Condensed Matter Theory problem set 2

Dr. Tilman Enss & Valentin Kasper
Institut für Theoretische Physik, Universität Heidelberg
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Problem 4: Kronig-Penney model

A simple model for a periodic potential in one dimension is the Kronig-Penney (Dirac comb) model ($\lambda > 0$),

$$V(x) = \lambda \frac{\hbar^2}{m} \sum_{j=-\infty}^{\infty} \delta(x - ja). \tag{1}$$

(a) The wavefunction in the region $0 < x < a$ can be written as $\psi(x) = Ae^{iQx} + Be^{-iQx}$ with wavenumber $Q = \sqrt{2mE}/\hbar > 0$. Use the Bloch condition $\psi(x + a) = e^{ika}\psi(x)$ for crystal momentum $\hbar k$ to find the wavefunction in the region $a < x < 2a$. The conditions that $\psi(x)$ is continuous at $x = a$ and that $\psi'(x)$ jumps by $2\lambda\psi(a)$ at $x = a$ give a homogeneous linear system; solve it and find the implicit relation between the crystal momentum and the allowed values of Q and thereby E. Show that this relation can be written in the form

$$\cos(ka) = \frac{\cos[Qa + \delta(Q)]}{|t(Q)|} =: \mu(Q) \tag{2}$$

with $|t(Q)| = \cos\delta(Q) = \left(1 + (\frac{\lambda}{Q})^2\right)^{-1/2}$.

(b) Show that $t(Q) = |t(Q)|e^{i\delta(Q)}$ is precisely the transmission amplitude across a *single* δ potential.

(c) Plot $\mu(Q)$ as a function of $x = Qa$ for $\lambda a = 5$ and sketch the allowed and forbidden energy bands. Make a free-hand sketch of the corresponding band dispersion E vs. ka. Can electrons move in the limit $Q \to 0$? How does the band structure change for $\lambda \to 0$?

(continued)

Problem 5: Tight-binding model

Consider a simple cubic lattice in d dimensions with lattice constant a.

(a) Show that a tight-binding model with nearest-neighbor hopping $-J$ has the band energy

$$\varepsilon_{\boldsymbol{k}} = -2J \sum_{\ell=1}^{d} \cos(k_\ell a). \tag{3}$$

(b) Compute the density of states for a single spin,

$$g(\varepsilon) = \int_{1.\ \mathrm{BZ}} \frac{d^d k}{(2\pi)^d}\, \delta(\varepsilon - \varepsilon_{\boldsymbol{k}}), \tag{4}$$

explicitly in one dimension (the wavevector integral runs over the first Brillouin zone; set $\hbar = 1$). How does it behave near the boundaries of the band on the energy axis ($\varepsilon \approx \pm 2J$)?

(c) In two dimensions, draw the first Brillouin zone and qualitatively sketch the Fermi surface at zero temperature for an almost empty band; a half-filled band; and an almost completely filled band. Argue whether the density of states has van Hove singularities *(a)* at the boundaries of the band on the energy axis ($\varepsilon \approx -4J$: expand $\varepsilon_{\boldsymbol{k}}$ to second order in $\boldsymbol{k}$ around $\boldsymbol{k} = 0$ and compute (4)); and *(b)* at the center of the band on the energy axis ($\varepsilon \approx 0$: expand $\varepsilon_{\boldsymbol{k}}$ to second order around the point $k_x = \pi/a$, $k_y = 0$ or equivalent).