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

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

The Parameter C_α is a not yet specified normalization constant.

(b) Calculate the normalization constant C_α.

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

$$= C_\alpha \sum_{n=0}^{\infty} \alpha^n \frac{a(a^\dagger)^n}{n!} |\varphi_0\rangle$$

$$= C_\alpha \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} \left[(a^\dagger)^n a + n(a^\dagger)^{n-1}\right] |\varphi_0\rangle$$

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

$$= C_\alpha \sum_{n=1}^{\infty} \frac{\alpha^n}{(n-1)!} (a^\dagger)^{n-1} |\varphi_0\rangle = \alpha|\alpha\rangle$$

$$a(a^\dagger)^n = (a^\dagger a + 1)(a^\dagger)^{n-1}$$

$$= a^\dagger(a^\dagger a + 1)(a^\dagger)^{n-2} + (a^\dagger)^{n-1}$$

$$= \dots = (a^\dagger)^n a + n(a^\dagger)^{n-1}$$

b) $$\langle\alpha|\alpha\rangle = \left(\sum_{k=0}^{\infty} \langle\varphi_0| \frac{(\alpha^*)^k a^k}{k!}\right)\left(\sum_{n=0}^{\infty} \frac{\alpha^n (a^\dagger)^n}{n!} |\varphi_0\rangle\right) |C_\alpha|^2$$

$$= |C_\alpha|^2 \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} \frac{1}{k!\,n!} \langle\varphi_0|\alpha^n (\alpha^*)^k\, a^k (a^\dagger)^n |\varphi_0\rangle$$

Note that this vanishes for $k \neq n$!

$$= |C_\alpha|^2 \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{(n!)^2} \langle\varphi_0| a^n (a^\dagger)^n |\varphi_0\rangle$$

$$= |C_\alpha|^2 \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{(n!)^2}\, n! = |C_\alpha|^2 e^{\alpha^2}$$

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 $\hat{O}$.

$$|kq\rangle = |k\rangle \otimes |q\rangle \pm |k\rangle \otimes |q\rangle$$

$$\langle qk|\hat{O}|pr\rangle = \frac{1}{2}\Big(\langle q| \otimes \langle k| \mp \langle k| \otimes \langle q| \Big)\hat{O}$$

$$\langle xy|kq\rangle = \frac{1}{\sqrt{2}}\Big(\langle x|k\rangle\langle y|q\rangle + \langle x|q\rangle\langle y|k\rangle \Big)$$

$$\hat{O} = \sum_{ijmn} O_{ijmn} |ij\rangle\langle mn|$$

$$\langle qk|\hat{O}|pr\rangle = \sum_{ijmn} O_{ijmn} \langle qk|ij\rangle\langle mn|pr\rangle$$

$$= \frac{1}{2}\sum_{ijmn} O_{ijmn} \left(\delta_{qi}\delta_{kj} + \delta_{qj}\delta_{ki}\right)\left(\delta \ldots\right)$$

$$= \frac{1}{2}\left(O_{qkpr} + O_{kqpr} + O_{qkrp} + O_{kqrp} \right)$$

$$|kq\rangle = a_k^{\dagger} a_q^{\dagger}$$

$$\hat{O} = \frac{1}{2}\sum_{ijmn} O_{ijmn}\, a_i^{\dagger} \hat{a}_j\, a_m a_n$$

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.

$$[H, N] = \Big[H, \sum_n a_n^\dagger a_n\Big]$$

$$= \sum_k E_k \Big[a_k^\dagger a_k, \sum_n a_n^\dagger a_n\Big] + \frac{1}{2}\sum_{kqpr} V_{kqpr}\Big[a_k^\dagger a_q^\dagger a_p a_r, \sum_n a_n^\dagger a_n\Big]$$

$$= \sum_k \sum_n E_k \underbrace{[a_k^\dagger a_k, a_n^\dagger a_n]}_{0} + \frac{1}{2}\sum_{kqprn} V_{kqpr}[a_k^\dagger a_q^\dagger a_p a_r, a_n^\dagger a_n]$$

$$[a_k^\dagger a_q^\dagger a_p a_r, a_n^\dagger a_n] = [a_k^\dagger a_q^\dagger a_p a_r, a_n^\dagger] a_n + a_n^\dagger [a_k^\dagger a_q^\dagger a_p a_r, a_n]$$

$$[a_k^\dagger a_q^\dagger a_p a_r, a_n^\dagger] = a_k^\dagger a_q^\dagger a_p [a_r, a_n^\dagger] + a_k^\dagger a_q^\dagger [a_p, a_n^\dagger] a_r + a_k^\dagger \cancel{[a_q^\dagger, a_n^\dagger]}^{\to 0} a_p a_r + \cancel{[a_k^\dagger, a_n^\dagger]}^{\to 0} a_q^\dagger a_p a_r$$

