

From Atoms to Bands: Modeling Electron Behavior in Crystalline Solids

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INTRODUCTION

In this study, we model the behavior of electrons in a 1D crystal lattice, described by the periodic potential energy:

$$V(x) = -100 \cdot (1 - \cos(2\pi x)) \quad (1)$$

which allows us to examine the behavior of electrons as they move through this periodic environment. The objective is to find the energy spectrum for different lengths of the lattice (a), and different number of electrons, Z . The electron's behavior is modeled with the time-independent Schrödinger equation ($S.E.$): $\hat{H}\Psi(x) = E\Psi(x)$. In our model, the Hamiltonian \hat{H} is composed of kinetic \hat{T} and potential \hat{V} energy terms: $\hat{H} = \hat{T} + \hat{V}$. Numerical methods are employed to solve the $S.E.$ for this system. We aim to demonstrate how discrete energy levels can merge into bands, creating the distinct electronic structures characteristic of conductors, semiconductors, and insulators.

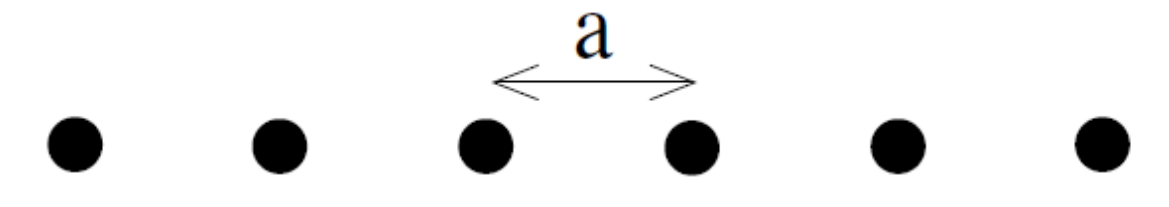


Figure 1. Crystal lattice with lattice parameter a and N lattice sites [2].

THEORETICAL BACKGROUND

- In the study of the band structure of solids, the **nearly free electron model** is commonly used. This model allows us to understand the electron behavior in a nearly free state and the energy-momentum relationship of electrons in solids.
- The **band structure** describes how the energy of an electron varies with its wave vector, and explains the conductive and insulative properties of materials based on the allowed and forbidden energy bands. The **Fermi level** is the highest occupied energy level at absolute zero temperature, while the **density of states** indicates how many states are available at each energy level.
- The electrons can occupy quantum states according to the **Pauli exclusion principle**, which states that no two electrons with the same spin can occupy the same quantum state simultaneously. In a periodic potential, the energy states available to electrons are quantized and form bands.

METHODOLOGY

Discretization of the Schrödinger Equation:

The time-independent $S.E.$ is given by:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (2)$$

The second derivative can be approximated using finite differences [1]. For a grid of points x_i where $i = 1, 2, \dots, N$ and $x_{i+1} - x_i = \Delta x$, the second derivative of ψ at x_i can be approximated as:

$$\frac{d^2\psi}{dx^2}(x_i) \approx \frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1}))}{(\Delta x)^2} \quad (3)$$

Using this approximation, the $S.E.$ can be written in matrix form as $H\psi = E\psi$ where H is the Hamiltonian matrix whose elements are:

- $H_{ii} = \frac{\hbar^2}{2m(\Delta x)^2} + V(x_i)$ for the diagonal elements
- $H_{i,i+1} = H_{i+1,i} = -\frac{\hbar^2}{2m(\Delta x)^2}$ for the off-diagonal elements that are adjacent to the diagonal
- $H_{i,j} = 0$ for all other off-diagonal elements

The matrix is diagonalized to find the energy levels (eigenvalues) and the corresponding wavefunctions (eigenvectors).

