

## 4261 HW 6

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### 1a

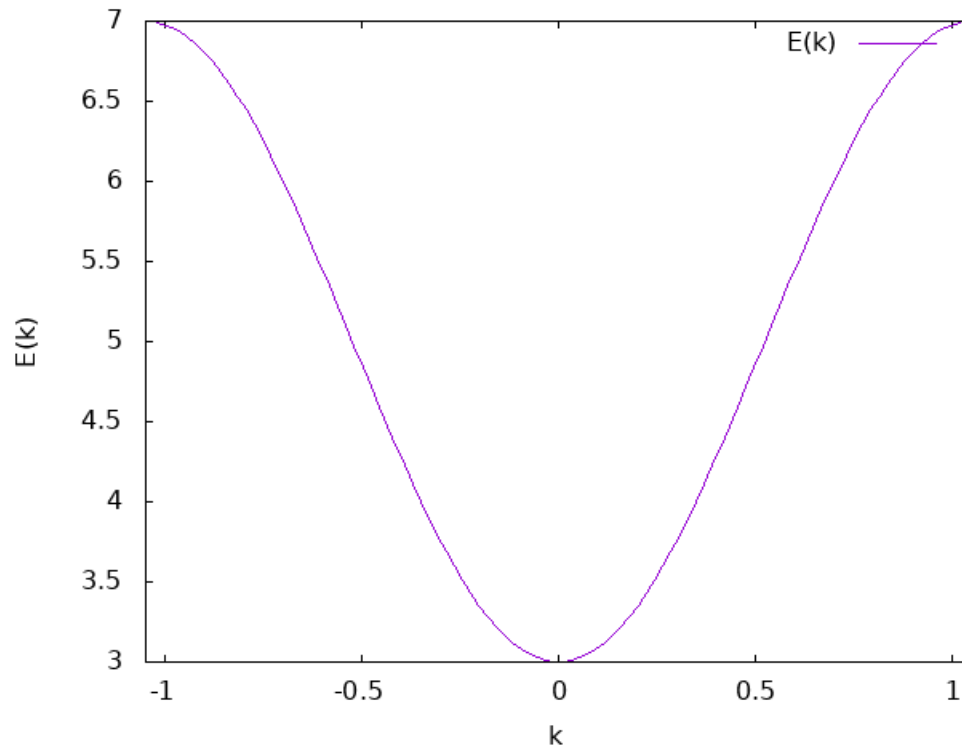
We have an effective Schrödinger equation, following the cited problem,

$$E\phi_n = \epsilon\phi_n - t(\phi_{n+1} + \phi_{n-1})$$

Applying the ansatz  $\phi_n = e^{ikna}/\sqrt{N}$ , where  $N$  is some normalization constant, we get

$$Ee^{ikna} = \epsilon e^{ikna} - te^{ik(n+1)a} - te^{ik(n-1)a} \Leftrightarrow E = \epsilon - t(e^{ika} + e^{-ika}) = \epsilon - 2t \cos(ka)$$

A plot with random values for the constants appears below.



If there are  $N$  sites, and we have periodic boundary conditions  $k = k + 2\pi/a$ , the total system  $k$  is quantized as  $k = 2\pi m/(Na)$ , i.e. there are  $N$  values of  $k$  corresponding bijectively to  $N$  eigenstates of the system. Approximating  $\cos x = 1 - x^2/2$  near zero,

$$E(k) \approx \epsilon - 2t + tk^2a^2$$

Comparing this to the free electron dispersion,

$$\frac{\hbar^2 k^2}{2m^*} = ta^2 k^2 \Leftrightarrow m^* = \frac{\hbar^2}{2ta^2}$$

The density of states is by definition

$$g(E) = \frac{dN}{dE} = \frac{dN}{dk} \frac{dk}{dE}$$

The first term is constant, since the number of states per unit  $k$  is constant; it is equal to  $Na/2\pi$ . The second is, from the dispersion relation,  $1/2ta \sin(ka)$ , so in total we have

$$g(E) = \frac{N}{4\pi t \sin(ka)}$$

Monovalent atoms imply half-filled bands, in which case the Fermi surface (the boundary between filled and unfilled states) occurs halfway through the first Brillouin zone at  $k = \pi/2a$  and  $k = -\pi/2a$ , which corresponds to a density of states  $N/4\pi t$ . Heat capacity in terms of the density of states is, following section 4.2,

$$C_V = \gamma k_B^2 g(E_F) TV = \gamma k_B^2 NTV/4\pi t$$

If the atoms are divalent, then the band is fully filled, which means there's no way the energy of the system can change as the temperature changes, i.e.  $C_V = 0$ . Similarly, the spin susceptibility is also zero, since there are no available states for the electrons to move into and align with the applied magnetic field, i.e.  $M(H) = 0$ .

