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October 2013 - Entrance Examination: Condensed Matter

Solve at least one of the following problems. Write out solutions clearly and concisely. State each approximation used. Diagrams welcome. Number page, problem, and question clearly. Do not write your name on the problem sheet, but use extra envelope.

Problem 1: Model bound state in momentum space.

It is very common, in condensed matter physics problems, to encounter scattering of electrons or other quantum particles on some very localized attractive potential, for example due to an impurity, which may or may not give rise to a bound state. The present problem presents the simplest such case, whose exact solution, which is easiest to achieve in momentum space, contains interesting information about the bound state wavefunction and the binding energy dependence upon the particle mass and the potential strength.

1) Write the one dimensional Schrödinger equation for a particle of mass m moving in a time independent potential $V(x)$.

2) By Fourier transforming the wavefunction $\Psi(x) \to \hat{\Psi}(k)$ and the potential $V(x) \to \hat{V}(k)$, write the same Schrödinger equation now in momentum space.

Consider now an attractive δ-function potential $V(x) = -V_0\delta(x)$, with $V_0 > 0$ (dimensionally, an energy times a length), and the corresponding momentum space Schrödinger equation.

4) Solve it to find the ground (bound) state wavefunction $\hat{\Psi}_0(k)$, and its real space Fourier transform $\Psi_0(x)$.

5) Determine the corresponding ground state energy $-|E_0| < 0$, and comment on the dependence of $|E_0|$ (the "binding energy") upon the particle mass m and the potential strength V_0.

6) Are there other bound states? How many?

Hint: Use a book of integrals, if you prefer.

Problem 2: Quantum fluctuations of a dipole at a metal surface

Consider a system of two point particles of opposite charge, $\pm e$, and equal mass, m, placed ad a distance d from each other and whose center of mass is at a distance $z \gg d$ from a metal surface.

1. Write the expression of the potential energy of the system as a function of z and of the angle θ between the dipole of the system and and the normal to the metal surface.

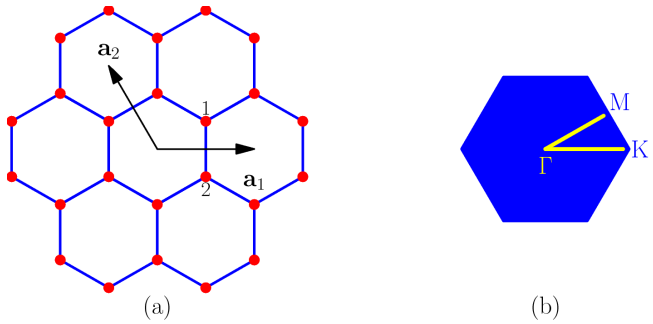
2. Find the classical equilibrium configuration(s) of the system as a function of z.

3. Write down the quantum Hamiltonian of the system and find the eigenvalues considering the distance z fixed and in the limit of small oscillations (*i.e.* in the limit of small deviations of θ from the equilibrium value). State explicitly the conditions that the system has to fulfill in order for the small oscillation approximation to hold.

4. Write down the expression of the ground-state energy of the system, as a function of z, taking into account quantum fluctuation (*i.e.* zero-point motion) effects.

Problem 3: Electronic structure of graphene

Graphene is a layer of carbon atoms as shown in Figure (a):



(a) (b)

This structure can be described by an hexagonal Bravais lattice and two atoms per cell. The lattice is described by the primitive vectors $\mathbf{a}_1 = a(1,0)$ and $\mathbf{a}_2 = a(-\frac{1}{2}, \frac{\sqrt{3}}{2})$, and the positions of the two atoms are: $\mathbf{d}_1 = a(\frac{1}{2}, \frac{1}{2\sqrt{3}})$ and $\mathbf{d}_2 = a(\frac{1}{2}, -\frac{1}{2\sqrt{3}})$.

