固体物理第六次作业

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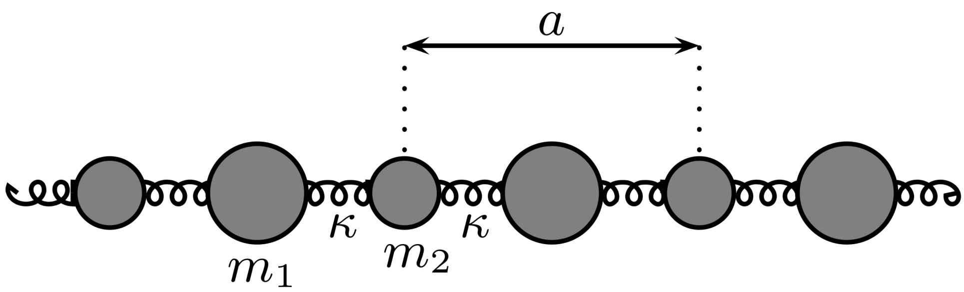
1 (10.1) **Normal modes of a One-Dimensional Diatomic Chain**

(a) What is the difference between an acoustic mode and an optical mode.

▷ Describe how particles move in each case.

(b) Derive the dispersion relation for the longitudinal oscillations if a one-dimensional diatomic mass-and-spring crystal where the unit cell is of length a and each unit cell contains one atom of mass m_1 and one atom of mass m_2 connected together by springs with spring constant κ, as shown in the figure (all springs are the same, and motion of particles is in one dimension only).



(c) Determine the frequencies of the acoustic and optical modes at $k = 0$ as well as the Brillouin zone boundary

▷ Describe the motion of the masses in each case (see margin note 4 of this chapter!)

▷ Determine the sound velocity and show that the group velocity is zero at the zone boundary

(d) Sketch the dispersion in both reduced and extended zone scheme.

▷ If there are N unit cells, how many different normal modes are there?

▷ How many *branches* of excitations are there ? I.e., in reduced zone scheme, how many modes are there at each k?

(e) What happens when $m_1 = m_2$?

(a) For the acoustic mode, all atoms in the unit cell move in-phase with each other at $k = 0$, whereas for optical modes they move out of phase with each other at $k = 0$. Generally, an acoustic mode is any mode that has linear dispersion as $k \to 0$.
即对于声学模式，元胞中所有的原子在 $k = 0$ 时以同相位移动，对于光学模式，不同的原子在 $k = 0$ 时以不同的相位移动。

(b) 考虑第 n 个质量为 m_1 的原子与第 n 个质量为 m_2 的原子，牛顿第二定律方程为:

$$m_1\delta\ddot{x}_n = \kappa(\delta y_n - \delta x_n) + \kappa(\delta y_{n-1} - \delta x_n),$$

$$m_2\delta\ddot{y}_n = \kappa(\delta x_{n+1} - \delta y_n) + \kappa(\delta x_n - \delta y_n).$$

通解为:

$$\delta x_n = A_x e^{i(\omega t - kna)},\ \delta y_n = A_y e^{i(\omega t - kna)}.$$

代入方程可得:

$$-m_1\omega^2 A_x = \kappa(1+e^{ika})A_y - 2\kappa A_x,$$
$$-m_2\omega^2 A_y = \kappa(1+e^{-ika})A_x - 2\kappa A_y.$$

关于 A_x,A_y 的方程组有非零解,则行列式为 0:

$$\begin{vmatrix} m_1\omega^2 - 2\kappa & \kappa(1+e^{ika}) \\ \kappa(1+e^{-ika}) & m_2\omega^2 - 2\kappa \end{vmatrix} = (m_1\omega^2 - 2\kappa)(m_2\omega^2 - 2\kappa) - 4\kappa^2\cos^2\frac{ka}{2} = 0.$$

可以解得色散关系为:

$$\omega^2 = \frac{\kappa}{m_1 m_2}(m_1 + m_2 \pm \sqrt{m_1^2 + m_2^2 + 2m_1 m_2\cos(ka)}).$$