CONCLUSIONS

- The discretization of energy levels into bands is a consequence of the periodic potential in a crystalline solid.
- For $Z = N$ only half of the states are occupied up to the Fermi energy, the system behaves similarly to metals or semimetals, where electrons at the Fermi level are available for conduction. For $Z = 2N$, the system resembles an insulator or a fully occupied valence band in semiconductors, all states are filled, and there are no available states at the Fermi level for electrons to jump to at low temperatures, inhibiting conductivity.

RESULTS

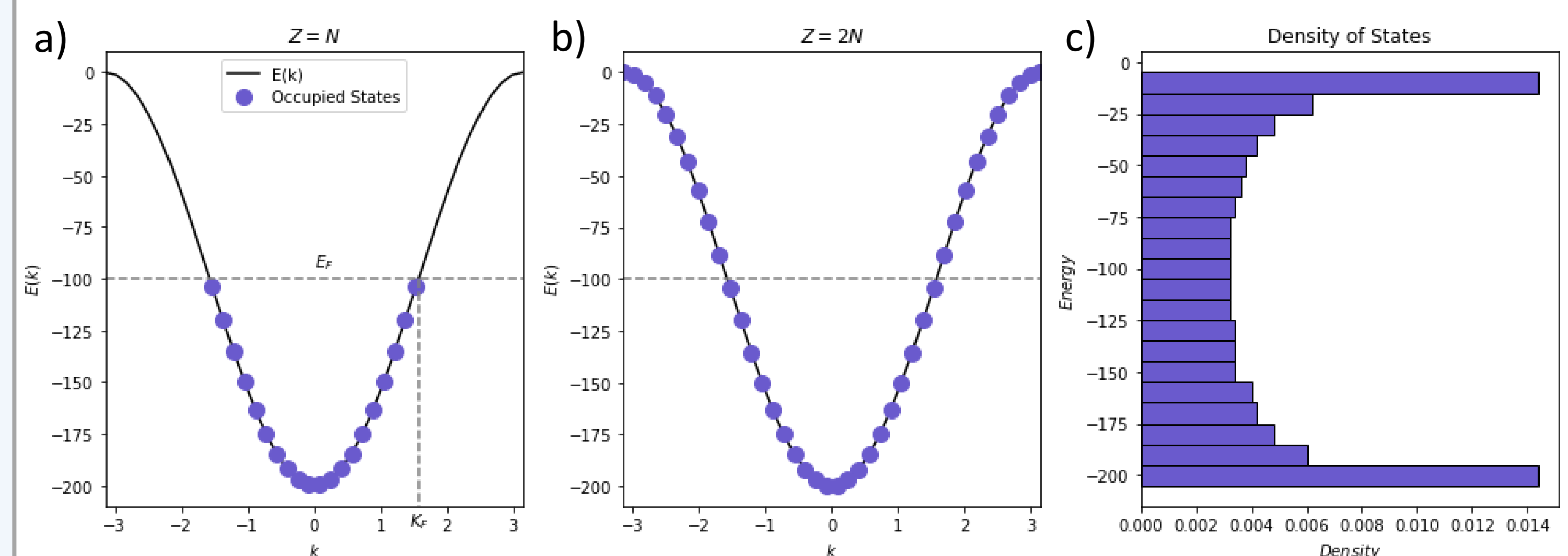


Figure 2. a) Energy spectrum for $Z = N = 40$, b) Energy spectrum for $Z = 2N = 80$, c) Density of states for $N = 100$. The lattice parameter is $a = 1$ for all cases. E_F is the Fermi level, and k_F is the Fermi wavevector

The 5 lowest energy levels for $N = 40$ are: -199.7, -197.1, -191.9, -184.5, and -174.85 (a.u)