The wave-function of an electron in graphene has the Bloch form and is the solution of the Schrödinger equation: $H|\psi_{\mathbf{k},n}\rangle = \varepsilon_{\mathbf{k},n}|\psi_{\mathbf{k},n}\rangle$, where $\mathbf{k}$ is a wave-vector in the Brillouin zone (shown in Figure (b)). In order to solve approximatively this equation we consider a simple tight-binding model with a p_z orbital in each carbon atom, $\phi_{p_z}(\mathbf{r})$, and we assume that: $\langle\phi_{p_z}(\mathbf{r}-\mathbf{R})|H|\phi_{p_z}(\mathbf{r}-\mathbf{R})\rangle = \varepsilon_{2p}$ when the orbitals are centered on the same atom, while $\langle\phi_{p_z}(\mathbf{r}-\mathbf{R})|H|\phi_{p_z}(\mathbf{r}-\mathbf{R}')\rangle = -\gamma_0$ when $|\mathbf{R}-\mathbf{R}'| = \frac{a}{\sqrt{3}}$ (nearest neighbors atoms) and zero otherwise. Moreover, we assume that $\langle\phi_{p_z}(\mathbf{r}-\mathbf{R})|\phi_{p_z}(\mathbf{r}-\mathbf{R}')\rangle = \delta_{\mathbf{R},\mathbf{R}'}$.

1) Searching the solutions as tight-binding combinations:

$$\psi_{\mathbf{k},n}(\mathbf{r}) = \sum_{\mu} e^{i\mathbf{k}\mathbf{R}_\mu} \left[c_1(\mathbf{k},n)\phi_{p_z}(\mathbf{r}-\mathbf{R}_\mu-\mathbf{d}_1) + c_2(\mathbf{k},n)\phi_{p_z}(\mathbf{r}-\mathbf{R}_\mu-\mathbf{d}_2)\right], \quad (1)$$

where the sum is over all the Bravais lattice vectors $\mathbf{R}_\mu$, write the equations for the two coefficients $c_1(\mathbf{k},n)$ and $c_2(\mathbf{k},n)$ in terms of ε_{2p} and γ_0. (Hint: substitute the solution in the Schrödinger equation).

2) Find the eigenvalues $\varepsilon_{\mathbf{k},1}$ and $\varepsilon_{\mathbf{k},2}$ as a function of $\mathbf{k}$ and plot them along the lines $M-\Gamma-K$ shown in Figure (b). You can make the plot for $\varepsilon_{2p} = 0$.

3) Now take $\mathbf{q} = \mathbf{k} - \mathbf{k}_0$, where $\mathbf{k}_0$ is the point K. Show that, for small $|\mathbf{q}|$, $\varepsilon_{\mathbf{q},1} = \alpha|\mathbf{q}|$ and $\varepsilon_{\mathbf{q},2} = -\alpha|\mathbf{q}|$ and find the value of α as a function of γ_0 and a. Which is the speed of a Bloch electron in one of these bands?

4) Expand the 2×2 matrix found at point [1)] in a Taylor series about $\mathbf{k}_0$, diagonalize it and find the eigenvalues showing that they coincide with those found at point [3)]. Find also the eigenvectors of this simplified Hamiltonian.

Problem 4: Two interacting electrons in a magnetic field

Two electrons move in the two dimensional $x-y$ plane and are described by the Hamiltonian

$$H = \sum_{i=1}^{2} \frac{1}{2m} \left[\Big(-i\hbar\, \boldsymbol{\nabla}_i + \frac{e}{c}\, \mathbf{A}(\mathbf{r}_i \Big)^2 - g\, \mu_B\, B\, s_i^z \right] + \frac{K}{2}\, (\mathbf{r}_1 - \mathbf{r}_2)^2, \tag{2}$$

where $\mathbf{r}_i = (x_i, y_i, 0)$ is the coordinate of the electron $i = 1, 2$, $-i\hbar\, \boldsymbol{\nabla}_i = -i\hbar\, (\, \partial/\partial x_i,\, \partial/\partial y_i, 0)$ its conjugate momentum and s_i^z its spin projection in the z-direction. The vector potential $\mathbf{A}(\mathbf{r})$ corresponds to a constant magnetic field directed perpendicular to the $x-y$ plane, i.e.

$$\boldsymbol{\nabla} \wedge \mathbf{A}(\mathbf{r}) = \mathbf{B}(\mathbf{r}) = (0, 0, B).$$

The last term in Eq. (2) describes a *fictitious* harmonic attraction between the two electrons.

Questions:

1) Find eigenvalues and eigenfunctions of the Hamiltonian Eq. (2) in the two possible spin sectors, i.e. when the two spin-1/2 electrons are coupled into a spin singlet or triplet configuration;

2) Find the condition for which the actual ground state is a spin singlet.