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Theoretical Solid-State Physics, Herbstsemester 2012

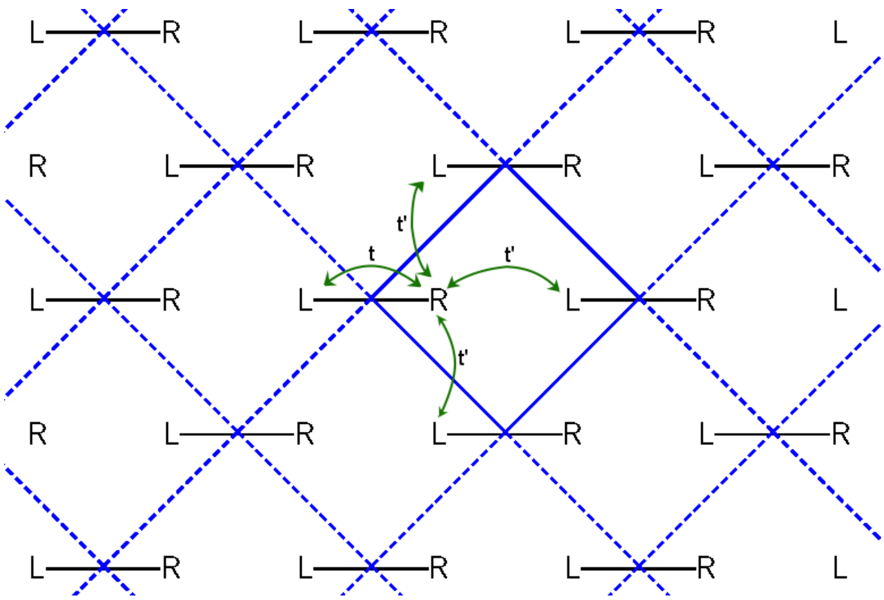
Blatt 2

Abgabe: 4. Oktober, 12:00H (Treppenhaus 4. Stock)
Tutor: Patrick Hofer Zi.: 4.13

(1) **Tight-binding electrons on a checkerboard lattice** (5 Punkte)
Consider tightly-bound electrons on a "checkerboard lattice" (see figure below). This lattice consists of two sublattices L and R, such that only the sites belonging to two different sublattices are connected through nonzero hopping (bipartite lattice). Let a be the distance between the nearest-neighbor L and R sites.

(a) Set up the nearest-neighbor tight-binding Hamiltonian that describes this system and write it in the second-quantization notation. Assume one electronic orbital per site and the on-site energies ε_{L} and ε_{R}. Assume also that the hopping integral t between the L and R sites within the same "LR-dimer" is in general different than the one between the L and R sites that do not belong to the same dimer (t').

(b) Perform a Fourier transformation to **k**-space and diagonalize the Hamiltonian of the system. Plot or draw the obtained Bloch bands along high-symmetry directions for $\varepsilon_{\mathrm{L}} = \varepsilon_{\mathrm{R}}$ and $\varepsilon_{\mathrm{L,R}} = \varepsilon \pm \delta$. Also comment on the special case t'=t.



(2) **Critical points and singularities in the density-of-states** (5 Punkte)

The density-of-states for a single band with dispersion $E(\boldsymbol{k})$ is given by

$$D(E) = 2\sum_{\boldsymbol{k}} \delta(E(\boldsymbol{k}) - E) = 2\int_{E(\boldsymbol{k})\equiv E} \frac{V}{(2\pi)^d} \frac{dS}{|\boldsymbol{\nabla}_{\boldsymbol{k}} E(\boldsymbol{k})|} ,$$

where d denotes the dimension, V the system volume, and $\int dS$ a surface integral (thus the surface element dS has dimension $d-1$). The last equation indicates that the singular points (usually called critical points) in the density-of-states are described by $\boldsymbol{\nabla}_{\boldsymbol{k}} E(\boldsymbol{k}) = 0$. Around such a critical point $E = E_c$, the band dispersion can be expanded as

$$E(\boldsymbol{k}) = E_c \pm \frac{\hbar^2 k_x^2}{2m_x} \pm \frac{\hbar^2 k_y^2}{2m_y} \pm \frac{\hbar^2 k_z^2}{2m_z} + \mathcal{O}(k_x^3, k_y^3, k_z^3) .$$

For simplicity, the last expansion was written under the assumption that $\mathbf{k}_c = 0$, i.e., that the origin of the $\mathbf{k}$-space coincides with the critical point under consideration.

(a) Discuss the last expansion and relate the number of plus/minus signs to the nature of the critical point [i.e., whether it is a minimum, a maximum, or a saddle-point of the band dispersion $E(\boldsymbol{k})$] in 1D, 2D, and 3D.

(b) Derive the density-of-states $D(E)$ in the vicinity of band minima and maxima (not saddle-points !) in 1D and 2D. In the 2D case, make use of polar coordinates to simplify the derivation.

Hint: use the relation for the delta function

$$\delta[f(x)] = \sum_n \frac{\delta(x - x_n)}{|f'(x_n)|} ,$$

where x_n are the zeroes of the function $f(x)$.