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

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

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 $\mathbf{k}_f = (\pi/a, \pi/a)$:

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

(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:

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

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

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

(a) The approximate form of the transcendental equation (applying the conditions mentioned above):

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

(b) The energy of the lowest energy band at $k = 0$.

(c) The band gap at $k = \pi/a$.

Hint: For the last two questions, you can consider that $P = q^2 ba/2 \ll 1$.

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