

Estado Sólido I

Tarea 5: Electrón en un Potencial Periódico

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Nombre del Estudiante: _____

Problema 1 *Square lattice*

Consider a square lattice in two dimensions with the crystal potential

$$U(x, y) = -4U \cos(2\pi x/a) \cos(2\pi y/a).$$

Apply the secular equation,

$$\left(\frac{\hbar^2 k^2}{2m} - \epsilon \right) C_{\mathbf{k}} + \sum_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}} V_{\mathbf{G}} = 0,$$

and find the following:

- (a) The energy spectrum ϵ around the corner point of the Brillouin zone $\mathbf{k} = \mathbf{k}_f + \delta$, with $\mathbf{k}_f = (\pi/a, \pi/a)$:

$$\epsilon = \frac{\hbar^2}{2m} (k_f^2 + \delta^2) \pm U \left[1 + \frac{4}{U^2} \left(\frac{\hbar^2 k_f^2}{2m} \right) \left(\frac{\hbar^2 \delta^2}{2m} \right) \right]^{1/2}.$$

- (b) The energy gap $\Delta\epsilon$ at \mathbf{k}_f .

Hint: δ can be consider as in same direction as \mathbf{k}_f .

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Problema 2 *Kronig-Penney model*

For the square-well periodic potential (Kronig-Penney potential), find the general trascendental equation that comes as a result of applying the boundary and periodic conditions to the wave functions in the real space:

$$[(q^2 - \kappa^2) / 2q\kappa] \text{Senh } qb \text{Sen } \kappa a + \text{Cosh } qb \text{Cos } \kappa a = \text{Cos } k(a + b).$$

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Problema 3 *Delta-function potential for the Kronig-Penney model*

Applying the delta-function approximation for the square-well periodic potential (Kronig-Penney): $b \rightarrow 0$ and $U_0 \rightarrow \infty$, demonstrate,

- (a) $P = q^2ba/2$ is a finite quantity (does not diverge).
- (b) $q \gg \kappa$.
- (c) $bq \ll 1$.
- (d) The approximate form of the transcendental equation (applying the conditions mentioned above):

$$\frac{P}{\kappa a} \text{Sen } \kappa a + \text{Cos } \kappa a = \text{Cos } ka.$$

- (e) The energy of the lowest energy band at $k = 0$.
- (f) The band gap at $k = \pi/a$.

Hint: For the last two questions, you can consider that $P \ll 1$.

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