Solid State Theory

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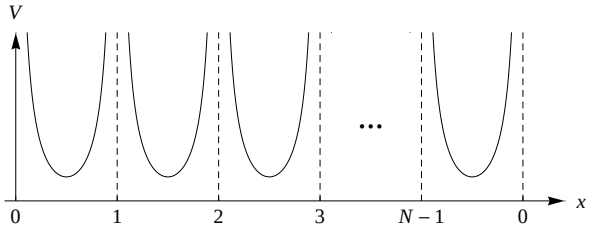
Exercise 1: Bloch waves in 1d

Consider a potential $V_0(x)$, $0 < x < 1$, that diverges for $x = 0$ and $x = 1$ and has a discrete spectrum of energies E_i ($E_0 < E_1 < \dots$) with non-degenerate eigenstates $\phi_i(x)$. When continued to a periodic potential $V(x) := V_0(x - n)$ for $n < x < n + 1$ as shown in the figure below, together with periodic boundary conditions $N \equiv 0$, the Hamiltonian $H = -\frac{\hbar}{2m}\frac{d^2}{dx^2} + V(x)$ commutes with discrete translations T_n, where $(T_n\psi)(x) := \psi(x - n)$.



a) What are the possible energies of a particle in this periodic potential? What is the degeneracy D of these energies? Write down a set of D orthogonal eigenstates that span the eigenspace corresponding to a fixed energy. [Hint: one of them may be chosen to be $\phi_i(x)$] (3 points)

b) Denoting $\phi_i^n(x) := \phi_i(x-n)$, what is the matrix of T_1 with respect to the basis $\{\phi_i^0(x), \dots, \phi_i^{N-1}(x)\}$ of states with fixed energy E_i? (2 points)

c) Show that the eigenvalues of the matrix in b) are given by $\exp(2\pi i \frac{n}{N})$, where $n = 0, \dots, N - 1$ [Hint: two useful facts are that the determinant of an upper triangular matrix is given by the product of its diagonal entries and that taking the transpose matrix does not change the determinant] (3 points)

d) Using c), determine the eigenvectors of the matrix in b) (2 points)

e) Using the fact that $T_n = (T_1)^n$, determine the eigenvalues and eigenvectors of the matrix of T_n, again with respect to $\{\phi_i^1(x), \dots, \phi_i^{N-1}(x)\}$. (2 points)

f) Write down a basis of the total Hilbert space that diagonalises every operator in the set $\{H, T_1, T_2, \dots, T_{N-1}\}$. (1 point)

g) Bloch's theorem claims that every state in f) can be written in the form $\exp(ikx)u(x)$ for some real number k and periodic function $u(x)$ (which differ for different states). Verify this statement by identifying k and $u(x)$ for each state found in f) and sketch the dispersion relation $E(k)$ (3 points)

Exercise 2*: Tight-binding model

Assume that by changing the periodic potential $V(x)$ in exercise 1 to be finite (but large) for $x = 1, 2, \ldots, N-1$, the states $\phi_0^n(x)$ change to another orthonormal set $\psi_0^n(x) := \psi_0(x-n)$, for some $\psi_0(x)$ (almost) localised to the interval $[0,1]$. These new states differ from the completely localised ones by "leaking" into other sites, i.e. $\psi_0^n(x) \neq 0$ for $x \notin [n, n+1]$ is possible. In the tight-binding approximation, this (small) leaking is implemented in the Hamiltonian by a "hopping" parameter $t > 0$, such that $H\psi_0^n(x) = E_0\psi_0^n(x) - t\psi_0^{n-1}(x) - t\psi_0^{n+1}(x)$.

a) For which values of $k \in \mathbb{R}$ does $\xi_k(x) := \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{ikx}\psi_0^n(x)$ give an energy eigenstate? Determine the energy for each of these values. (2 bonus points)

b) Sketch the energy dispersion. (1 bonus point)

Exercise 3: The Fourier-transformed Schrödinger equation

Consider a one-dimensional (finite) lattice with the periodic potential $V_1(x)$ given by

$$V_1(x) = \sum_{n=1}^{N} \alpha\, \delta(x - na) \quad , \quad \alpha < 0 \ ,$$

which corresponds to the attractive Kronig-Penney model.

a) Calculate the Fourier coefficients V_g of the potential $V_1(x)$. (1 point)

b) The Fourier-transformed Schrödinger equation

$$\left[\frac{\hbar^2}{2m}\left(\vec{k} - \vec{G}_0\right)^2 - E\right] c_{\vec{k}-\vec{G}_0} + \sum_{\vec{G}} V_{\vec{G}-\vec{G}_0} c_{\vec{k}-\vec{G}} = 0 \ ,$$

can be written in a matrix representation as

$$(V + T)\vec{c}_{\vec{k}} = E\vec{c}_{\vec{k}} \ ,$$

with the components of the vector $\vec{c}_{\vec{k}}$ given by the $c_{\vec{k}-\vec{G}}$. What is the form of the matrix elements of T (in general)? Give the expressions of the matrix elements of V for the potential $V_1(x)$. (2 points)

c) In the nearly-free electron model, the effect of the potential is taken into account within second-order perturbation theory. Calculate the splittings of the energy bands close to the zone boundary due to the potential $V_1(x)$. (4 points)

d*) Consider now a potential of the form

$$V_2(x) = \alpha \cos\left(\frac{2\pi}{a}x\right) \quad , \quad \alpha < 0 \ ,$$

Calculate the splittings of the energy bands close to the zone boundary due to the potential $V_2(x)$ following the steps in a) to c) above. (3 bonus points)

Exercise 4*: Single electron in a periodic potential – numerical solution

Consider the potential $V_2(x)$ of exercise 3d), with the periodic boundary conditions replaced by *fixed* boundary conditions for the wave function $\psi(x)$:

$$\psi(0) = 0 \ , \ \psi(Na) = 0 \ .$$

Using standard numerical algorithms for the solution of ordinary differential equations, calculate the spectrum of eigenenergies E_n, and the corresponding wave functions $\psi_n(x)$. (up to 10 bonus points)