$$= \delta_{rn} a_k^\dagger a_q^\dagger a_p + \delta_{pn} a_k^\dagger a_q^\dagger a_r$$

$$[a_k^\dagger a_q^\dagger a_p a_r, a_n] = a_k^\dagger a_q^\dagger a_p \cancel{[a_r, a_n]}^{\to 0} + a_k^\dagger a_q^\dagger \cancel{[a_p, a_n]}^{\to 0} a_r + a_k^\dagger [a_q^\dagger, a_n] a_p a_r + [a_k^\dagger, a_n] a_q^\dagger a_p a_r$$

$$= -a_k^\dagger a_p a_r \delta_{qn} - \delta_{kn} a_q^\dagger a_p a_r$$

$$[a_k^\dagger a_q^\dagger a_p a_r, a_n^\dagger a_n] = \delta_{rn} \cancel{a_k^\dagger a_q^\dagger a_p a_n} + \delta_{pn} \cancel{a_k^\dagger a_q^\dagger a_r a_n} - \delta_{qn} \cancel{a_n^\dagger a_k^\dagger a_p a_r} - \delta_{kn} \cancel{a_n^\dagger a_q^\dagger a_p a_r}$$

Im fermionischen Fall

$$[a_k^\dagger a_q^\dagger a_p a_r, a_n^\dagger] = a_k^\dagger \{a_q^\dagger a_p a_r, a_n^\dagger\} - \cancelto{0}{\{a_k^\dagger, a_n^\dagger\}} a_q^\dagger a_p a_r$$

$$= a_k^\dagger \left[a_q^\dagger \{a_p a_r, a_n^\dagger\} - \cancelto{0}{\{a_q^\dagger, a_n^\dagger\}} a_p a_r \right]$$

$$= a_k^\dagger a_q^\dagger \left[a_p \{a_r, a_n^\dagger\} - \{a_p, a_n^\dagger\} a_r \right]$$

$$= a_k^\dagger a_q^\dagger a_p \delta_{rn} - a_k^\dagger a_q^\dagger a_r \delta_{pn}$$

$$[a_k^\dagger a_q^\dagger a_p a_r, a_n] = a_k^\dagger a_q^\dagger a_p \cancelto{0}{\{a_r, a_n\}} - \{a_k^\dagger a_q^\dagger a_p, a_n\} a_r$$

$$= - \left[a_k^\dagger a_q^\dagger \cancelto{0}{\{a_p, a_n\}} - \{a_k^\dagger a_q^\dagger, a_n\} a_p \right] a_r$$

$$= \left[a_k^\dagger \{a_q^\dagger, a_n\} - \{a_k^\dagger, a_n\} a_q^\dagger \right] a_p a_r$$

$$= \delta_{qn} a_k^\dagger a_p a_r - \delta_{kn} a_q^\dagger a_p a_r$$

$$[a_k^\dagger a_q^\dagger a_p a_r, a_n^\dagger a_n] = \delta_{rn} a_k^\dagger a_q^\dagger a_p a_n - \delta_{pn} a_k^\dagger a_q^\dagger a_r a_n$$

$$+ \delta_{qn} a_n^\dagger a_k^\dagger a_p a_r - \delta_{kn} a_n^\dagger a_q^\dagger a_p a_r$$

$$= 0$$

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).

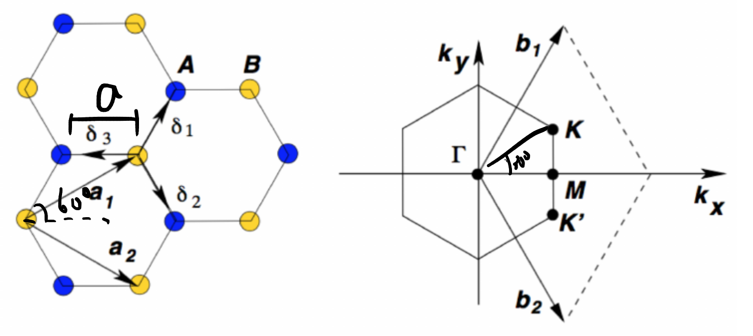

Figure 1: Left: Lattice structure of graphene made out of two interpenetrating triangular lattices ($\mathbf{a}_1$ and $\mathbf{a}_2$ are the lattice unit vectors, and $\boldsymbol{\delta}_i$, $i = 1, 2, 3$ are the nearest neighbour vectors). Right: corresponding Brillouin zone. The Dirac cones are located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

$$\vec{\delta}_1 = a\begin{pmatrix}\cos 60° \\ \sin 60°\end{pmatrix} = \frac{a}{2}\begin{pmatrix}1 \\ \sqrt{3}\end{pmatrix}$$

$$\vec{\delta}_2 = a\begin{pmatrix}\cos 60° \\ -\sin 60°\end{pmatrix} = \frac{a}{2}\begin{pmatrix}1 \\ -\sqrt{3}\end{pmatrix}$$

$$\vec{\delta}_3 = \begin{pmatrix}-a \\ 0\end{pmatrix}$$

$$\vec{a}_1 = \vec{\delta}_1 - \vec{\delta}_3 = \frac{a}{2}\begin{pmatrix}3 \\ \sqrt{3}\end{pmatrix}$$

$$\vec{a}_2 = \frac{a}{2}\begin{pmatrix}3 \\ -\sqrt{3}\end{pmatrix}$$

(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).

