HW2 solution

MTLE-6120: Spring 2018

Due: Feb 5, 2018

1. **Counting waves**

   We showed in class that for waves trapped in a 3D box, the number of wave vectors $\vec{k}$ with magnitude between k and $k + \mathrm{d}k$ is $k^2\mathrm{d}k/(2\pi^2)$ per unit volume, independent of box size (not counting the factor of 2 for polarizations here). What are the corresponding numbers for waves in 2D and 1D boxes? Optional: derive the general result for d dimensions.

   For waves in a 2D box of length L, the area in the first quadrant of k space between k and $k + \mathrm{d}k$ is $(2\pi k\mathrm{d}k)/4$. The area per k is $(\pi/L)^2$, so that the required number of waves per unit area is

$$N_{2\mathrm{D}}(k)\mathrm{d}k = \frac{2\pi k\mathrm{d}k}{4} \cdot \frac{1}{(\pi/L)^2} \cdot \frac{1}{L^2} = \frac{k\mathrm{d}k}{2\pi}$$

   Similarly, for waves in a 1D box of length L, the length in the positive half of k space between k and $k + \mathrm{d}k$ is just $\mathrm{d}k$. The length per k is (π/L), so that the required number of waves per unit length is

$$N_{1\mathrm{D}}(k)\mathrm{d}k = \mathrm{d}k \cdot \frac{1}{(\pi/L)} \cdot \frac{1}{L} = \frac{\mathrm{d}k}{\pi}$$

   The general case for d dimensions will also follow the same logic above, once we know the formula for a 'surface area of a sphere in d dimensions'; that must be of the form $A_d(r) = c_d r^{d-1}$, where c_d is some constant for each dimension (we all know $c_1 = 2$, $c_2 = 2\pi$, $c_3 = 4\pi$). A neat trick to determine this constant in general is to compare the integral of a Gaussian over all of d dimensional space between spherical and cartesian coordinates,

$$\int \mathrm{d}\vec{r} e^{-|\vec{r}|^2} = \int \mathrm{d}\vec{r} e^{-(x_1^2+x_2^2+\ldots+x_d^2)}.$$

   On the left side, the spherical symmetry allows us to write $\mathrm{d}\vec{r} = A_d(r)\mathrm{d}r$, while on the right side, we separate in Cartesian coodinates $\mathrm{d}\vec{r} = \mathrm{d}x_1\mathrm{d}x_2\ldots\mathrm{d}x_d$. Therefore:

$$\begin{aligned}
\int_0^\infty A_d(r)\mathrm{d}r e^{-r^2} &= \int \mathrm{d}x_1\mathrm{d}x_2\ldots\mathrm{d}x_d e^{-(x_1^2+x_2^2+\ldots+x_d^2)} \\
\int_0^\infty c_d r^{d-1}\mathrm{d}r e^{-r^2} &= \int_{-\infty}^\infty \mathrm{d}x_1 e^{-x_1^2} \int_{-\infty}^\infty \mathrm{d}x_2 e^{-x_2^2} \ldots \int_{-\infty}^\infty \mathrm{d}x_d e^{-x_d^2} \\
\int_0^\infty c_d(\sqrt{s})^{d-1}\frac{\mathrm{d}s}{2\sqrt{s}} e^{-s} &= (\sqrt{\pi})^d \qquad \text{(Substituting } s = r^2\text{)} \\
c_d \int_0^\infty \mathrm{d}s s^{d/2-1} e^{-s} &= 2\pi^{d/2} \\
\Rightarrow \qquad c_d &= \frac{2\pi^{d/2}}{\Gamma(d/2)}
\end{aligned}$$

   Then it follows that the number of waves per unit 'volume' of a d-dimensional box is

$$N_{d\mathrm{D}}(k)\mathrm{d}k = \frac{2\pi^{d/2}k^{d-1}\mathrm{d}k}{\Gamma(d/2)2^d} \cdot \frac{1}{(\pi/L)^d} \cdot \frac{1}{L^d} = \frac{(k/2)^{d-1}\mathrm{d}k}{\Gamma(d/2)\pi^{d/2}}.$$

Using $\Gamma(1/2) = \sqrt{\pi}$, $\Gamma(1) = 1$ and $\Gamma(3/2) = \sqrt{\pi}/2$, we can easily see that it reduces to the 1, 2 and 3D versions we derived before.

