Übung Quantenmechanik 2 WS 2024/25

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1. Bosonic coherent states

A coherent state $|\alpha\rangle$ is an eigenvector of the annihilation operator a defined by $a\,|\alpha\rangle = \alpha\,|\alpha\rangle$. The bosonic annihilation operator satisfies the canonical commutation relation $[a, a^\dagger] = 1$. The ground-state of the system is denoted by $|\varphi_0\rangle$ (remember: $a\,|\varphi_0\rangle = 0$).

(a) Show that the state $|\alpha\rangle$ is given by

$$|\alpha\rangle = C_\alpha \sum_{n=0}^{\infty} \frac{\left(\alpha a^\dagger\right)^n}{n!}\,|\varphi_0\rangle\,. \tag{1}$$

The Parameter C_α is a not yet specified normalization constant.

(b) Calculate the normalization constant C_α.

2. Matrix elements in the second quantization formalism

Demonstrate that, for symmetrized or antisymmetrized 2-particle states, the 2-particle operator written in second quantization has the same matrix elements as the operator written in first quantization.

Hint:

- Write down the generic symmetrized or antisymmetrized 2-particle state $|kq\rangle$ in the first quantization formalism, i.e. $\langle xy|kq\rangle$, as well as the expectation value $\langle qk|\hat{O}|pr\rangle$ of a given operator $\hat{O}$.

- Define the state $|kq\rangle$ in second quantization starting from the vacuum $|0\rangle$, and write down the generic 2-particle operator $\hat{O}$.

3. Conservation of the total number of particles

Demonstrate that given the Hamiltonian

$$\hat{H} = \sum_k E_k a_k^\dagger a_k + \frac{1}{2}\sum_{kqpr} a_k^\dagger a_q^\dagger V_{kqpr} a_p a_r$$

both for bosons and fermions, it holds that $[\hat{H}, \hat{N}] = 0$, with $\hat{N} = \sum_k a_k^\dagger a_k$ being the total number operator.

Hint:

- Make use of the following relationships: Given three operators $\hat{A}$, $\hat{B}$ and $\hat{C}$, use $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$ and $[\hat{A}\hat{B}, \hat{C}] = \hat{A}\{\hat{B}, \hat{C}\} - \{\hat{A}, \hat{C}\}\hat{B}$, which are useful for the bosonic and fermionic case, respectively.

4. Application I: The band structure of Graphene

Graphene is a material made of a single atomic layer. This two dimensional system is made of Carbon atoms, arranged in a honeycomb lattice, as depicted in Fig. 1 (left).

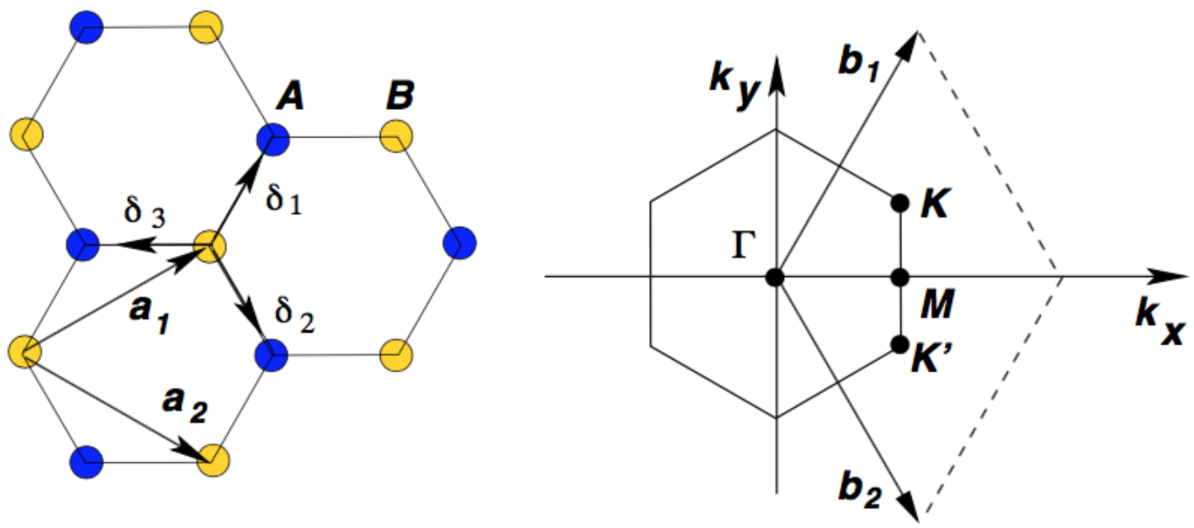

Figure 1: Left: Lattice structure of graphene made out of two interpenetrating triangular lattices ($\mathbf{a}_1$ and $\mathbf{a}_2$ are the lattice unit vectors, and $\boldsymbol{\delta}_i$, $i = 1, 2, 3$ are the nearest neighbour vectors). Right: corresponding Brillouin zone. The Dirac cones are located at the K and K' points.

