Exercise 4 for Theoretical Solid State Physics in Summer 2021

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Submission: 07.05.2021, 12:00 in the P.O. Box Giesen on D.10 or by e-mail
Discussion: 10.05.2021, 14:15

1. **Lattice structures (6 Points)**
   Here we study some problems occurring in cubic structures.
   (a) fcc lattice: What is the filling ratio of this lattice with hard spheres of identical (and maximal) radius placed at the lattice sites?
   (b) Independent spins in crystal fields: Consider a local spin $\vec{S}$ with Hamiltonian
   $$H = J\left(S_x^4 + S_y^4 + S_z^4\right),$$
   where $\vec{S}^2 = S(S+1)$ and S takes a half-inter or an integer value. The dimension of the Hilbert space is $2S+1$. What are the eigenvalues and their degeneracies for instance in the case $S = 5/2$? (It is absolutely acceptable if you use the QM definitions of the spin matrices and computer algebra for the calculation.)

2. **Kronig-Penney model (14 Points)**
   The Kronig-Penney model is a simple, one-dimensional model for the understanding of the band structure in a solid state. Consider an electron of mass m, which moves in the periodic potential
   $$V(x) = aV_0 \sum_{n\in\mathbb{Z}} \delta(x - an).$$
   $V_0 > 0$ is the strength of the potential and a is the lattice constant.
   (a) Use dimensionless units, so that the stationary Schrödinger equation takes the form
   $$H\phi(y) = \left(-\partial_y^2 + 2c\sum_{n\in\mathbb{Z}} \delta(y-n)\right)\phi(y) = q^2\phi(y).$$
   What is the relation between x and y, V_0 and c and q^2 and E?

(b) Impose the continuity condition $\phi(1^+) = \phi(1^-)$ and $\phi'(1^+) - \phi'(1^-) = 2c\phi(1)$ (why?).

(c) Because of the periodicity of the potential, H commutes with the translation operator defined by

$$T\phi(y) = \phi(y-1).$$

Consequently H and T have a common system of eigenfunctions. The eigenvalues are:

$$H\phi(y) = q^2\phi(y) \tag{1}$$

$$T\phi(y) = e^{-ik}\phi(y) \tag{2}$$

Determine the solutions of (1) and (2) as a function of k and q. What is the relation between k and q?

(d) Justify why k must be real, so that $\phi(y)$ is a bounded, normalizable state. Can q be complex? Discuss the dispersion relation from (c) graphically.