(c) 当 $k=0$ 时,$\cos(ka)=1$,则频率为:

$$\omega_- = 0,\ \omega_+ = \sqrt{\frac{2\kappa(m_1+m_2)}{m_1 m_2}}.$$

其中 ω_- 为声学模式频率,ω_+ 为光学模式频率。

在布里渊区边界上时,有:$\cos(ka)=-1$,则频率为:

$$\omega_- = \sqrt{\frac{\kappa(m_1+m_2-|m_1-m_2|)}{m_1 m_2}},\ \omega_+ = \sqrt{\frac{\kappa(m_1+m_2+|m_1-m_2|)}{m_1 m_2}}.$$

其中 ω_- 为声学模式频率,ω_+ 为光学模式频率。

①当 $k=0$,$\omega=\omega_-=0$ 时,有 $A_x=A_y$,即两种质量不同的原子以相同的频率,相同的振幅运动。

②当 $k=0$,$\omega=\omega_+=\sqrt{\frac{2\kappa(m_1+m_2)}{m_1 m_2}}$ 时,有 $A_x=-\frac{m_2}{m_1}A_y$,即两种质量不同的原子以相反的方向振动,质量更重的原子振幅较小。

当 $\cos(ka)=-1$ 时,不妨令 $m_1<m_2$,则有:$\omega_-=\sqrt{\frac{2\kappa}{m_2}}, \omega_+=\sqrt{\frac{2\kappa}{m_1}}$.

③当 $\cos(ka)=-1$,$\omega=\omega_-=\sqrt{\frac{2\kappa}{m_2}}$ 时,有 $A_x=0$,最近邻两个质量为 m_2 的原子运动方向相反。

④当 $\cos(ka)=-1$,$\omega=\omega_+=\sqrt{\frac{2\kappa}{m_1}}$ 时,有 $A_y=0$,最近邻两个质量为 m_1 的原子运动方向相反。

声速为:

$$v_{sound} = \lim_{k\to 0}\frac{d\omega_-}{dk} = \sqrt{\frac{a^2\kappa}{2(m_1+m_2)}}.$$

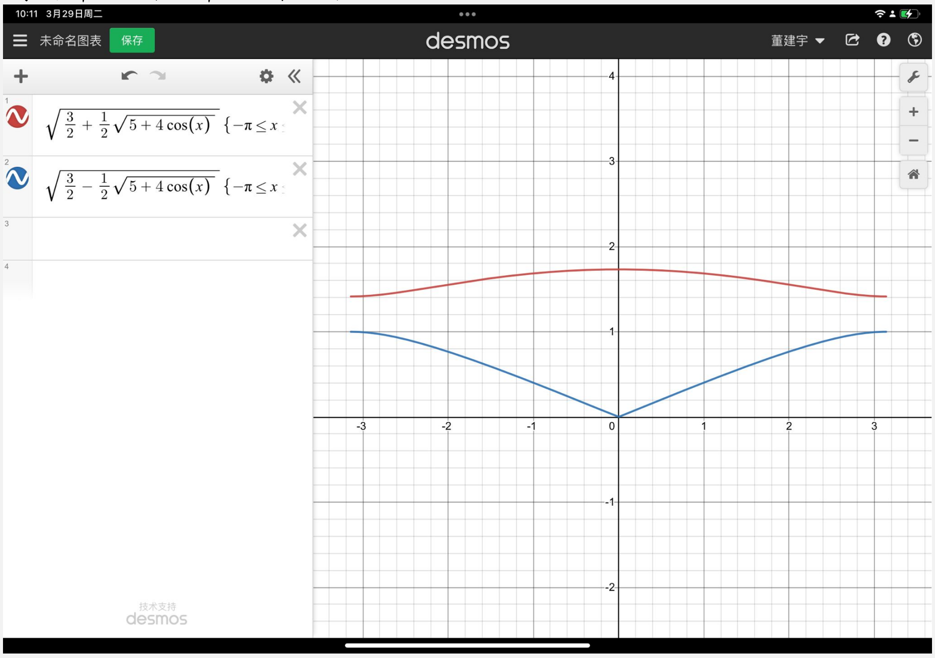
由于群速度包涵 $\sin(ka)$ 因子,则在布里渊区边界处有 $v_{group}=0$。

原子链密度可以写为:$\rho=\frac{m_1+m_2}{a}$,压缩系数满足:$\frac{1}{\beta}=-L\frac{\partial F}{\partial L}=2Na\frac{\kappa a/2}{2Na}=\frac{\kappa a}{2}$。则有:

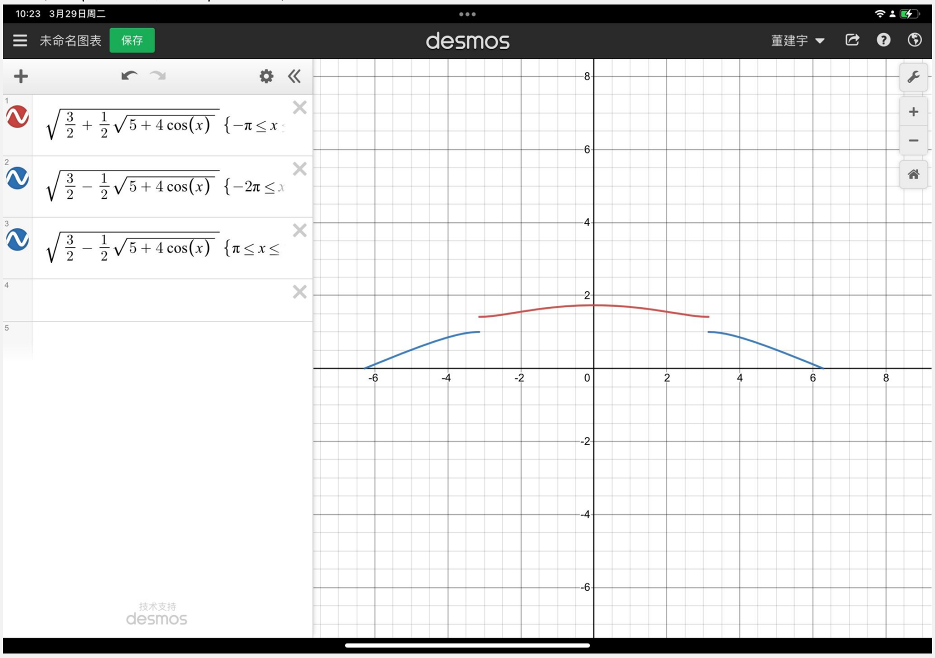
$$\rho\beta = \frac{2(m_1+m_2)}{\kappa a^2} = v_s^{-2}.$$

(d) 令 $m_2 = 2m_1 = 2m$, $x = ka$，则纵坐标为 $\omega/\sqrt{\kappa/m}$。

简约布里渊区中绘图如下:



扩展布里渊区中绘图如下:

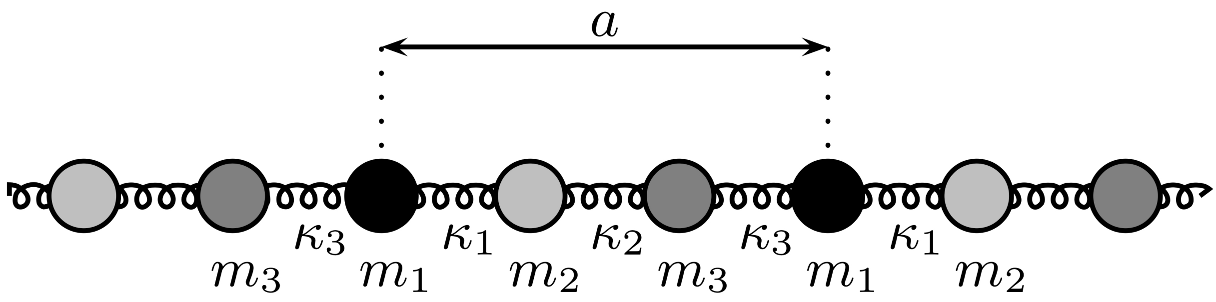


如果有 N 个元胞，则有 $2N$ 个原子，即有 $2N$ 个简正模式。在 reduced zone scheme 中，每一个 k 对应两个模式，即有 2 个分支。

(e) 当 $m_1 = m_2$ 时，系统变为相同原子的一位原子链，晶格常数变为 $a/2$。布里渊区的宽度变为 2 倍。同时，布里渊区边界处的间隙消失，两个分支变为单个分支。

2 (10.5) Triatomic Chain

Consider a mass-and-spring model with three different masses and three different springs per unit cell as shown in this diagram.



As usual, assume that the masses move only in one dimension.

(a) At $k = 0$ how many optical modes are there? Calculate the energies of these modes. Hind: you will get a cubic equation. However, you already know one of the roots since it is the energy of the acoustic mode at $k = 0$.