## 1b

Our unit cell is now expanded to include two adjacent atoms, so we have a system of effective Schrödinger equations of the same type as above:

$$E\phi_{n,A} = \epsilon_A \phi_{n,A} - t(\phi_{n,B} + \phi_{n-1,B})$$

$$E\phi_{n,B} = \epsilon_B \phi_{n,B} - t(\phi_{n+1,A} + \phi_{n,A})$$

where  $\phi_{n,A}$  ( $\phi_{n,B}$ ) denotes the contribution to the  $n$ th site wave function from atom  $A$  ( $B$ ). Using ansätze

$$\phi_{n,A} = Ae^{ikna}$$

$$\phi_{n,B} = Be^{ikna}$$

we have

$$AEe^{ikna} = \epsilon_A Ae^{ikna} - tB(e^{ikna} + e^{ik(n-1)a}) \Leftrightarrow E = \epsilon_A - t\frac{B}{A}(1 + e^{-ika})$$

$$BEe^{ikna} = \epsilon_B Be^{ikna} - tA(e^{ik(n+1)a} + e^{ikna}) \Leftrightarrow E = \epsilon_B - t\frac{A}{B}(e^{ika} + 1)$$

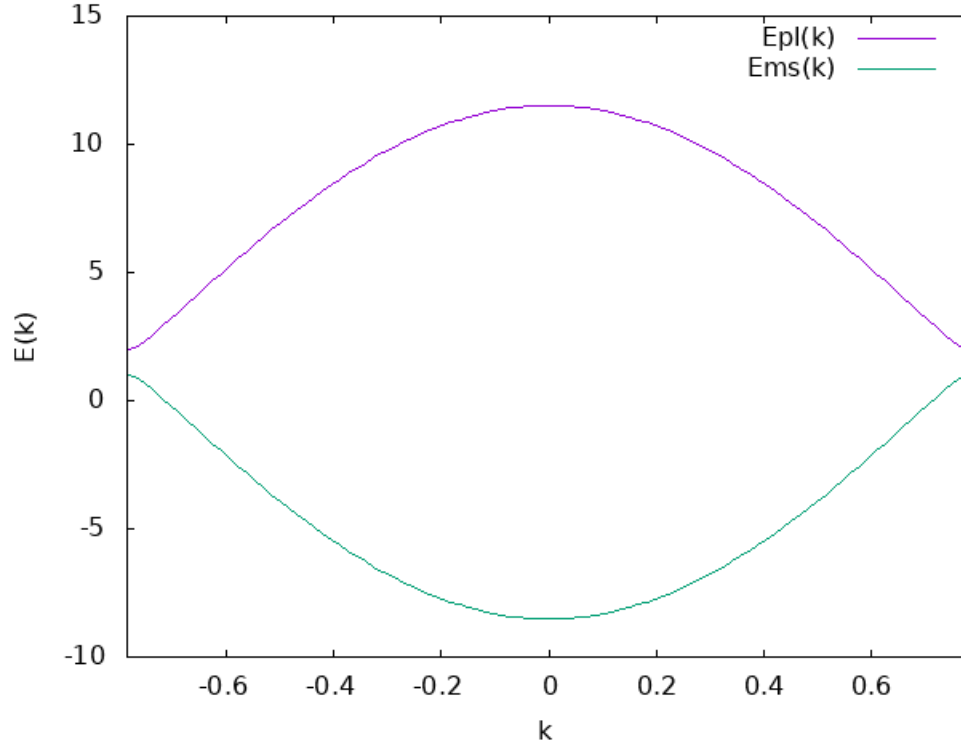
This system may be written in matrix form as

$$E \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \epsilon_A & -t(1 + e^{-ika}) \\ -t(1 + e^{ika}) & \epsilon_B \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}$$

