Homework 6 Solutions

1. The one-dimensional Kronig-Penney model yields the useful expression

$$\frac{Q^2 - K^2}{2QK} \sinh Qb \sin Ka + \cosh Qb \cos Ka = \cos k(a+b)$$

where $K = (2mU)^{1/2}/\hbar$ and $Q = [2m(V_B - U)]^{1/2}/\hbar$ K = (2mU)$^{1/2}$. This can be solved for k as a function of U easily, and has been carried out using Microsoft Excel for the present purposes.

(a) The "band structure" of U vs k is shown in Fig. 1 for V_B = 10 eV, a = 4.0 Ang, and b = 1.0 Ang. The plot is carried out between k = 0 and k = π/d, where d = a + b is the period. The numerical value is 6.28x10^9 m^{-1} ?

(b) Clearly the lowest energy state is the one in the first band (n = 1) at k = 0 Fig. 1. From the plot for the n = 1 band in Fig. 1(b), we see that U(k=0) = 1.09 eV. The bandwidth is 0.53 eV. The effective mass at k = 0 is found to be m* ≈ 1.49 m_e by numerical differentiation at k = 0 using m* ≡ $\hbar^2(\partial^2 U/\partial k^2)^{-1}$ and the following formula from elementary calculus:

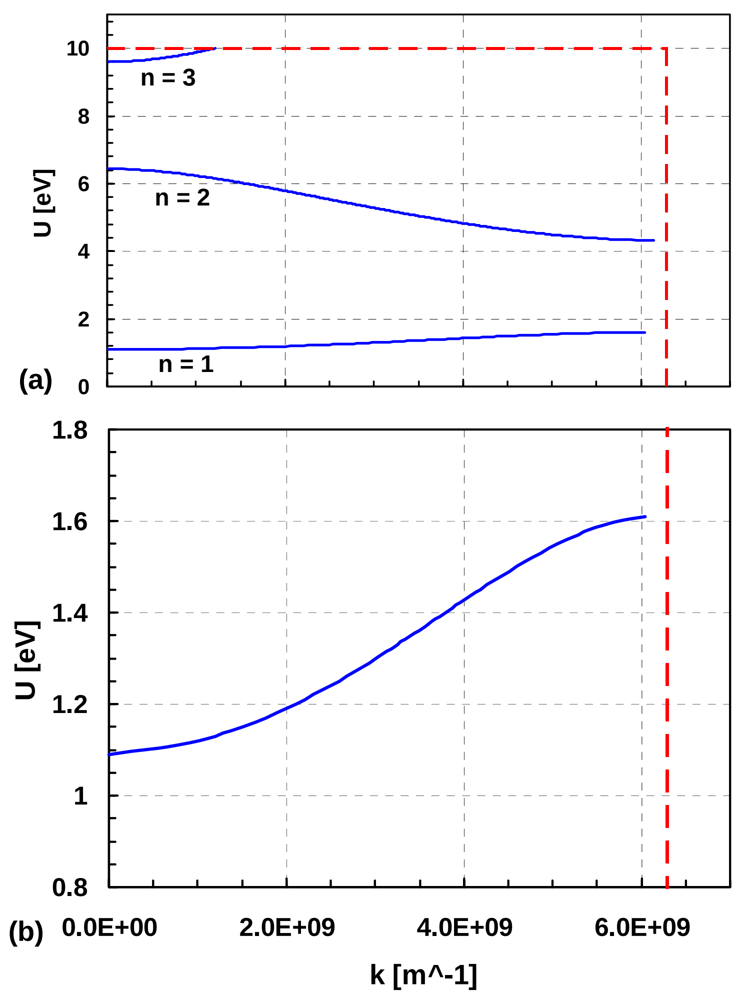

Fig. 1. (a) Band structure from Kronig-Penney model in Problem 1. (b) Expanded view of the n=1 band.

$$\left.\frac{d^2 f}{dx^2}\right|_{x=x_j} \approx \frac{\dfrac{f_{j+2}-f_j}{x_{j+2}-x_j} - \dfrac{f_j - f_{j-2}}{x_j - x_{j-2}}}{x_{j+1}-x_{j-1}}$$

At the highest energy in the first band [which occurs at k = π/(a+b)], the same formula leads to $m^* \approx -0.86\ m_e$ - a negative result because the U vs k curve is concave-down at this point !

(c) There are two complete bands between U = 0 and 10 eV, and one partial band (n=3) ? From Fig. 1(a), the bandwidth of the (complete) n = 2 band is 2.14 eV. This is ~ 4-times greater than the bandwidth of n =1, consistent with the fact that the higher bands place the electrons closer to the top of the barriers where they can tunnel through much easier. The greater tunneling leads to more "mixing" of the energy levels in adjacent wells and, therefore, to greater bandwidth.

(d) From Fig. 1(a), the energy gap between the top of the 1st band and the bottom of the 2nd band is ≈ 2.70 eV.