2. **Photoelectric effect and quantum efficiency: Kasap 3.8**

   (a) Longest wavelength λ_0 corresponds to minimum photon energy E_0, which must equal the work function $\phi_0 = 1.9$ eV. So

   $$\lambda_0 = hc/E_0 = \frac{6.626 \times 10^{-34}\ \text{Js} \cdot 3 \times 10^8\ \text{m/s}}{1.9 \cdot 1.602 \times 10^{-19}\ \text{J}} = 653\ \text{nm}$$

   In fact, it is useful to note the value of $hc = 1241\ \text{nm} \cdot \text{eV}$ to convert between wavelengths and photon energies. So $E_0 = 1.9$ eV corresponds to $1241/1.9 = 653$ nm.

   (b) Blue radiation of wavelength 450 nm has photon energy $1241/450 = 2.76$ eV. Since the work function is 1.9 eV, the ejected electrons have kinetic energy $2.76 - 1.9 = 0.86$ eV. It would therefore take a potential of 0.86 V to stop them.

   (c) Given intensity $\mathcal{I}$ on area A, the incident power is $\mathcal{I}A$. This corresponds to a photon incident rate of $\mathcal{I}A/E_{\text{photon}}$. The quantum efficiency QE determines the fraction of photons converted to electrons, so the electron generation rate is $\text{QE} \cdot \mathcal{I}A/E_{\text{photon}}$. Correspondingly the photocurrent is

   $$e\frac{\text{QE} \cdot \mathcal{I}A}{E_{\text{photon}}} = e\frac{(25\%)(30\ \text{mW/cm}^2)(\pi(6\ \text{mm})^2/4)}{2.76\ \text{eV}} = \frac{(0.25)(300\ \text{J/s/m}^2)(9\pi \times 10^{-6}\ \text{m}^2)}{2.76\ \text{V}} \approx 0.77\ \text{mA}$$

3. **Scattering by a δ-atom**

   (a) Consider an electron with energy $E = \frac{\hbar^2 k^2}{2m} > 0$ incident from the left ($-\infty$) towards a δ-atom given by the potential $-V_0\delta(x)$, with strength parametrized using the parameter $q = 2mV_0/\hbar^2$. Find the wavefunction $\psi(x)$ (expressed in k and q, rather than E and V_0 for convenience). Can you normalize it?
   At $x \neq 0$, the wavefunctions are $e^{\pm ikx}$. So we can assume the general form

   $$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ Ce^{ikx} + De^{-ikx}, & x > 0 \end{cases}$$

   The incident electron corresponds to Ae^{ikx}, which could reflect to Be^{-ikx} and transmit to Ce^{ikx}. But it cannot produce De^{-ikx}, which is an electron incident from the right ($+\infty$), so set $D = 0$. At $x = 0$, the wavefunction should be continuous, which yields $A + B = C + D = C$, so that

   $$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ (A+B)e^{ikx}, & x > 0 \end{cases}$$

   In class, we derived the derivative discontinuity condition

   $$\psi'(0^+) - \psi'(0^-) = \frac{-2mV_0}{\hbar^2}\psi(0) \equiv -q\psi(0)$$

   Substituting $\psi(x)$ yields

   $$ik(A+B) - (ikA - ikB) = -q(A+B)$$

   which simplifies to $B = -qA/(2ik+q)$. Therefore

   $$\psi(x) = A\begin{cases} e^{ikx} - \frac{q}{2ik+q}e^{-ikx}, & x < 0 \\ \frac{2ik}{2ik+q}e^{ikx}, & x > 0 \end{cases}$$

   Usually A would now be determined by normalizing the wavefunction. However, this wavefunction is present in all of space and cannot be normalized in the conventional way. (A naive attempt would lead to $A \to 0$.)

(b) What are the probabilities of the electron getting reflected and transmitted? Describe and explain their qualitative dependence on the energy of the electron. What would the corresponding probabilities be in the classical case?

The incident wave had amplitude A, and the reflected wave had amplitude B, so the reflection probability is

$$R \equiv \left|\frac{B}{A}\right|^2 = \frac{q^2}{4k^2 + q^2}.$$

Similarly the transmission probability is

$$T \equiv \left|\frac{A+B}{A}\right|^2 = \frac{4k^2}{4k^2 + q^2}.$$

As expected, $R + T = 1$.

For energy $E \to 0$, $k = 0$, which corresponds to $R = 1$ and $T = 0$ i.e. perfect reflection. As energy increases, k increases, which causes R to decrease and T to increase. For energy $E \to \infty$, $k \to \infty$ which results in $R = 0$ and $T = 1$ i.e. perfect transmission. As the electron energy increases, it is less affected by the potential and has a greater tendency to continue in its original direction (transmission).

Classically the electron would always transmit $T = 1$ and $R = 0$. (It will roll into the bottom of the well gaining kinetic energy, and then roll back up converting that back to potential energy, and continue onwards with its original kinetic (and total) energy.)

(c) Consider the opposite potential $+V_0\delta(x)$. What is the electron wavefunction? What are the probabilities of the electron getting reflected and transmitted? What would the corresponding probabilities be in the classical case?