(b) If all the masses are the same and $\kappa_1 = \kappa_2$ determine the frequencies of all three modes at the zone boundary $k = \pi/a$. You will have a cubic equation, but you should be able to guess one root which corresponds to a particularly simple normal mode.

(c) If all three spring constants are the same, and $m_1 = m_2$ determine the frequencies of all three modes at the zone boundary $k = \pi/a$. Again you should be able to guess one of the roots.

(a) 当 $k = 0$ 时，有两个光学模式。考虑第 n 个元胞，由牛顿第二定律得:

$$\begin{aligned} m_1\delta\ddot{x}_n &= \kappa_1(\delta y_n - \delta x_n) + \kappa_3(\delta z_{n-1} - \delta x_n), \\ m_2\delta\ddot{y}_n &= \kappa_2(\delta z_n - \delta y_n) + \kappa_1(\delta x_n - \delta y_n), \\ m_3\delta\ddot{z}_n &= \kappa_3(\delta x_{n+1} - \delta z_n) + \kappa_2(\delta y_n - \delta z_n). \end{aligned}$$

通解为:

$$\delta x_n = A_x e^{i(\omega t - kna)},\ \delta y_n = A_y e^{i(\omega t - kna)},\ \delta z_n = A_z e^{i(\omega t - kna)}.$$

代入方程可得:

$$\begin{aligned} &(\kappa_1 + \kappa_3 - m_1\omega^2)A_x - \kappa_1 A_y - \kappa_3 e^{ika} A_z = 0, \\ &-\kappa_1 A_x + (\kappa_1 + \kappa_2 - m_2\omega^2)A_y - \kappa_2 A_z = 0, \\ &-\kappa_3 e^{-ika} A_x - \kappa_2 A_y + (\kappa_2 + \kappa_3 - m_3\omega^2)A_z = 0. \end{aligned}$$

方程组存在非零解，则有:

$$\begin{vmatrix} \kappa_1 + \kappa_3 - m_1\omega^2 & -\kappa_1 & -\kappa_3 e^{ika} \\ -\kappa_1 & \kappa_1 + \kappa_2 - m_2\omega^2 & -\kappa_2 \\ -\kappa_3 e^{-ika} & -\kappa_2 & \kappa_2 + \kappa_3 - m_3\omega^2 \end{vmatrix} = 0.$$

即

$$-m_1m_2m_3\omega^6+(m_1m_2(\kappa_2+\kappa_3)+m_1m_3(\kappa_1+\kappa_2)+m_2m_3(\kappa_1+\kappa_3))\omega^4$$
$$-(m_1+m_2+m_3)(\kappa_1\kappa_2+\kappa_1\kappa_3+\kappa_2\kappa_3)\omega^2+2\kappa_1\kappa_2\kappa_3(1-\cos(ka))=0.$$

当 $k=0$ 时，有:

$$-\omega^6+\left(\frac{\kappa_3+\kappa_1}{m_1}+\frac{\kappa_1+\kappa_2}{m_2}+\frac{\kappa_2+\kappa_3}{m_3}\right)\omega^4-\frac{(m_1+m_2+m_3)(\kappa_1\kappa_2+\kappa_1\kappa_3+\kappa_2\kappa_3)}{m_1m_2m_3}\omega^2=0.$$

易知对于声学模式有:

$$\omega_{acoustic}=0$$

则可以解得两个光学模式频率为:

$$\omega_\pm=\sqrt{\frac{1}{2}(\alpha\pm\sqrt{\alpha^2-4\beta})}.$$

其中

$$\alpha=\frac{\kappa_3+\kappa_1}{m_1}+\frac{\kappa_1+\kappa_2}{m_2}+\frac{\kappa_2+\kappa_3}{m_3},$$
$$\beta=\frac{4(m_1+m_2+m_3)(\kappa_1\kappa_2+\kappa_1\kappa_3+\kappa_2\kappa_3)}{m_1m_2m_3}.$$

则能量为:

$$E_\pm=\hbar\omega_\pm.$$

(b) 如果质量全一样，且 $\kappa_1=\kappa_2$，频率满足的方程为:

$$m^3\omega^6-m^2(4\kappa_1+2\kappa_3)\omega^4+3m(\kappa_1^2+2\kappa_1\kappa_3)\omega^2-4\kappa_1^2\kappa_3=0.$$