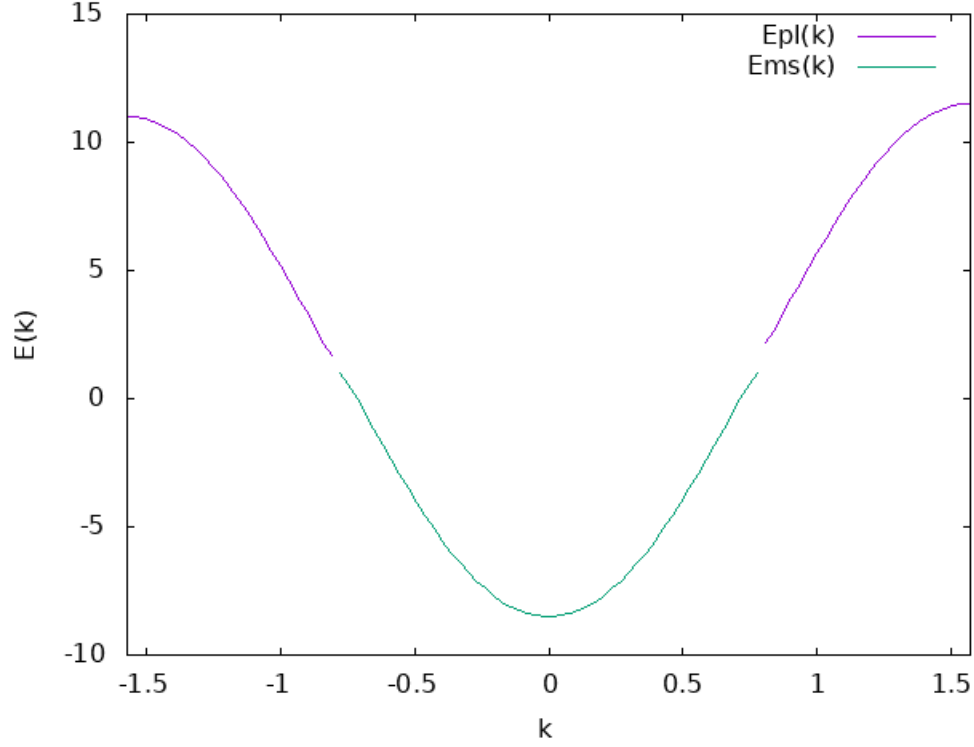
This is just the expression that  $E$  is an eigenvalue of the matrix; we may solve for its value by computing

$$\begin{aligned} 0 &= \begin{vmatrix} \epsilon_A - E & -t(1 + e^{-ika}) \\ -t(1 + e^{ika}) & \epsilon_B - E \end{vmatrix} \Leftrightarrow 0 = (\epsilon_A - E)(\epsilon_B - E) - t^2(1 + e^{-ika})(1 + e^{ika}) \\ &\Leftrightarrow 0 = \epsilon_A \epsilon_B - (\epsilon_A + \epsilon_B)E + E^2 - t^2(1 + e^{ika} + e^{-ika} + 1) \\ &\Leftrightarrow 0 = \epsilon_A \epsilon_B - t^2(2 + 2\cos(ka)) - (\epsilon_A + \epsilon_B)E + E^2 \\ &\Leftrightarrow E = \frac{\epsilon_A + \epsilon_B \pm \sqrt{(\epsilon_A + \epsilon_B)^2 - 4(\epsilon_A \epsilon_B - t^2[2 + 2\cos(ka)])}}{2} \end{aligned}$$

Plotting this for random values of the constants, we obtain in the reduced zone scheme



and in the extended zone scheme



In the limit as  $t \rightarrow 0$ ,  $E \rightarrow \epsilon_A + \epsilon_B$  for the positive branch and  $E \rightarrow 0$  for the negative branch. Near the minimum, we can expand near  $k = 0$   $\cos(ka) \approx 1 - k^2 a^2 / 2$  to get

$$E \approx (\epsilon_A + \epsilon_B)/2 - \frac{1}{2} \sqrt{(\epsilon_A - \epsilon_B)^2 + 4t^2[4 - k^2 a^2]}$$

Expanding again using  $\sqrt{a+x} \approx \sqrt{a} + \frac{x}{2\sqrt{a}}$ ,

$$E \approx (\epsilon_A + \epsilon_B)/2 - \frac{\sqrt{(\epsilon_A - \epsilon_B)^2 + 16t^2}}{2} + \frac{1}{2} \frac{4t^2 a^2 k^2}{2\sqrt{(\epsilon_A - \epsilon_B)^2 + 16t^2}} = \text{const} + \frac{t^2 a^2 k^2}{\sqrt{(\epsilon_A - \epsilon_B)^2 + 16t^2}}$$

Setting the quadratic part of this equation equal to the free electron dispersion,

$$\frac{\hbar^2 k^2}{2m^*} = \frac{t^2 a^2 k^2}{\sqrt{(\epsilon_A - \epsilon_B)^2 + 16t^2}} \Leftrightarrow m^* = \frac{\hbar^2 \sqrt{(\epsilon_A - \epsilon_B)^2 + 16t^2}}{2a^2 t^2}$$

If each atom is monovalent, there are two electrons per unit cell, filling the band and resulting in an insulator. If  $\epsilon_A = \epsilon_B$ , we recover the previous problem's monatomic tight-binding chain solution, and the material becomes a metal.