Sei $\vec{b}_i = \begin{pmatrix}b_{i1} \\ b_{i2}\end{pmatrix}$

$$\vec{b}_1 \cdot \vec{a}_1 = \frac{a}{2}\left[3 b_{11} + \sqrt{3}\, b_{12}\right] = 2\pi$$

$$\vec{b}_1 \cdot \vec{a}_2 = \frac{a}{2}\left[3 b_{11} - \sqrt{3}\, b_{12}\right] = 0$$

$$3 a b_{11} = 2\pi$$

$$\sqrt{3}\, a b_{12} = 2\pi$$

$$\vec{b}_1 = \frac{2\pi}{a}\begin{pmatrix}1/3 \\ 1/\sqrt{3}\end{pmatrix} = \frac{2\pi}{a\sqrt{3}}\begin{pmatrix}\sqrt{3} \\ 1\end{pmatrix}$$

$$\vec{b}_2 \cdot \vec{a}_1 = \frac{a}{2}\left[3 b_{21} + \sqrt{3}\, b_{22}\right] = 0$$

$$\vec{b}_2 \cdot \vec{a}_2 = \frac{a}{2}\left[3 b_{21} - \sqrt{3}\, b_{22}\right] = 2\pi$$

$$\vec{b}_2 = \frac{2\pi}{a\sqrt{3}} \begin{pmatrix} \sqrt{3} \\ -1 \end{pmatrix}$$

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

$$\vec{\Gamma}_\Gamma = 0$$

$$\vec{\Gamma}_M = \frac{1}{2}\left(\vec{b}_1 + \vec{b}_2\right) = \frac{2\pi}{a\sqrt{3}} \begin{pmatrix} \sqrt{3} \\ 0 \end{pmatrix} = \frac{2\pi}{a} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\vec{\Gamma}_K = \frac{2\pi}{a} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{2\pi}{a} \tan 30^\circ \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$= \frac{2\pi}{a} \begin{pmatrix} 1 \\ 1/\sqrt{3} \end{pmatrix}$$

$$\vec{\Gamma}_{K'} = \frac{2\pi}{a} \begin{pmatrix} 1 \\ -1/\sqrt{3} \end{pmatrix}$$

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.

$$H = -t \sum_{R,\delta} A(R)^\dagger B(R+\delta) + h.c.$$

$$= -\frac{t}{N} \sum_{R,\delta} \sum_{k_1 \in BZ} \sum_{k_2 \in BZ} A(k_1)^\dagger e^{-ik_1 R} B(k_2) e^{ik_2(R+\delta)} + h.c.$$

$$= -\frac{t}{N} \sum_{R,\delta} \sum_{k_1 \in BZ} \sum_{k_2 \in BZ} A(k_1)^\dagger B(k_2) e^{i(k_2 - k_1)R} e^{ik_2\delta} + h.c.$$

$$= -t \sum_{\delta} \sum_{k_1 \in BZ} \sum_{k_2 \in BZ} A(k_1)^\dagger B(k_2)\, \delta_{k_1,k_2} e^{ik_2\delta} + h.c.$$

$$= -t \sum_{\delta} \sum_{k \in BZ} A(k)^\dagger B(k) e^{ik\delta} + h.c.$$

$$= -t \sum_{k \in BZ} \sum_{\delta} \left[A(k)^\dagger B(k)\, e^{ik\delta} + B(k)^\dagger A(k) e^{-ik\delta} \right]$$

$$\sum_\delta e^{ik\delta} = e^{i\left[\frac{k_x a}{2} + \frac{\sqrt{3}k_y a}{2}\right]} + e^{i\left[\frac{k_x a}{2} - \frac{\sqrt{3}k_y a}{2}\right]} + e^{-ik_x a}$$

$$= e^{-ik_x a} + 2e^{i\frac{k_x a}{2}} \cos\frac{\sqrt{3}k_y a}{2} = f(\vec{k})$$

$$\sum_\delta e^{-ik\delta} = e^{ik_x a} + 2e^{-\frac{ik_x a}{2}} \cos\frac{\sqrt{3}k_y a}{2} = f^*(\vec{k})$$

Daher $\quad H = \sum_k \Psi^\dagger(\vec{k})\, h(\vec{k})\, \Psi(\vec{k})$

(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).

$$\varepsilon_\pm(\vec{k}) = \pm |f(\vec{k})|$$