Theory of Quantum Matter

Lecturer: Prof. Otfried Gühne (Mon 14:00, Fri 10:00, Room D120)
Exercises: Chau Nguyen (Fri 14:00, Room B030) **Sheet 5**

Hand in: Mon 19.11.2018 *(questions marked as $*$ are optional)*
Discussion date: Fri 23.11.2018

7. Tight-binding approximation for electrons in the Kronig–Penny potential

(a) (10pts) Show that for the δ-Dirac potential, $V(x) = -S\delta(x)$ with $S > 0$, there is a single bound state. Find the corresponding energy E and wave function $\phi(x)$.

(c) (20pts) Now we consider a periodic lattice of δ-Dirac potentials with spatial period d, $V(x) = -\sum_{n=-\infty}^{+\infty} S\delta(x - nd)$. In the tight-binding approximation, we use the wavefunctions $\phi(x-nd)$ as basis. Compute that wavefunction overlaps $s_{mn} = \langle \phi(x - md), \phi(x - nd) \rangle$ and the matrix elements $H_{mn} = \langle \phi(x - md), H\phi(x - nd) \rangle$.

(d) (5pts) Compute and sketch the energy band in the tight-binding approximation. For simplicity, we consider only upto nearest neighbour hoopings ($H_{mn} = 0$ if $|m - n| \geq 2$) and ignore the wavefunction overlaps ($s_{mn} = 0$ if $m \neq n$).

8. Tight-binding approximation for some lattices

Consider the tight-binding approximation for a certain lattice. Let H be the Hamiltonian of an electron in the lattice and $\phi(\vec{r})$ be the local atomic wavefunction. To aid the computation, we assume: $\left\langle \phi(\vec{r} - \vec{R}), H\phi(\vec{r} - \vec{R}) \right\rangle = 0$ (this is obtained by redefining an additive constant in the Hamiltonian), $\left\langle \phi(\vec{r} - \vec{R}'), H\phi(\vec{r} - \vec{R}) \right\rangle = -t$ if $\vec{R}'$ and $\vec{R}$ are nearest neighbours in the lattices (nearest neighbour hooping approximation) and $\left\langle \phi(\vec{r} - \vec{R}'), \phi(\vec{r} - \vec{R}) \right\rangle = \delta_{\vec{R},\vec{R}'}$ (orthogonality approximation). In the tight-binding approximation:

(a) ($*$) Compute the energy band for the square lattice in the plane.

(b) (5pts) Compute the energy band for the triangular lattice in the plane defined by two basic vectors $\vec{a}$ and $\vec{b}$ of the same length and angle of $\pi/6$.