## 2

From the periodic boundary conditions, we have in any dimension

$$e^{ik(x+L)} = e^{ikx} \Leftrightarrow e^{ikL} = 1 \Leftrightarrow kL = 2\pi n \Leftrightarrow k = 2\pi n/L$$

i.e. each eigenstate corresponds to a volume  $(2\pi/L)^3$  in  $k$ -space; the first Brillouin zone ranges from  $-\pi/a$  to  $\pi/a$  in each direction and so has volume  $(2\pi/a)^3$ . Dividing by the  $k$ -volume per eigenstate, there are  $(L/a)^3$  eigenstates in the first Brillouin zone. But this is exactly the expression for the number of primitive unit cells in the sample, which is the desired result.

## 3

Since the potential is weak, the motion of the electrons is approximately free, and so a plane-wave state is a good approximation to the solution. Degenerate second-order perturbation theory implies that wave functions near the zone boundary may be decomposed

$$\Psi = A|k\rangle + B|k+G\rangle = Ae^{ikx} + Be^{i(k+G)x}$$

We have an effective Schrödinger equation

$$\begin{pmatrix} \epsilon_0(k) & V_G^* \\ V_G & \epsilon_0(k+G) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = E \begin{pmatrix} A \\ B \end{pmatrix}$$

which is an eigenvalue problem equivalent to

$$\begin{aligned} 0 &= \begin{vmatrix} \epsilon_0(k) - E & V_G^* \\ V_G & \epsilon_0(k+G) - E \end{vmatrix} = \epsilon_0(k)\epsilon_0(k+G) - [\epsilon_0(k) + \epsilon_0(k+G)]E + E^2 - |V_G|^2 \\ &\Leftrightarrow E = \frac{\epsilon_0(k) + \epsilon_0(k+G) \pm \sqrt{[\epsilon_0(k) + \epsilon_0(k+G)]^2 - 4(\epsilon_0(k)\epsilon_0(k+G) - |V_G|^2)}}{2} \\ &= \frac{1}{2} \left( \epsilon_0(k) + \epsilon_0(k+G) \pm \sqrt{[\epsilon_0(k) - \epsilon_0(k+G)]^2 + 4|V_G|^2} \right) \end{aligned}$$

Exactly on the Brillouin zone boundary,  $\epsilon_0(k) = \epsilon_0(k+G)$ , so

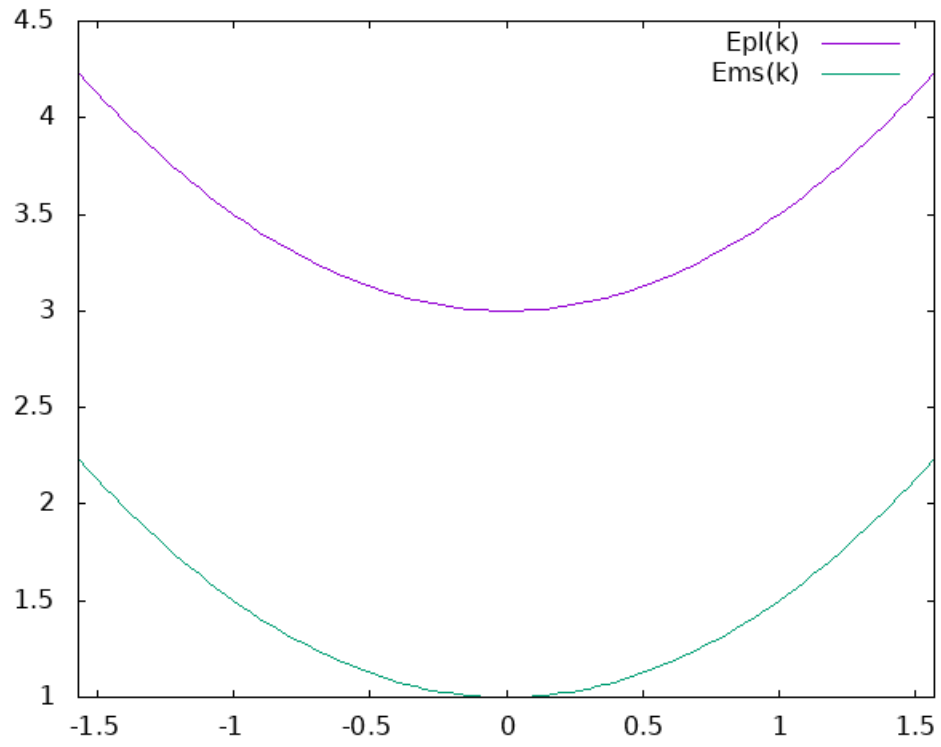
$$E = \epsilon \pm |V_G|$$

Applying the dispersion of the free electron,

$$E = \frac{\hbar^2 k^2}{2m} + V_0 \pm |V_G|$$

The states are separated by  $2|V_G|$  because the potential  $V_G$  causes the scattered state to interfere with the incident state, producing two states with different energies. With a rather exaggerated

band gap, the dispersion in the reduced zone scheme is sketched as



and in the extended zone scheme as

