Fundamentals of Nanoelectronics

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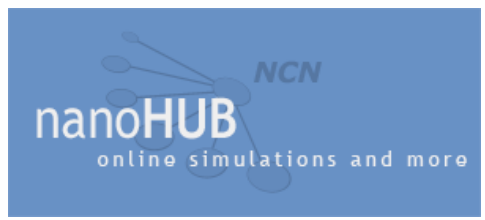
Lecture 17: Bandstructure 2

Ref. Chapter 5.1

Network for Computational Nanotechnology

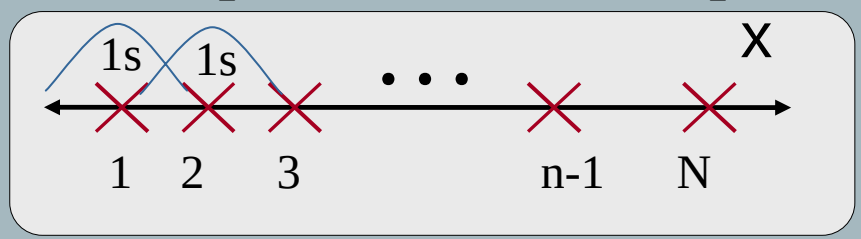


Review

00:03

• The principle of bandstructure helps us to find the eigenvalues of a periodic matrix. This is important for us because solids that we are interested in have periodic structures. Consider the example of last day:

$$E\begin{bmatrix}\phi_1\\ \phi_2\\ \vdots\\ \phi_N\end{bmatrix}=\begin{bmatrix}\varepsilon & t & 0 & 0 & 0 & 0\\ t & \varepsilon & t & 0 & 0 & 0\\ 0 & t & \varepsilon & t & & \\ 0 & & \ddots & \ddots & \ddots & \\ 0 & & & & & \\ 0 & & & & & \end{bmatrix}\begin{bmatrix}\phi_1\\ \phi_2\\ \vdots\\ \phi_N\end{bmatrix}$$



• Regardless of the details of the problem, the matrix that we write will be periodic.

• Notice that as long as every row looks the same, the principle of bandstructure applies regardless of how each row looks. The nth row is:

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

• This solution satisfies the Schrödinger equation if the E-k relationship below is met.

$$\phi_n = e^{inka}\phi_0 \quad (2)$$

$$E = te^{-ika} + \varepsilon + te^{ika}$$

• 2 in 1 →

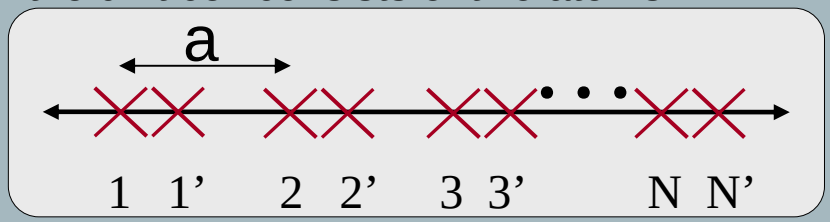
$$\boxed{E = \varepsilon + 2t\cos ka}$$

• As long as the above E-k relationship is met, the solution we chose will satisfy the Schrödinger equation.