注意到一种振动模式为与两个劲度系数 κ_1 连接的质量为 m_2 的原子保持不动，与劲度系数为 κ_3 连接的两个原子作为一个整体振动，且相邻两个元胞中与劲度系数 κ_3 连接的原子运动方向相反。则该振动频率为:

$$\omega_1^2=\frac{\kappa_1}{m}.$$

则有剩余两种频率满足:

$$\omega^4-\frac{3\kappa_1+2\kappa_3}{m}\omega^2+\frac{4\kappa_1\kappa_3}{m^2}=0.$$

则有:

$$\omega_{b,\pm}^2=\frac{3\kappa_1+2\kappa_2\pm\sqrt{9\kappa_1^2-4\kappa_1\kappa_3+4\kappa_3^2}}{2m}.$$

(c) 如果劲度系数全一样，且 $m_1=m_2$，频率满足的方程为:

$$m_1^2m_3\omega^6-\kappa(4m_1m_3+2m_1^2)\omega^4+3\kappa^2(2m_1+m_3)\omega^2-4\kappa^2=0.$$

注意到一种振动模式为质量为 m_3 的原子不动，质量相等的两个相邻原子作为一个整体，且相邻两个元胞中质量为 m_1 的原子振动方向相反。则该振动频率为:

$$\omega_1^2 = \frac{\kappa}{m_1}.$$

则剩余两种频率满足:

$$\omega^4 - \frac{\kappa(2m_1+3m_3)}{m_1 m_3}\omega^2 + \frac{4\kappa^2}{m_1 m_3} = 0.$$

则有:

$$\omega_{c,\pm}^2 = \frac{\kappa(2m_1+3m_3 \pm \sqrt{4m_1^2 - 4m_1 m_3 + 9m_3^2})}{2m_1 m_3}.$$

3 (11.2) Diatomic Tight Binding Chain

We now generalize the calculation of the previous exercise to a one-dimensional diatomic solid which might look as follows:

$$-A-B-A-B-A-B-$$

Suppose that the onsite energy of type A is different from the onsite energy of type B. I.e., $\langle n|\, H\, |n\rangle$ is ϵ_A for n being on a site of type A and is ϵ_B for n being on a site of type B. (All hopping matrix elements $-t$ are still identical to each other.)

▷ Calculate the new dispersion relation. (This is extremely similar to Exercise 10.1. If you are stuck, try studying that exercise again.)

▷ Sketch this dispersion relation in both the reduced and extended zone schemes.

▷ What happens if $\epsilon_A = \epsilon_B$?

▷ What happens in the "atomic" limit when t become very small.

▷ What is the effective mass of an electron near the bottom of the lower band?

▷ If each atom (of either type) is monovalent, is the system a metal or an insulator?

▷ Given the results of this exercise, explain why LiF (which has very ionic bonds) is an extremely good insulator.

▷ 记 $|n_A\rangle$ 表示第 n 个元胞中原子 A 的态，$|n_B\rangle$ 表示第 n 个元胞中原子 B 的态，则系统态矢量为:

$$|\Psi\rangle = \sum_n (a_n\,|n_A\rangle + b_n\,|n_B\rangle).$$

Hamiltonian 为

$$H = \begin{pmatrix} \epsilon_A & -t & 0 & 0 & \cdots & 0 & -t \\ -t & \epsilon_B & -t & 0 & \cdots & 0 & 0 \\ 0 & -t & \epsilon_A & -t & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \epsilon_A & -t \\ -t & 0 & 0 & 0 & \cdots & -t & \epsilon_B \end{pmatrix}.$$

则有:

$$Ea_n = \epsilon_A a_n - t(b_n + b_{n-1})$$
$$Eb_n = \epsilon_B b_n - t(a_n + a_{n+1})$$

其中

$$a_n = Ae^{ikna},\ b_n = Be^{ikna}.$$

代入方程可得:

$$(\epsilon_A - E)A + t(1 + e^{-ika})B = 0$$
$$t(1 + e^{ika})A + (\epsilon_B - E)B = 0$$