(e) From Fig. 1(a) the lowest and highest energies of the 2nd band occur at $k = k_N = \pi/d$ and k = 0, respectively. The effective masses at these energies are $m^* = 0.31\ m_e$, and $m^* = -0.16\ m_e$, respectively. From the numerical 1st derivative, and the formula $v_g = \hbar^{-1}(\partial U / \partial k)$ we find maximum values of $v_g = 1.98\text{x}10^5$ m/s (at $k = 3.72\text{x}10^9\ m^{-1}$) in the 1st band, and v_g = -$7.74\text{x}10^5$ m/s (maximum negative, at $k = 2.39\text{x}10^9\ m^{-1}$) in the 2nd band.

2.

(a) If V_B in problem 1 is raised 10 times to 100 eV with a and b kept the same, the bandwidth of the n =1 and n = 2 bands tends towards zero. This is consistent with the fact that such high barriers cause the wells to become isolated, each behaving like a "particle-in-a-box". The n = 1 and n = 2 levels behave as shown in Fig. 2 (a) with $U_1 \approx 1.95$ eV, and $U_2 \approx 7.79$ eV. The "particle-in-a-box" result is simply $U_n = (n\hbar\pi / 2mL)^2$. Substitution of L = 4 Ang yields U_1 = 2.35 eV, and U_2 = 9.40 eV.

(b) If V_B is kept at 10 eV but b is increased 10 times to 10 Ang, the energy levels should approach those of an isolated *quantum well*. The solution is similar qualitatively to 2(a) but U_1 goes to 1.36 eV, U_2 goes to 5.20 eV and U_3 goes to 9.88 eV. Referring to Saxon, Elementary Quantum Mechanics, we find that the quantum well problem involves solving an implicit equation that results in U_1 = 1.36, U_2 = 5.20 and U_3 = 9.93, in perfect agreement for U_1 and U_2.

(c) If V_B is kept at 10 eV and b at 1 Ang, but a is reduced 10 times to 0.4 Ang, the Kronig-Penney solution becomes the curve in 2(b). The lowest allowed energy level is 6.95 eV in the n = 1 band, and there are no other bands. The bandwidth of n =1 in Fig. 2(b) is 1.86 eV. Finally, if a is reduced all the way down to 0.004 Ang, we find a lowest allowed energy level right below the top of the barrier at 9.97 eV ? This is a reflection of the fundamental principle of quantum mechanics that all binding potentials, no matter how narrow or shallow, *have at least one bound state* ?