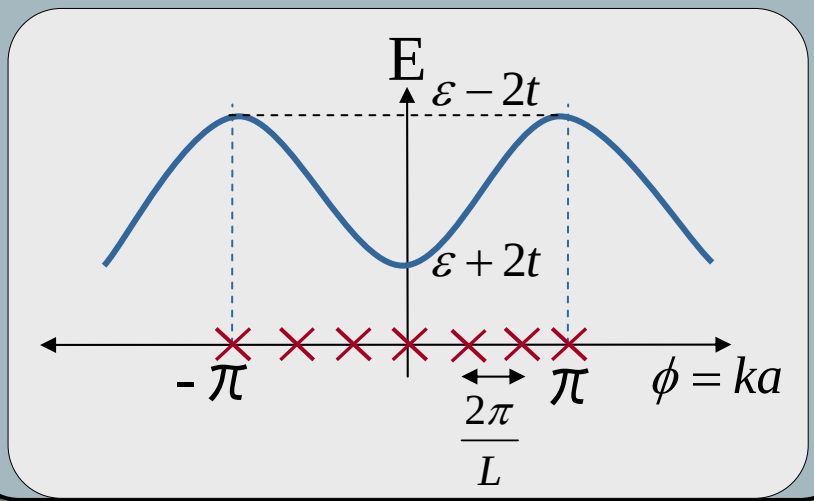
Review

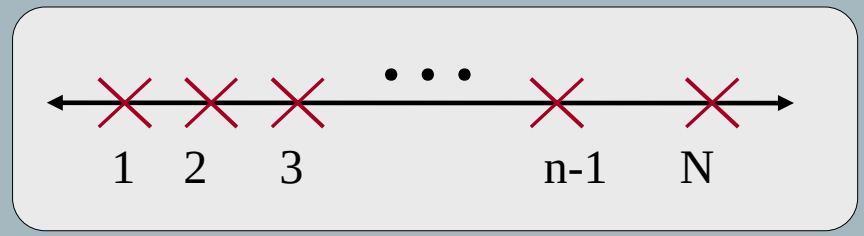
05:30

- What we'll learn today is a generalization of bandstructure method to a solid where the unit cell consists of two atoms.



- The above dimerized solid is semiconductor whereas for the old case shown below the solid is metallic. To know why consider:





- For the above solid the eigenvalues are given by:

$$E = \varepsilon + 2t\cos ka$$

Periodic Boundary Condition

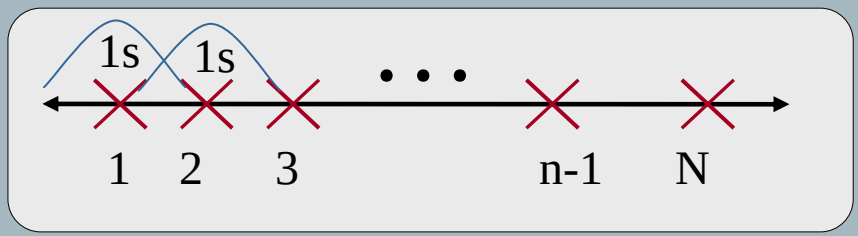
$$\phi_{n+N} = \phi_n \Rightarrow e^{iNka} = 1 \Rightarrow Nka = 2\pi\upsilon$$

$$k = \frac{2\pi}{Na}\upsilon \qquad \nu : \text{integer}$$

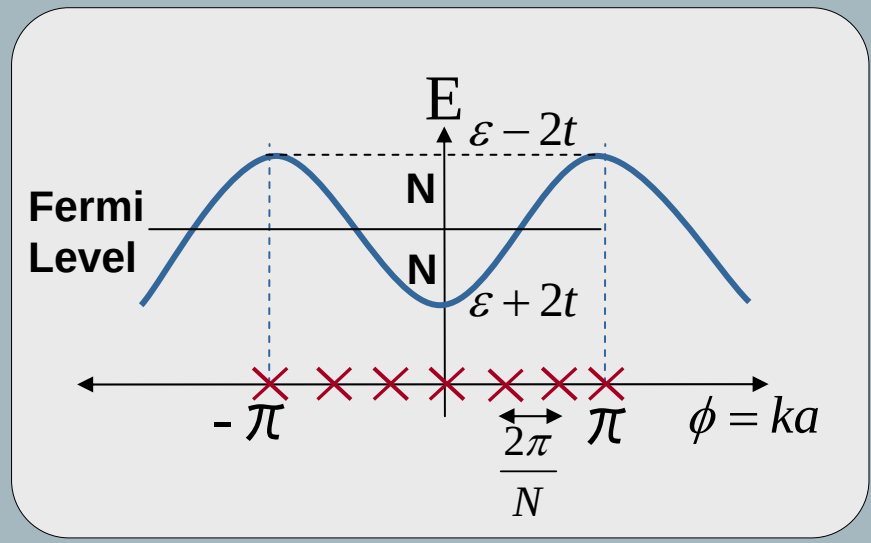
Array of H Atoms - Metallic Conduction

13:58

• How can we tell if a solid is metallic or not? Well, we'd have to investigate the energy levels around the Fermi level. If there are lots of levels around the Fermi energy, then the solid conducts well, otherwise it will conduct poorly.
• Where would the chemical potential be for this simple structure?



