Lecture 19 Highlights
Phys 402

WKB Approximation

We now go back to one-dimensional quantum mechanics and investigate some very useful approximation schemes. Note that the Schrödinger equation for the hydrogen atom reduces, in part, to a one-dimensional Schrödinger problem for the radial coordinate, so these approximation schemes can also work for aspects of 3D problems.

WKB Approximation Applied to Tunneling

We are now going to use the WKB approximation to calculate tunneling rates through odd-shaped barriers. You encountered tunneling before in Phys 401, including:

1) Section 2.5 where tunneling through a delta-function barrier of the form $V(x) = \alpha\,\delta(x)$ (with $\alpha > 0$). The result for the transmission probability is $T = \dfrac{1}{1 + E_0 / E}$, where E is the energy of the particle and $E_0 = m\alpha^2 / 2\hbar^2$ is a characteristic energy in the problem.

2) Problem 2.33 Tunneling through a rectangular barrier of height V_0 and width a. The transmission probability is $T = \dfrac{1}{1 + \dfrac{V_0^2}{4E(V_0 - E)}\sinh^2\left(\dfrac{a}{\hbar}\sqrt{2m(V_0 - E)}\right)}$ valid for $E < V_0$.

Consider the WKB approximation for particles in the "classically forbidden" region, $E < V(x)$. In this region the kinetic energy $p^2 / 2m$ is negative, which can be interpreted as resulting from an imaginary momentum $p = \sqrt{2m(E - V(x))}$. In this case the WKB solutions we found last time become:

$$\psi(x) = \frac{D}{\sqrt{|p_{class}(x)|}} \exp\left[\pm \frac{1}{\hbar}\int^{x} |p_{class}(x')|\,dx'\right],$$

with $|p_{class}| = \sqrt{2m(V(x) - E)}$, which is real and positive under the barrier. Notice that the complex exponential has now become a positive or negative exponential because the solutions are no longer running waves.

Consider a barrier of width a with an arbitrary potential on top, $V(x)$, as discussed on pages 358-361 of Griffiths. For energies E less than the minimum of $V(x)$, and for barriers that are sufficiently tall and thick, the transmission probability is dominated by the negative exponential term;

$T \propto e^{-2\gamma}$, where $\gamma = \dfrac{1}{\hbar}\displaystyle\int_0^a |p_{class}(x')|\,dx'$, where the integral is taken over the entire width of the potential barrier (0 to a).

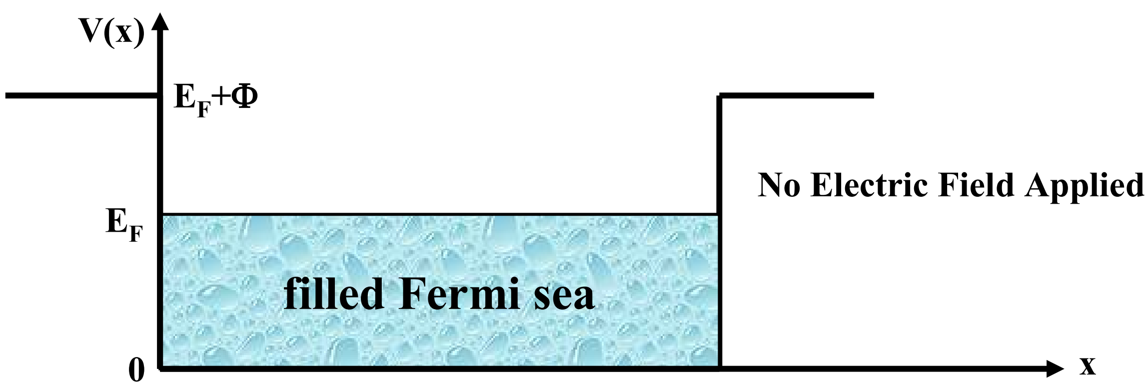
Going back to the flat-top barrier of problem 2.33 to test this result, the transmission probability in the WKB approximation (after doing the integral with $V(x) = V_0$) is

$T \propto e^{-\frac{2a}{\hbar}\sqrt{2m(V_0 - E)}}$. If we expand the exact result given above in the limit of tall and wide barrier (i.e. $\frac{a}{\hbar}\sqrt{2m(V_0 - E)} >> 1$), the result is $T \cong \frac{4E(V_0 - E)}{V_0^2} e^{-\frac{2a}{\hbar}\sqrt{2m(V_0 - E)}}$. The pre-factor is on the order of 1, so the exponential dominates, and is in agreement with the WKB approximate result.