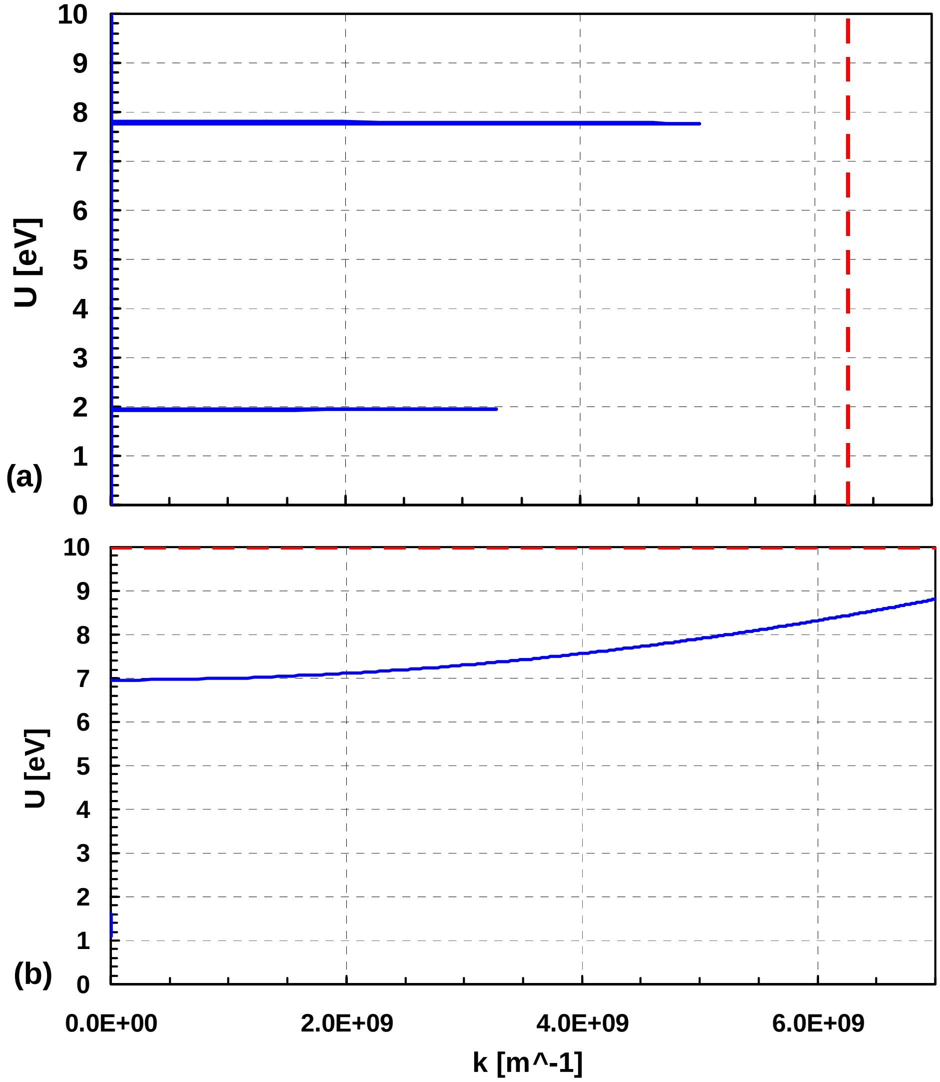

Fig. 2. (a) Kronig-Penney solution in the "particle-in-a-box" limit of V_B = 100 eV. (b) Kronig-Penney solution in the limit of a = 0.4 Ang.

3. Density of Levels

(a) If the Fermi surface is spherical and lies entirely within one zone (primitive cell) then

$$g_n(U) = g(U) = \oint_{S_U} \frac{dS}{4\pi^3} \frac{1}{\left|\vec{\nabla} U(\vec{k})\right|}$$ where n has one unique value

If $U(\vec{k}) = \hbar^2 |\vec{k}|^2 / 2m$, then $\vec{\nabla} U(\vec{k}) = \frac{\hbar^2}{m}(k_x \hat{x} + k_y \hat{y} + k_z \hat{z})$

So that $$\left|\vec{\nabla}U\left(\vec{k}\right)\right| = \frac{\hbar^2}{m}\sqrt{k_x^2 + k_y^2 + k_z^2}$$

We want to evaluate this gradient at the Fermi surface for which $\left|\vec{\nabla}U\left(\vec{k}\right)\right| = \frac{\hbar^2}{m}\sqrt{k_F^2} = \frac{\hbar^2}{m}k_F$

In k space, we have $dS = k^2 \sin\theta d\theta d\phi$ and $dS\big|_{K=K_F} = k_F^2 \sin\theta d\theta d\phi$

So that $g\left(U_F\right) = \int_0^{\pi}\int_0^{2\pi}\frac{mk_F^2 \sin\theta d\theta d\phi}{\hbar^2 4\pi^3 k_F}$

$$g\left(U_f\right) = \frac{m}{\hbar^2}k_F\frac{1}{4\pi^3}\int_0^{\pi}\sin\theta d\theta\int_0^{2\pi}d\phi = \frac{m}{\hbar^2}k_F\frac{1}{4\pi^3}(2)(2\pi) = \frac{mk_F}{\hbar^2\pi^2}$$

(b) For rhombohedral crystal and small k

$$U_n\left(\vec{k}\right) = U_0 + \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right)$$

We find g $_n$(U) the easy way. By definition $g_n\left(U\right) = \frac{dN_n\left(U\right)}{dU}$

where N(U) is the # allowed states inside constant.energy surface

In this case $U_n\left(\vec{k}\right) = \mathrm{U}$, with U held constant constant, defines an ellipsoid in k space:

$\frac{k_x^2}{a^2} + \frac{k_y^2}{b^2} + \frac{k_z^2}{c^2} = 1$, where $a = \sqrt{\frac{2m_x}{\hbar^2}\left(U - U_0\right)}$, $b = \sqrt{\frac{2m_y}{\hbar^2}\left(U - U_0\right)}$, and

$c = \sqrt{\frac{2m_z}{\hbar^2}\left(U - U_0\right)}$. From Geometry, the volume of any ellipsoid is 4/3 π a b c. So

$$N\left(U\right) = \left(\frac{L}{2\pi}\right)^3\frac{4}{3}\pi abc = \frac{V}{8\pi^3}\frac{4}{3}\pi\sqrt{m_x m_y m_z}\left(\frac{2\left(U - U_0\right)}{\hbar^2}\right)^{3/2}$$

$$g\left(U\right) = \frac{1}{V}\frac{dN\left(U\right)}{dU} = \frac{1}{4\pi^2}\left(\frac{2}{\hbar^2}\right)^{3/2}\sqrt{m_x m_y m_z}\left(U - U_0\right)^{1/2}$$

For N total electrons we have the definition

$$N_{tot} = N\left(U_F\right) = \frac{V}{8\pi^3}\frac{4}{3}\pi\sqrt{m_x m_y m_z}\left(\frac{2\left(U_F - U_0\right)}{\hbar^2}\right)^{3/2} \quad \text{or} \quad n = \frac{\sqrt{m_x m_y m_z}}{6\pi}\left(\frac{2\left(U_F - U_0\right)}{\hbar^2}\right)^{3/2}$$

So, $$g\left(U_F\right) = \frac{3}{2}\frac{\sqrt{m_x m_y m_z}}{6\pi}\left(\frac{2}{\hbar^2}\right)^{3/2}\frac{\left(U_F - U_0\right)^{3/2}}{U_F - U_0} = \frac{3}{2}\left(\frac{n}{U_F - U_0}\right)$$