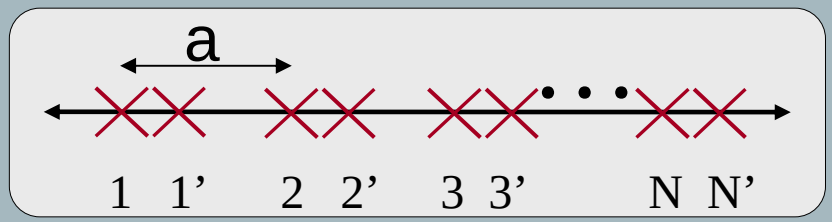
• By definition, the Fermi energy is where, above it all levels are empty and below it all levels are full (at absolute 0).



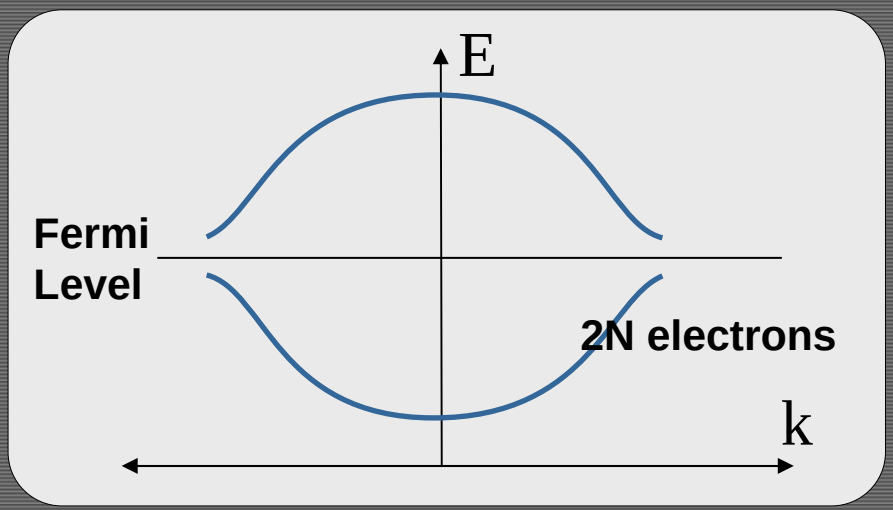
• Since there are lots of levels around Fermi level, in this case the solid will conduct well.

Dimerized Solid - Semi-Conduction

• In the case of dimerized solid, there are two atoms per unit cell. So N unit cells will consist of 2N Hydrogen atoms.



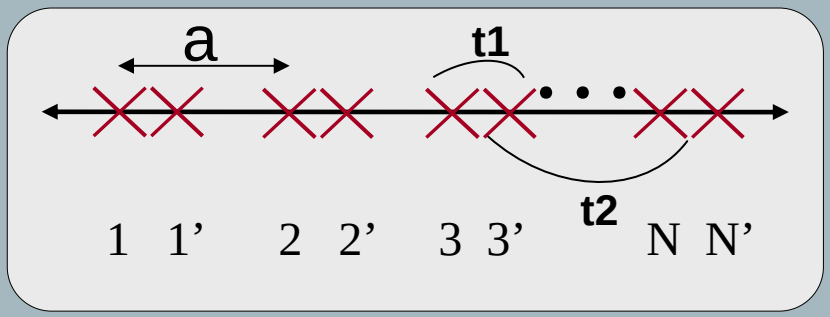
• What we will see shortly is that the energy levels of a dimerized solid look like:



• In this case, the Fermi energy lies between the two bands of allowed energy levels. Since there are not levels around the Fermi energy, the solid will not conduct.

Dimerized Solid - Schrödinger Equation

• Next we want to find the dispersion relation for the dimerized solid:



$$E\begin{Bmatrix}\phi_1\\ \phi_1'\\ \vdots\\ \phi_N\\ \phi_N'\end{Bmatrix}=\begin{bmatrix}\varepsilon & t_1 & & & \\ t_1 & \varepsilon & t_2 & & \\ & t_2 & \varepsilon & \ddots & \\ & & \ddots & \ddots & \end{bmatrix}\begin{Bmatrix}\phi_1\\ \phi_1'\\ \vdots\\ \phi_N\\ \phi_N'\end{Bmatrix}$$

• We see that now every other row in the matrix is the same not every row. To use the principle of bandstructure every row must look the same. To get this configuration we can do this:

$$E\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_N\end{Bmatrix}=\begin{bmatrix}\alpha & \beta & & \\ \beta^+ & \alpha & \beta & \\ & \beta^+ & \alpha & \ddots \\ & & \ddots & \ddots \end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_N\end{Bmatrix}$$