The honeycomb lattice is actually an hexagonal lattice with a basis of two ions (A in blue and B in yellow in Fig. 1 left) in each unit cell.

(a) If a is the distance between nearest neighbours, write down the cartesian components of the primitive lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, as well as the nearest neighbour vectors $\boldsymbol{\delta}_i$.

(b) Compute the reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ knowing that $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$, where $i = 1, 2$, $j = 1, 2$ and δ_{ij} is the Kronecker delta function. The first Brillouin zone generated by the reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ is shown in Fig. 1 (right).

(c) Compute the coordinates of the Γ, M, K and K' special points in the Brillouin zone.

We directly work in second quantization, and we can define the annihilation operators of an electron at the orbital (mainly of p_z character) centered around the atom A at position $\mathbf{R}$ and the atom B at position $\mathbf{R}'$:

$$\hat{A}(\mathbf{R}), \hat{B}(\mathbf{R}') \quad .$$

Such operators satisfy the following non-vanishing fermionic anticommutation rules:

$$\{\hat{A}(\mathbf{R}), \hat{A}(\mathbf{R}')^\dagger\} = \{\hat{B}(\mathbf{R}), \hat{B}(\mathbf{R}')^\dagger\} = \delta_{\mathbf{R},\mathbf{R}'} \quad .$$

Notice that the nearest neighbor of an ion of type A is always an ion of type B (and vice versa). The graphene tight-binding Hamiltonian in the second quantization formalism is then given by

$$H = -t \sum_{\langle \mathbf{R},\mathbf{R}' \rangle} \hat{A}(\mathbf{R})^\dagger \hat{B}(\mathbf{R}') + h.c. = -t \sum_{\mathbf{R},\boldsymbol{\delta}} \hat{A}(\mathbf{R})^\dagger \hat{B}(\mathbf{R} + \boldsymbol{\delta}) + h.c. \quad , \tag{2}$$

where t is the hopping integral for an electron destroyed on the B atom with position $\mathbf{R}'$ and created on the A atom with position $\mathbf{R}$, $\langle \mathbf{R}, \mathbf{R}' \rangle$ refers to all the nearest neighbour A/B couples, and $h.c.$ is a shorthand notation for hermitian conjugate. Since the system is translationally invariant, we can define the annihilation and creation operators in the Fourier space (reciprocal space):

$$\hat{A}(\mathbf{R}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in BZ} \hat{A}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{R}} \quad , \quad \hat{B}(\mathbf{R}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in BZ} \hat{B}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{R}} \tag{3}$$

such that $\{\hat{A}(\mathbf{k}), \hat{A}(\mathbf{k}')^\dagger\} = \{\hat{B}(\mathbf{k}), \hat{B}(\mathbf{k}')^\dagger\} = \delta_{\mathbf{k},\mathbf{k}'}$, where N is the number of unit cells and $\mathbf{k}$ is defined in the first Brillouin zone (see Fig. 1 right).

(d) Rewrite the tight-binding Hamiltonian (2) in terms of the Fourier space operators $\hat{A}(\mathbf{k})$ and $\hat{B}(\mathbf{k})$.
Hint: Make use of the fact that $\frac{1}{N}\sum_{\mathbf{R}} e^{i(\mathbf{q}-\mathbf{k})\cdot\mathbf{R}} = \delta_{\mathbf{q},\mathbf{k}}$, where $\delta_{\mathbf{q},\mathbf{k}}$ is the so-called lattice delta function.

(e) By defining $\psi(\mathbf{k}) = (\hat{A}(\mathbf{k}), \hat{B}(\mathbf{k}))^T$ recast the Hamiltonian in the form

$$H = \sum_{\mathbf{k}} \psi^\dagger(\mathbf{k}) h(\mathbf{k}) \psi(\mathbf{k}) \quad , \quad h(\mathbf{k}) = \begin{bmatrix} 0 & f(\mathbf{k}) \\ f^*(\mathbf{k}) & 0 \end{bmatrix} \tag{4}$$

and give an explicit expression for $f(\mathbf{k})$. The matrix $h(\mathbf{k})$ is called the Bloch Hamiltonian [**Solution**: $f(\mathbf{k}) = -t(e^{-ik_x a} + 2e^{ik_x a/2}\cos\frac{k_y a\sqrt{3}}{2})$].

(f) Diagonalize the Hamiltonian $h(\mathbf{k})$ and compute the graphene eigenvalues $\varepsilon_{\pm}(\mathbf{k})$. Demonstrate that $\varepsilon_{\pm}(\mathbf{k})$ are degenerate and equal to zero when $\mathbf{k}$ is equal to K and K' special points in the Brillouin zone (see Fig. 1 right). Plot the eigenvalues along the path $\Gamma \to \mathrm{K} \to \mathrm{M} \to \Gamma$ (the resulting plot, in units of the hopping integral t, is called the tight-binding band structure of graphene).

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