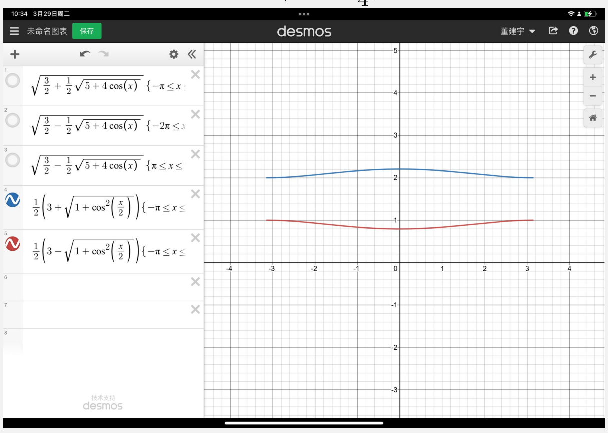
方程组存在非零解，则有:

$$\begin{vmatrix} \epsilon_A - E & t(1+e^{-ika}) \\ t(1+e^{ika}) & \epsilon_B - E \end{vmatrix} = E^2 - (\epsilon_A + \epsilon_B)E + \epsilon_A\epsilon_B - 4t^2\cos^2(ka/2) = 0.$$

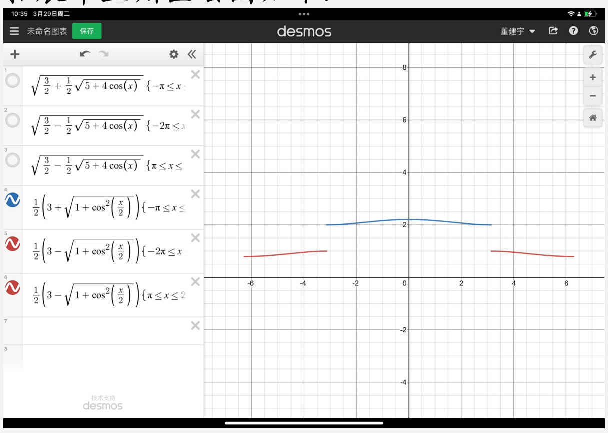
可以解得:

$$E_\pm = \frac{1}{2}(\epsilon_A + \epsilon_B \pm \sqrt{(\epsilon_A - \epsilon_B)^2 + 16t^2\cos^2(ka/2)}).$$

▷ 选取 $\epsilon_A = 2\epsilon_B = 2$, $t = \frac{1}{4}$, 简约布里渊区绘图如下:



拓展布里渊区绘图如下:



▷ 当 $\epsilon_A = \epsilon_B = \epsilon$ 时，系统变为单原子链，有:

$$E_{\pm} = \epsilon \pm 2|t\cos(ka/2)|.$$

▷ 当 t 为无穷小量时，E_+ 与 E_- 将变得非常接近。

▷ 计算 $\frac{dE_-}{dk}$ 得:

$$\frac{dE_-}{dk} = \frac{2at^2\sin(ka)}{\sqrt{(\epsilon_A-\epsilon_B)^2+16t^2\cos^2(ka/2)}}.$$

在 $k \to 0$ 的极限下，有:

$$\frac{dE_-}{dk} = \frac{2ka^2t^2}{\sqrt{(\epsilon_A-\epsilon_B)^2+16t^2}}.$$

即有:

$$E_- = Constant + \frac{dE_-}{dk}k = Constant + \frac{2k^2a^2t^2}{\sqrt{(\epsilon_A-\epsilon_B)^2+16t^2}}.$$

则有:

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

即有效质量为:

$$m^* = \frac{\hbar^2\sqrt{(\epsilon_A-\epsilon_B)^2+16t^2}}{4a^2t^2.}$$

▷ 如果每个原子都有一个价电子，那么每个元胞中恰好有两个价电子，恰好能填满能量较低的能级，如果 $\epsilon_A = \epsilon_B$，则只要加电场就可以产生电流，即为导体；如果 ϵ_A 与 ϵ_B 相差不大，则可以消耗一部分能量用于激发，余下能量可以产生电流，即为半导体；如果 ϵ_A 与 ϵ_B 相差很大，则电子很难跃迁到高能级，即为绝缘体。

▷ 对于 LiF，Li 电负性很小，而 F 颠覆性很大，则有:

$$\epsilon_F >> \epsilon_{Li}.$$

即 LiF 为绝缘体。

4 **(11.4)**

(a) Consider an atom with two orbitals, A and B having eigenenergies ϵ^A_{atomic} and ϵ^B_{atomic}. Now suppose we make a one-dimensional chain of such atoms and let us assume that these orbitals remain orthogonal. We imagine hopping amplitudes t_{AA} which allows an electron on orbital A of a given atom to hop to orbital A on the neighboring atom. Similarly we imagine a hopping amplitude t_{BB} that allows an electron on orbital B of a given atom to hop to orbital B on the neighboring atom. (We assume that V_0, the energy shift of the atomic orbital due to neighboring atoms, is zero).