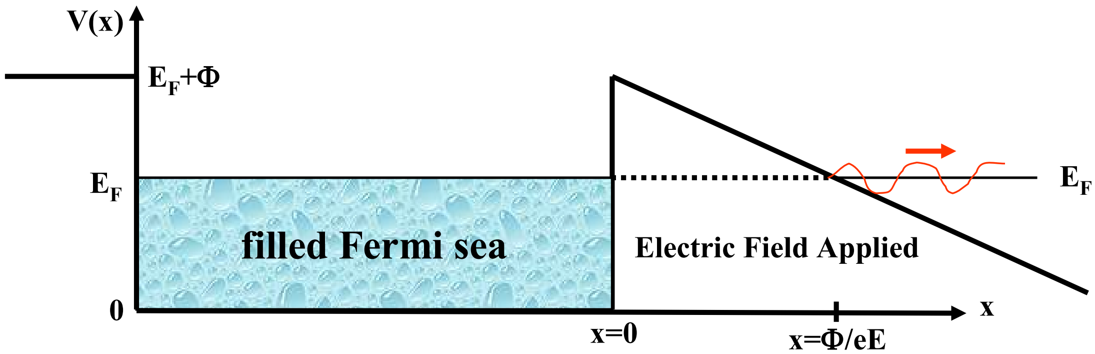
Fowler-Nordheim Tunneling

Consider the problem of cold emission from a metal. A metal is formed in to a sharp tip and held above a flat metallic counter-electrode, with a small gap. A large potential difference is maintained between the tip and the electrode, all in vacuum. The question is this: how much electrical current flows between the tip and the electrode as a function of the electric field?

We can roughly model a piece of metal as an infinite square well in which all of the identical spin-1/2 electrons with overlapping wavefunctions have to occupy unique quantum states (the Pauli Exclusion Principle). The highest occupied state of the metal is called the Fermi energy, and is typically on the scale of 5 to 10 eV. In reality it takes a finite amount of energy to extract an electron from a metal. Hence a metal can be better modeled as a potential well of depth $E_F + \Phi$, where E_F is the Fermi energy and Φ is the work function of the metal (see the Figure below). The work function is the energy required to remove an electron from the Fermi energy in the metal and to set it free. Work functions are typically on the order of a few electron volts for metals. For Cu, Ag, Au and Pb they are between 4 and 5 eV. At zero temperature all of the states below the Fermi energy are occupied and all those above are un-occupied.



If an electric field is applied to the surface of a metal, the potential is modified and it becomes possible for electrons to tunnel out of the metal into free space (this is called cold emission by Fowler-Nordheim tunneling). We take this radical 1D approximation to describe the tunneling of electrons out of the metal tip and through the vacuum tunnel barrier.



Note that the tunnel barrier is not a "flat top" but instead triangular shaped. The potential in the space between the tip and the flat electrode is given by $V(x) = E_F + \Phi - e\mathcal{E}x$, where $\mathcal{E}$ is the applied electric field. The calculation of the Fowler-Nordheim tunneling rate is a job for the WKB approximation! We see that electrons at the Fermi energy have the highest tunneling probability because they see the shortest and most narrow tunnel barrier of all the electrons in the metal. Hence we confine the tunneling estimate to just those electrons. The tunneling probability is given in WKB by,

$$T \propto e^{-2\gamma}, \text{ where } \gamma = \frac{1}{\hbar}\int_0^a |p_{class}(x')|dx' = \frac{1}{\hbar}\int_0^a \sqrt{2m(V(x)-E)}\,dx',$$

and in this case $\gamma = \frac{1}{\hbar}\int_0^{\Phi/e\mathcal{E}} \sqrt{2m(E_F + \Phi - e\mathcal{E}x' - E_F)}dx'$. Again we assume that the electrons at $E = E_F$ dominate the tunneling process. The upper limit of the integral is the point in x where the Fermi energy is equal to the potential outside the metal (a classical turning point). The integral can be solved by standard methods and the result is;

$$T = exp\left[-\frac{4}{3}\frac{\sqrt{2m}}{\hbar}\frac{\Phi^{3/2}}{e\mathcal{E}}\right]$$

The tunneling current is proportional to the transmission probability. Hence the log of the tunnel current should be proportional to the inverse of the electric field strength. This is the characteristic of Fowler-Nordheim tunneling, and data showing this behavior is posted on the class web site. As the electric field strength grows, the barrier gets narrower and a bit shorter, allowing for more tunneling out of the metal tip.

Another example of tunneling rate estimates is the radioactive alpha-particle decay of heavy nuclei. In this case, the nucleus can be approximately described as a finite square well for the identical neutrons and for the identical protons, both of which are spin-1/2 particles. There is a Fermi energy for both neutrons and protons in the nucleus. It can happen that an alpha particle (bound state of two protons and two neutrons) can tunnel out of the nucleus. Once it escapes, there is a strong Coulomb repulsion between the +2e alpha particle and the charge +(Z-2)e resulting nucleus. The combination of the finite square well and the Coulomb repulsion, $V(r) = \frac{+2e(Z-2)e}{4\pi\varepsilon_0 r}$, creates a (nearly) triangular barrier that the alpha particle must tunnel through. This produces an exponential relationship between the half-life of the nucleus against alpha decay, and the kinetic energy of the exiting alpha particle. The kinetic energy depends on the Fermi energy of the neutrons and protons in the original nucleus (see the diagram here), which in turn determines the height and width of the barrier, hence the half-life. The Fermi energy can be 'varied' by looking heavy atoms with different Z values (Th, U, Ac, Np), and various isotopes. The explanation of the plot of half-life vs. alpha particle kinetic energy was the first use of quantum tunneling to explain a physical phenomenon.