{2\gamma}}{4}$$

which now reduces our expression for the exact transmission to:

$$T \approx \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)}\frac{e^{2\gamma}}{4}} \approx \frac{1}{\frac{V_0^2 e^{2\gamma}}{16E(V_0-E)}} = \frac{16E(V_0 - E)}{V_0^2 e^{2\gamma}}$$

In the case where γ is very large, then we can effectively neglect the constants in front, meaning that our transmission now becomes

$$T \approx \frac{1}{e^{2\gamma}} = e^{-2\gamma}$$

which matches the WKB solution. $\square$

Problem 3

Use the WKB approximation to find the allowed energies of the harmonic oscillator.

Solution: Here, let E represent the energy of the particle. Then, since we know that $V(x) = \frac{1}{2}m\omega^2 x^2$, then we can easily solve for the turning points, which end up becoming:

$$a = \pm\sqrt{\frac{2E}{m\omega^2}}$$

Further, we have $p(x) = \sqrt{2m(E - \frac{1}{2}m\omega^2x^2)}$, so now we can solve the integral:

$$\int_{-a}^{a} \sqrt{2m(E - \frac{1}{2}m\omega^2x^2)}\ dx = 2\int_0^a \sqrt{2m(E - \frac{1}{2}m\omega^2x^2)}$$

This integral can be simplified by hand a little:

$$\begin{aligned}\int_{-a}^{a} \sqrt{2m(E - \frac{1}{2}m\omega^2x^2)}\ dx &= \int_{-a}^{a} \sqrt{m^2\omega^2\left(\frac{2E}{m\omega^2} - x^2\right)}\ dx \\ &= m\omega\int_{-a}^{a} \sqrt{a^2 - x^2}\ dx\end{aligned}$$

then, we can throw this into Mathematica:

$$m\omega\int_{-a}^{a} \sqrt{a^2 - x^2}dx = m\omega\frac{\pi a^2}{2}$$

Now, substituting back a:

$$m\omega\frac{\pi a^2}{2} = \frac{m\omega\pi}{2}\frac{2E}{m\omega^2} = \pi\frac{E}{\omega}$$

Now, since WKB requires that for a finite barrier, that we set $\int p dx = (n + 1/2)\pi\hbar$, then we have:

$$\frac{\pi E}{\omega} = \left(n + \frac{1}{2}\right)\pi\hbar$$

which implies that

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

which is the exact solution for the harmonic oscillator problem. □

Problem 4

In the phenomenon of *cold emission*, electrons are drawn from a metal (at room temperature) by an externally supported electric field. The potential well that the metal presents to the free electrons before the electric field is turned on is depicted in Fig. 2.5. After application of the constant electric field $\mathcal{E}$, the potential at the surface slopes down as shown in Fig. 7.38, thereby allowing electrons in the Fermi sea to "tunnel" through the potential barrier. If the surface of the metal is taken as the $x = 0$ plane, the new potential outside the surface is

$$V = \Phi + E_F - e\mathcal{E}x$$

where E_F is the Fermi level and Φ is the work function of the metal.

a) Use the WKB approximation to calculate the transmission coefficient for cold emission.

Solution: The WKB approximation says that for tunnelling, we have $T \approx e^{-2\gamma}$, and we define γ to be:

$$\gamma = \int_{x_1}^{x_2} \sqrt{\frac{2m}{\hbar^2}\left(V(x) - E\right)}\, dx$$

Applying this to our situation, we can see that the bounds of integration are from $x_1 = 0$ to $x_2 = \Phi/e\mathcal{E}$, and $V(x) = \Phi + E_F - e\mathcal{E}x$. Further, we only consider electrons at the top of the Fermi level, so therefore $E = E_F$ in our case. This means that the integral reduces to:

$$\gamma = \sqrt{\frac{2m}{\hbar^2}} \int_0^{\Phi/e\mathcal{E}} \sqrt{\Phi + E_F - e\mathcal{E}x - E_F}\, dx = \sqrt{\frac{2m}{\hbar^2}} \int_0^{\Phi/e\mathcal{E}} \sqrt{\Phi - e\mathcal{E}x}\, dx = \sqrt{\frac{2m}{\hbar^2}} \frac{2\Phi^{3/2}}{3e\mathcal{E}}$$

Rewriting this a bit, we get:

$$T = \exp\left(-\frac{4\sqrt{2m\Phi}}{3\hbar e\mathcal{E}}\right)$$

□

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b) Estimate the field strength $\mathcal{E}$, in volt/cm, necessary to draw current density of the order mA/cm^2 from a potassium surface. For J_{inc} (see Eq. 7.108: $T \equiv \left|\frac{J_{\text{trans}}}{J_{\text{inc}}}\right|$) use the expression $J_{inc} = env$, where n is the electron density and v is the speed of electrons at the top of the Fermi sea. The relevant expression for E_F may be found in Problem 2.42. Data for potassium is given in Section 2.3.

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3n}{8\pi}\right)^{\frac{2}{3}}$$

Solution: First, note that because we want J_{trans} on the order of mA/cm^2, then this is equivalent to wanting 10 A/m^2. This will be useful later on so that we don't have to worry too much about unit conversions. By the definition of the problem statement, we first write $J_{\text{inc}} \cdot T = J_{\text{trans}}$, and substituting in our equation for T, we get:

$$J_{\text{trans}} = J_{\text{inc}} \exp\left(-\frac{4\sqrt{2m\Phi}}{3\hbar e\mathcal{E}}\right)$$

Here, the only unknown quantity is J_{inc}, but we can solve for it in terms of other variables. Firstly, we know that we need to use $J_{\text{inc}} = env$, and solving for v by using the energy of particles at the top of the Fermi level:

$$v = \sqrt{\frac{2E_F}{m}}$$

We can also solve for n in terms of E_F using the expression in Problem 2.42:

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3m}{8\pi}\right)^{\frac{2}{3}}$$
$$\therefore n = \frac{16\sqrt{2}\pi}{3}\left(\frac{E_F m}{\hbar^2}\right)^{\frac{3}{2}}$$

therefore, now we can calculate J_{inc}:

$$J_{\text{inc}} = env = e\left(\frac{16\sqrt{2}\pi}{3}\left(\frac{mE_F}{\hbar^2}\right)^{\frac{3}{2}}\right)\sqrt{\frac{2E_F}{m}} = \frac{32e\pi}{3}\sqrt{\frac{E_F}{m}}\left(\frac{E_F m}{\hbar^2}\right)^{\frac{3}{2}} = \frac{32e\pi}{3}\frac{E_F^2 m}{\hbar^3}$$

Now we can finally just plug in values:

$$J_{\text{trans}} = 10\frac{\text{A}}{\text{m}^2} = J_{\text{inc}}T = \left(\frac{32e\pi m E_F^2}{3\hbar^3}\right)\exp\left(-\frac{4\sqrt{2m\Phi}}{2\hbar e\mathcal{E}}\right)$$

So again, now we can solve for $\mathcal{E}$ by throwing this into Mathematica once again:

$$\mathcal{E} = \frac{4\sqrt{2m\Phi^3}}{3e\hbar\ln\left(\frac{32em\pi}{3\hbar^2 J_{\text{inc}}}E_F^2\right)} = \frac{4\sqrt{2m\Phi^3}}{3e\hbar\ln\left(\frac{32em\pi}{30\hbar^2}E_F^2\right)}$$

Plugging this value into WolframAlpha, we get approximately -7.1×10^{-6} for $\mathcal{E}$, which is a very strong electric field. $\square$