▷ Calculate and sketch the dispersion of the two resulting bands.

▷ If the atom is diatomic, derive a condition on the quantities $\epsilon^A_{atomic} - \epsilon^B_{atomic}$, as well as t_{AA} and t_{BB} which determines whether the system is a metal or an insulator.

(b) Now suppose that there is in addition a hopping term t_{AB} which allows an electron in one atom in orbital A to hop to orbital B on the neighboring atom (and vice verse). What is the dispersion relation now?

(a) 由于态矢量仍满足正交关系，可分别对 A,B 列方程如下:

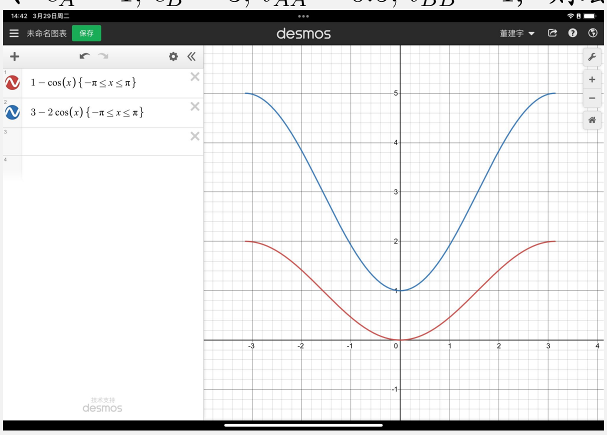
$$\begin{pmatrix} \epsilon_A & -t_{AA} & 0 & \cdots & -t_{AA} \\ -t_{AA} & \epsilon_A & -t_{AA} & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ -t_{AA} & 0 & 0 & \cdots & \epsilon_A \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} = E_A \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}$$

$$\begin{pmatrix} \epsilon_B & -t_{BB} & 0 & \cdots & -t_{BB} \\ -t_{BB} & \epsilon_B & -t_{BB} & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ -t_{BB} & 0 & 0 & \cdots & \epsilon_B \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix} = E_B \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$$

令 $a_n = Ae^{ikna}$, $b_n = Be^{ikna}$，可以解得:

$$E_A = \epsilon_A - 2t_{AA}\cos(ka),\ E_B = \epsilon_B - 2t_{BB}\cos(ka).$$

令 $\epsilon_A = 1$, $\epsilon_B = 3$, $t_{AA} = 0.5$, $t_{BB} = 1$，则绘图如下:



其中红线为 E_A，蓝线为 E_B。

如果该体系为绝缘体，则 E_A 与 E_B 不存在交叠部分，即:

$$\epsilon_A - 2|t_{AA}| > \epsilon_B + 2|t_{BB}|$$

或者

$$\epsilon_A + 2|t_{AA}| < \epsilon_B - 2|t_{BB}|$$

否则，如果满足

$$|\epsilon_A - \epsilon_B| > 2(|t_{AA}| + |t_{BB}|)$$

则体系为导体。

(b) 由题意可知，考虑第 n 个元胞中 A、B 原子，有:

$$\begin{aligned} &- t_{AA}^* a_{n-1} - t_{AB}^* b_{n-1} + \epsilon_A a_n - t_{AA} a_{n+1} - t_{AB} b_{n+1} = E a_n, \\ &- t_{AB}^* a_{n-1} - t_{BB}^* b_{n-1} + \epsilon_B b_n - t_{AB} a_{n+1} - t_{BB} b_{n+1} = E b_n. \end{aligned}$$

假设有:

$$a_n = A e^{ikna},\ b_n = B e^{ikna},$$

令

$$\begin{aligned} R_A &= t_{AA}^* e^{-ika} + t_{AA} e^{ika} = 2\mathbf{Re}(t_{AA} e^{ika}) \\ R_B &= t_{BB}^* e^{-ika} + t_{BB} e^{ika} = 2\mathbf{Re}(t_{BB} e^{ika}) \\ R_{AB} &= t_{AB}^* e^{-ika} + t_{AB} e^{ika} = 2\mathbf{Re}(t_{AB} e^{ika}) \end{aligned}$$