• What has happened is that by combining two elements of the wavevector into a new one we get:

$$\psi_1=\begin{Bmatrix}\phi_1\\ \phi_1'\end{Bmatrix}$$

• Similarly:

$$\alpha\equiv\begin{bmatrix}\varepsilon & t_1\\ t_1 & \varepsilon\end{bmatrix}\qquad\beta\equiv\begin{bmatrix}0 & 0\\ t_2 & 0\end{bmatrix}$$

Dimerized Solid: Dispersion Relation

27:08

• We can now use the principle of bandstructre to write the solution to the set of equations:

$$E\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \\ \psi_N\end{Bmatrix}=\begin{bmatrix}\alpha & \beta & & & \\ \beta^+ & \alpha & \beta & & \\ & \beta^+ & \alpha & \ddots & \\ & & \ddots & \ddots & \end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \\ \psi_N\end{Bmatrix}$$

• The claim is that the following will satisfy the equations:

$$\{\psi_n\}=\{\psi_0\}e^{inka} \qquad (1)$$

• Equation "n" reads:

$$E\{\psi_n\}= \qquad (2)$$

$$[\alpha]\{\psi_n\}+[\beta^+]\{\psi_{n-1}\}+[\beta]\{\psi_{n+1}\}$$

• Putting (1) in (2)→

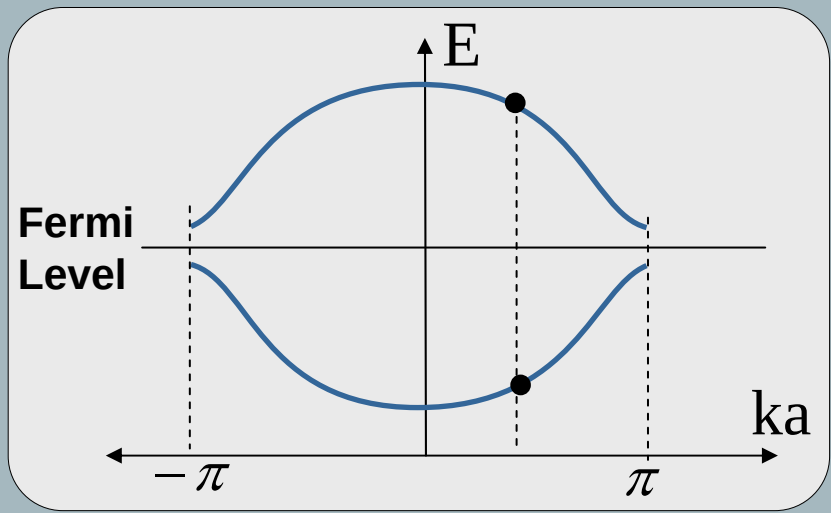
$$E\{\psi_0\}e^{inka}=[\alpha]\{\phi_0\}e^{inka}+$$

$$[\beta^+]\{\psi_0\}e^{i(n-1)ka}+[\beta]\{\phi_0\}e^{i(n+1)ka}$$

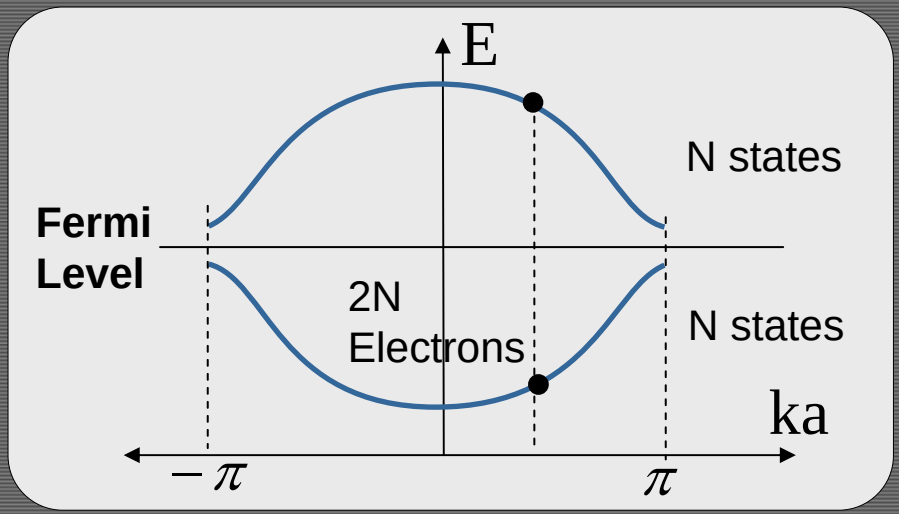
• Canceling the same factors from the two sides:

