SS2019: Solid State Theory
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Problem Set 3

1. **Reciprocal lattice** (2+2+2 points)

Consider a crystal defined by the following primitive vectors:

$$\vec{a}_1 = \frac{\sqrt{3}}{2}a\hat{x} + \frac{1}{2}a\hat{y}, \qquad \vec{a}_2 = -\frac{\sqrt{3}}{2}a\hat{x} + \frac{1}{2}a\hat{y}, \qquad \vec{a}_3 = a\hat{z}.$$

(a) Sketch the lattice in the x-y plane.

(b) What are the primitive vectors $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$ for the reciprocal lattice?

(c) Sketch the shape of the first Brillouin zone.

2. **Volume of the first Brillouin zone** (4 points)

For a crystal defined by the primitive vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$, the volume of the primitive cell is given by

$$V = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|.$$

Prove that the volume of the primitive cell for the reciprocal space is given by

$$\Omega \equiv |\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)| = \frac{(2\pi)^3}{V}.$$

Note that Ω is also the volume of the first Brillouin zone. Why?

3. **LCAO as a variational problem** (5+3 points)

The LCAO method can be naturally formulated as a variational problem. Consider the Hamiltonian H and a set of *non-orthogonal* wave functions $|\phi_a\rangle$ ($a = 1, \ldots, n$). The variational wave function is constructed as

$$|\psi\rangle = \sum_{a=1}^{n} c_a |\phi_a\rangle,$$

where c_a are variational parameters which should be determined by minimizing the variational energy

$$E[c^*, c] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

with respect to c_a and c_a^*.

Alternatively, you may formulate this variational problem by using a Lagrange multiplier λ to ensure that the variational ansatz $|\psi\rangle$ is normalized and considering the energy functional

$$E[c^*, c, \lambda] = \langle\psi|H|\psi\rangle - \lambda(\langle\psi|\psi\rangle - 1).$$

(a) Show that the optimal choice of variational parameters is determined by the secular equation

$$\sum_{b=1}^{n} (\langle\phi_a|H|\phi_b\rangle - E\langle\phi_a|\phi_b\rangle) c_b = 0,$$

whose nontrivial solution is obtained from

$$\det(\mathcal{H} - E\mathcal{S}) = 0.$$

Here $\mathcal{H}$ and $\mathcal{S}$ are $n \times n$ matrices with matrix elements $\mathcal{H}_{ab} = \langle \phi_a | H | \phi_b \rangle$ and $\mathcal{S}_{ab} = \langle \phi_a | \phi_b \rangle$, respectively.

(b) Show that one can turn the above secular equation (for the non-orthogonal basis) into an ordinary secular equation

$$\det(\mathcal{H}' - EI) = 0,$$

where I is the $n \times n$ identity matrix. What is $\mathcal{H}'$?

Hint: You may diagonalize the overlap matrix $\mathcal{S}$, which effectively orthogonalizes $|\phi_a\rangle$.