则有:

$$\begin{aligned} (E - \epsilon_A + T_{AA})A + T_{AB}B = 0 \\ T_{AB}A + (E - \epsilon_B + T_{BB})B = 0 \end{aligned}$$

方程组存在非零解，有:

$$\begin{vmatrix} E - \epsilon_A + T_{AA} & T_{AB} \\ T_{AB} & E - \epsilon_B + T_{BB} \end{vmatrix} = (E - \epsilon_A + T_{AA})(E - \epsilon_B + T_{BB}) - T_{AB}^2 = 0$$

可以解得:

$$E_\pm = \frac{1}{2}(\epsilon_A + \epsilon_B - T_{AA} - T_{BB} \pm \sqrt{(\epsilon_A - T_{AA} - \epsilon_B + T_{BB})^2 + 4T_{AB}^2}).$$

5 **(11.5)** Electronic Impurity State

Consider the one-dimensional tight binding Hamiltonian given in Eq. 11.4. Now consider the situation where one of the atoms in the chain (atom $n = 0$) is an impurity such that it has an atomic orbital energy which differs by Δ from all the other atomic orbital energies. In this case the Hamiltonian becomes

$$H_{n,m} = \epsilon_0 \delta_{n,m} - t(\delta_{n+1,m} + \delta_{n-1,m}) + \Delta \delta_{n,m} \delta_{n,0}.$$

(a) Using an ansatz

$$\phi_n = Ae^{-qa|n|}$$

with q real, and a the lattice constant, show that there is a localized eigenstate for any negative Δ, and find the eigenstate energy. This exercise is very similar to Exercise 9.6.

(b) Consider instead a continuum one-dimensional Hamiltonian with a delta-function potential

$$H = -\frac{\hbar^2}{2m^*}\partial_x^2 + (a\Delta)\delta(x).$$

Similarly show that there is a localized eigenstate for any negative Δ and find its energy. Compare your result to that of part (a).

(a) 当 $n \neq 0$ 时，有:

$$E\phi_n = \epsilon_0\phi_n - t(\phi_{n-1} + \phi_{n+1}).$$

带入

$$\phi_n = Ae^{-qa|n|}$$

可得:

$$E = \epsilon_0 - t(e^{-qa} + e^{qa}).$$

当 $n = 0$ 时，有:

$$E\phi_0 = (\epsilon_0 + \Delta)\phi_0 - t(\phi_{-1} + \phi_1)$$

则有:

$$E = \epsilon_0 + \Delta - 2te^{-qa}.$$

则可以解得:

$$\Delta = -2t\sinh(qa).$$

则对于每一个负的 Δ，都有

$$qa = \sinh^{-1}(-\Delta/(2t)).$$

即存在一个态，此态的能量为:

$$E_0 = \epsilon_0 - 2t\sqrt{1 + \frac{\Delta^2}{4t^2}}.$$

(b) 假设仍有:

$$\psi(x) = Ae^{-px}$$

则有:

$$-\frac{\hbar^2}{2m^*}\partial_x^2\psi(x) = -\frac{\hbar^2p^2}{2m^*}\psi(x)$$

即

$$E = -\frac{\hbar^2p^2}{2m^*}.$$

由于势能函数为 δ 函数，满足连续性条件有:

$$\frac{\partial}{\partial x}\psi(0+) - \frac{\partial}{\partial x}\psi(0-) = -2p = \frac{2m^*a\Delta}{\hbar^2}.$$

利用有效质量的表达式:

$$m^* = \frac{\hbar^2}{2a^2 t}$$

可得:

$$E_b = -\frac{\Delta^2}{4t}.$$

注意到，(a) 中当 $\Delta \to 0$ 时，有:

$$E_a = \epsilon_0 - 2t\sqrt{1+\frac{\Delta^2}{4t^2}} \approx \epsilon_0 - 2t(1+\Delta^2/(8t^2)) = \epsilon_0 - 2t - \frac{\Delta^2}{4t}.$$

选取合适的基态能量满足: $\epsilon_0 - 2t = 0$，则有:

$$E_a = -\frac{\Delta^2}{4t} = E_b.$$