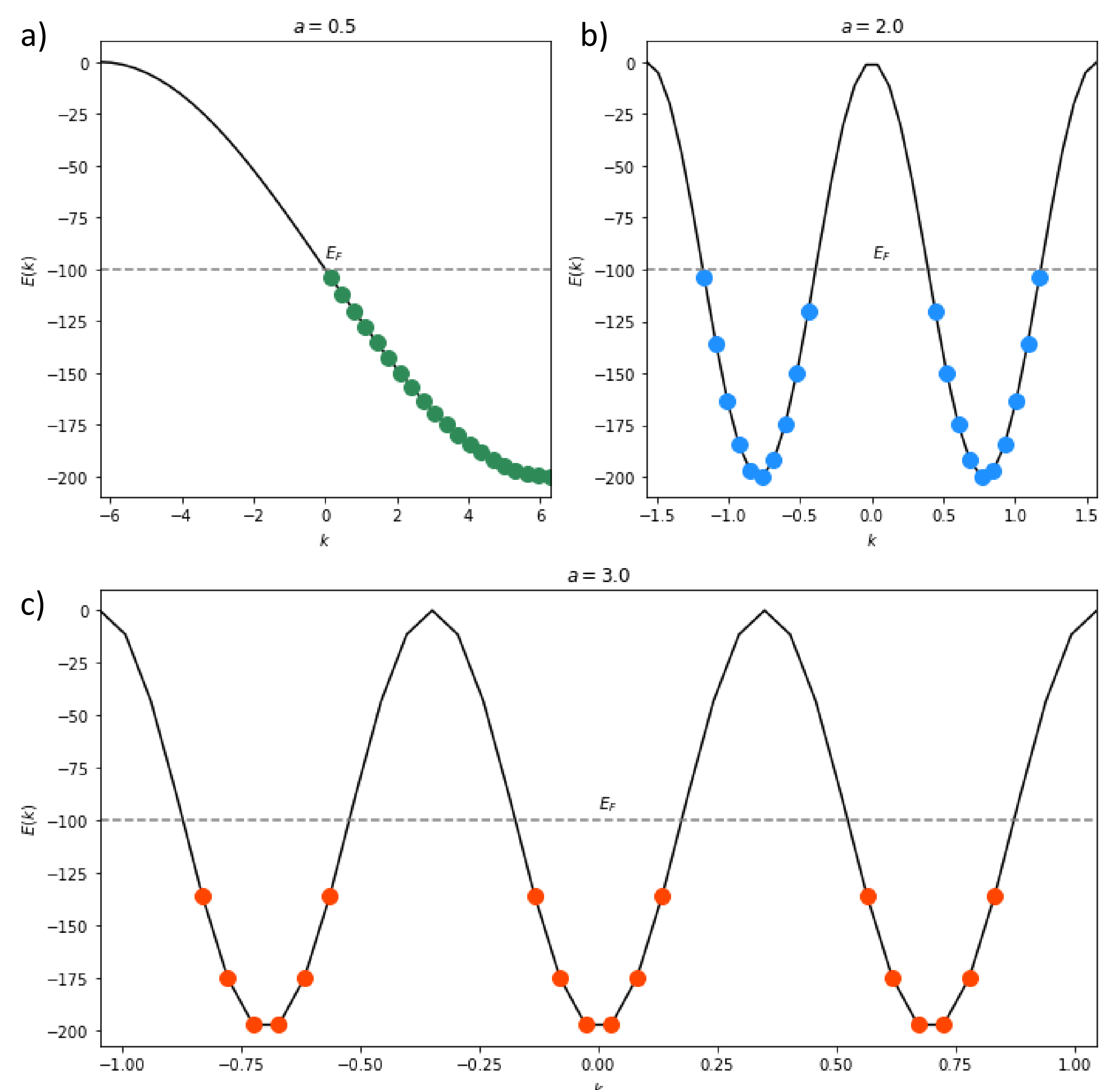


Figure 3. a) Energy spectrum for $a = 0.5$, b) Energy spectrum for $a = 2.0$, c) Energy spectrum for $a = 3.0$. $Z = N = 40$ was used for all cases

BIBLIOGRAPHY

- [1] Rafael Guardiola, Emili Higon, Josep Ros "Mètodes numèrics per a la física"
- [2] Tong, David. "Solid State Physics." University of Cambridge, Lent Term 2017