The only thing that changes is $V_0 \to -V_0$, which is equivalent to $q \to -q$. Therefore

$$\psi(x) = A \begin{cases} e^{ikx} + \frac{q}{2ik-q} e^{-ikx}, & x < 0 \\ \frac{2ik}{2ik-q} e^{ikx}, & x > 0 \end{cases}$$

The quantum reflection and transmission probabilities,

$$R = \frac{q^2}{4k^2 + q^2} \qquad \text{and} \qquad T = \frac{4k^2}{4k^2 + q^2},$$

remain unchanged!

Classically, the electron cannot cross an infinite potential and will always bounce back i.e. $T = 0$ and $R = 1$.

(d) Instead of a free electron with definite momentum k (and energy $E = \frac{\hbar^2 k^2}{2m}$) as considered above, consider a Gaussian wavepacket with coefficients

$$c_k = \frac{1}{\sqrt{\sigma_k \sqrt{2\pi}}} \exp \frac{-(k - k_0)^2}{2\sigma_k^2},$$

assuming that the spread in momentum $\sigma_k \ll k_0$ and q. Where is the electron as a function of time?

In class, we showed that for a wave $e^{i(kx - \omega t)}$, such a wavepacket takes the form

$$\frac{\exp \frac{-(x - \omega'(k_0)t)^2}{2\sigma_x^2}}{\sqrt{\sigma_x \sqrt{2\pi}}} e^{i(k_0 x - \omega(k_0)t)}$$

with $\sigma_x = 1/\sigma_k$.

For a single k, we already solved for the wavefunction

$$\psi(x) = A \begin{cases} e^{ikx} - \frac{q}{2ik+q} e^{-ikx}, & x < 0 \\ \frac{2ik}{2ik+q} e^{ikx}, & x > 0 \end{cases}$$

which contains $e^{\pm ikx}$ pieces for $x<0$ and $x>0$. Within the wavepacket, all the k are close to k_0 within width $\sigma_k \ll k_0$ and q. This means that the coefficients of the reflected and transmitted piece are approximately the same for each k as for the center k_0 i.e.

$$\psi(x) \approx A \begin{cases} e^{ikx} - \frac{q}{2ik_0+q} e^{-ikx}, & x<0 \\ \frac{2ik_0}{2ik_0+q} e^{ikx}, & x>0 \end{cases}$$

for all k that are relevant.

Now, we can combine each of the pieces into a wavepacket using the derivation from class, taking care to flip the sign of k_0 for the negative propagating wave:

$$\psi_{\text{packet}}(x,t) \approx \frac{A}{\sqrt{\sigma_x \sqrt{2\pi}}} \begin{cases} \begin{array}{l} \exp\left(\frac{-(x-\omega'(k_0)t)^2}{2\sigma_x^2}\right) e^{i(k_0x-\omega(k_0)t)} \\ \qquad -\frac{q}{2ik_0+q} \exp\left(\frac{-(x+\omega'(k_0)t)^2}{2\sigma_x^2}\right) e^{i(-k_0x-\omega(k_0)t)} \end{array}, & x<0 \\ \frac{2ik_0}{2ik_0+q} \exp\left(\frac{-(x-\omega'(k_0)t)^2}{2\sigma_x^2}\right) e^{i(k_0x-\omega(k_0)t)}, & x>0 \end{cases}$$

The first term for $x<0$ consists of a bunch centered at $x=v_g t$, where $v_g=\omega'(k_0)=\hbar k_0/m$, which has significant contribution for $x<0$ (the domain of this solution) only for $t<0$. So this is the incoming electron that lasts from $t=-\infty$ till $t=0$ when it 'collides' with the potential.

The second term for $x<0$ is centered at $x=-v_g t$, which has significant contribution in $x<0$ only for $t>0$. This corresponds to the reflected electron bunch which is produced at $t=0$ upon collision with the potential.

The single term for $x>0$ is centered at $x=v_g t$, which contributes for $x>0$ when $t>0$. Of course, this corresponds to the electron bunch transmitted after collision with the potential at $t=0$.

Collecting by time, the electron comes in as a wavepacket of width $\sigma_x/\sqrt{2}$ (where $\sqrt{2}$ is because of wavefunction squared) centered at $x=v_g t$, moving with velocity $v_g\hat{x}$ towards $x=0$ till $t=0$. For $t>0$, the electron is **either** in the reflected bunch centered at $x=-v_g t$ moving with velocity $-v_g\hat{x}$ **or** in the transmitted bunch centered at $x=v_g t$ moving with velocity $v_g\hat{x}$. The probability of which bunch it is in is precisely given by the reflection and transmission probabilities, R and T.