$$E\{\psi_0\}=[h]\{\psi_0\}$$

$$[h]\equiv[\alpha]+[\beta^+]e^{-ika}+[\beta]e^{+ika}$$

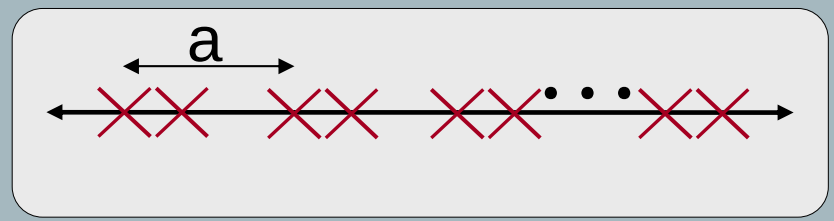


Dimerized Solid: E-k curve / Conduction



• There are 2N states available. There are total of 2N electrons. Each state can take two electrons. At temperature, the lower band is filled and the upper band is empty. Fermi levels lies between the two bands. Since there are no states around the Fermi level, the dimerized solid will not conduct well.

• The fact is that if we had a linear array of H atoms, it would be arranged like a dimerized solid and it won't conduct.



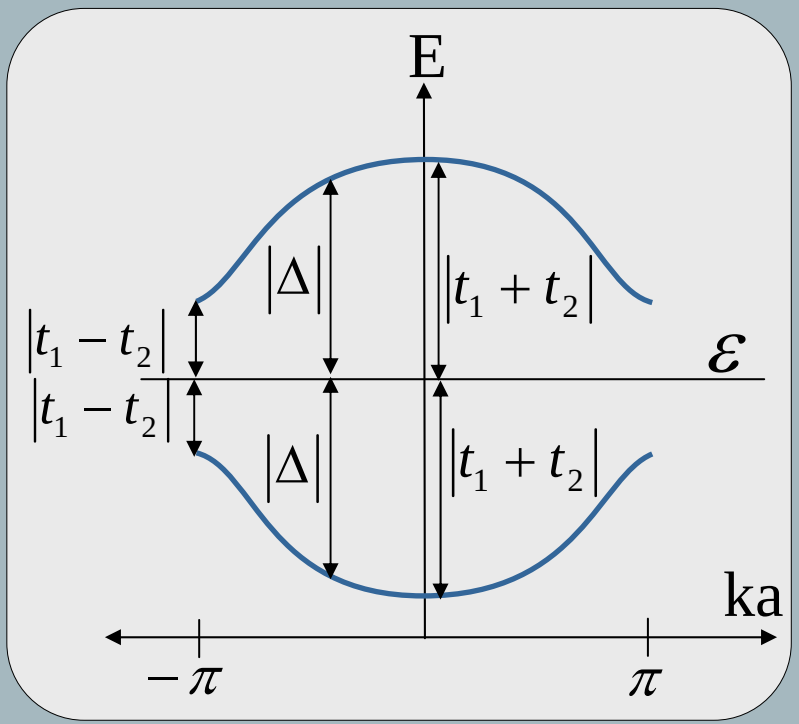
Dimerized Solid: Eigenvalues

- Next we want to find the eigenvalues. First, let's write matrix h(k):

$$[h(k)] \equiv [\alpha] + [\beta^+] e^{-ika} + [\beta] e^{+ika}$$

$$\alpha \equiv \begin{bmatrix} \varepsilon & t_1 \\ t_1 & \varepsilon \end{bmatrix} \qquad \beta \equiv \begin{bmatrix} 0 & 0 \\ t_2 & 0 \end{bmatrix} \qquad \beta^+ \equiv \begin{bmatrix} 0 & t_2 \\ 0 & 0 \end{bmatrix}$$

$$[h(k)] = \begin{bmatrix} \varepsilon & t_1 + t_2 e^{-ika} \\ t_1 + t_2 e^{+ika} & \varepsilon \end{bmatrix}$$



- Eigenvalues are:

$$E = \varepsilon \pm |\Delta| \qquad \Delta \equiv t_1 + t_2 e^{-ika}$$