Estado Sólido I
Tarea 5: Electrón en un Potencial Periódico

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Nombre del Estudiante: ______________________________

Problema 1 *Square lattice, free electron energies*

(a) Show for a simple square lattice (two dimensions) that the kinetic energy of a free electron at a corner of the first Brioullin zone is higher than that of an electron at midpoint of a side face of the zone by a factor of 2.

(b) What is the corresponding factor for a simple cubic lattice (three dimensions)?

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Problema 2 *Square lattice*

Consider a square lattice in two dimensions with the crystal potential

$$U(x, y) = -4U\mathrm{Cos}(2\pi x/a)\mathrm{Cos}(2\pi y/a).$$

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

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

as well as the energy gap at $\mathbf{k}_f$.
Hint: δ can be consider as in same direction as $\mathbf{k}_f$.

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Problema 3 *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:

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

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Problema 4 *Delta-function potential for the Kronig-Penney model*

Applying the delta-function approximation for the square-well periodic potential (Kronig-Penney), show or obtain:

(a) $P = q^2ba/2$ is a finite quantity (does not diverge).

(b) $q \gg \kappa$.

(c) $qb \ll 1$.

(d) The approximate form of the trascendental 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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