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Höhere Quantenmechanik

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Exercise sheet 9

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Evaluation der Lehrveranstaltung am 21.06.22
`https://itp.uni-frankfurt.de/~gros/Vorlesungen/QM_2/QM2_evaluation_22.pdf`

Exercise 1: spin operators for fermions *(12 Points)*

We consider a fermionic particle with spin $S = 1/2$ (e.g., an electron), which can be described by the annihilation and creation operators c_α and $c_\alpha^\dagger$. The index α can take the values $\alpha = 1 = \uparrow$ and $\alpha = 2 = \downarrow$, which indicate, respectively, whether the spin of the particle points up or down (with respect to a certain arbitrary S_z axis). The fermionic operators satisfy the anticommutation relation

$$[c_\alpha, c_\beta]_+ = 0 \qquad [c_\alpha^\dagger, c_\beta^\dagger]_+ = 0 \qquad [c_\alpha, c_\beta^\dagger]_+ = \delta_{\alpha,\beta} \tag{1}$$

We can define the spin operators for the fermionic particle as

$$S_a = \frac{\hbar}{2} \sum_{\alpha,\beta} c_\alpha^\dagger \sigma^a_{\alpha,\beta} c_\beta \tag{2}$$

where $a = x, y, z$ indicates the spin component and σ^a is the corresponding Pauli matrix. Within this notation, Greek indices run over $1, 2$ (or, equivalently, $\uparrow, \downarrow$), while Latin indices label the x, y, z components of the spin. Note: superscripts/subscripts don't have any special meaning!

(i) Show that the definition of Eq. (2) satisfies the usual commutation relations of the spin operators, i.e.

$$[S_x, S_y]_- = i\hbar S_z \qquad [S_y, S_z]_- = i\hbar S_x \qquad [S_z, S_x]_- = i\hbar S_y$$

(7 Points)

Hint 1: you can prove the three equations one by one, or, alternatively, you can pursue a general proof by starting from the expression

$$[S_a, S_b]_- = i\hbar \sum_{c=1}^{3} \varepsilon_{a,b,c} S_c,$$

where a, b, c are the component indices (1 for x, 2 for y, 3 for z), and $\varepsilon_{a,b,c}$ is the Levi-Civita symbol.

Hint 2: for three generic operators, A,B,C, the following properties of commutators and anticommutators hold

$$[A, BC]_- = [A, B]_- C + B[A, C]_-$$
$$[AB, C]_- = A[B, C]_- + [A, C]_- B$$
$$[AB, C]_- = A[B, C]_+ - [A, C]_+ B$$

For Pauli matrices, the following holds

$$\sigma^a \sigma^b = \delta_{a,b} \mathbb{1} + i \sum_c \varepsilon_{a,b,c} \sigma^c$$

where a, b, c are the component indices (1 for x, 2 for y, 3 for z), and $\mathbb{1}$ the identity matrix.

(ii) Apply the S_z operator to the state $|\uparrow\rangle = c^\dagger_\uparrow |0\rangle$ or $|\downarrow\rangle = c^\dagger_\downarrow |0\rangle$. What do you get? Comment the result. *(2 Points)*

(iii) How do the S_+ and S_- operators look like? Discuss the result. *(2 Points)*

(iv) Suppose that the spin-$\frac{1}{2}$ fermionic operators of this exercise create/destroy electrons in a certain s-orbital. The state $|\uparrow\downarrow\rangle = c^\dagger_\uparrow c^\dagger_\downarrow |0\rangle$ corresponds to a filled orbital (no other electrons can be added). What is the result of $S^2 |\uparrow\downarrow\rangle$ (with $S^2 = S_x^2 + S_y^2 + S_z^2$)? Don't do any calculation, just use physical arguments. *(1 Point)*

Exercise 2: one-body operators in second quantization, fields *(8 Points)*

As discussed in the lecture notes, in second quantization we define annihilation and creation operators by choosing a certain basis of single-particle states. Let us consider identical bosonic particles in this exercise. If we choose the complete orthonormal basis $\{|\alpha\rangle\}$, we can write the annihilation and creation operators as $\hat{b}_\alpha$ and $\hat{b}^\dagger_\alpha$, which respectively destroy and create a particle in the single-particle state $|\alpha\rangle$. These operators satisfy the commutation relations discussed in the notes. Many-particle states are then obtained by successive application of the creation operator on the vacuum state. Thanks to the commutation properties, the many-particle states satisfy the correct properties for identical particles, i.e., in the case of bosons they are symmetric under the exchange of two particles.

Obviously, the choice of the single-particle basis is not unique. We could choose another basis, $\{|n\rangle\}$, and write the transformation between the annihilation/creation operators in the two bases as follows

$$\hat{b}_n = \sum_\alpha \langle n|\alpha\rangle \hat{b}_\alpha$$
$$\hat{b}^\dagger_n = \sum_\alpha (\langle n|\alpha\rangle)^* \hat{b}^\dagger_\alpha = \sum_\alpha \langle \alpha|n\rangle \hat{b}^\dagger_\alpha$$

Note: in this exercise we use a "hat" to denote operators in order to avoid confusion.

(i) Consider the special case of the eigenbasis of the position operator $\hat{x}$, which we denote by $\{|x\rangle\}$. For simplicity, we imagine to be in one dimension. The annihilation and creation operators in the position basis are usually called *field operators* and written as

$$\hat{\psi}(x) = \sum_\alpha \langle x|\alpha\rangle \hat{b}_\alpha = \sum_\alpha \varphi_\alpha(x) \hat{b}_\alpha$$
$$\hat{\psi}^\dagger(x) = \sum_\alpha \langle \alpha|x\rangle \hat{b}^\dagger_\alpha = \sum_\alpha \varphi^*_\alpha(x) \hat{b}^\dagger_\alpha$$

They destroy or create a particle in the position x. Their expansion in terms of $\hat{b}_\alpha$ and $\hat{b}_\alpha^\dagger$ involves the wave functions $\varphi_\alpha(x)$ and $\varphi_\alpha^*(x)$.

Show that the following commutation relations hold

$$[\hat{\psi}(x), \hat{\psi}(x')]_- = 0 \qquad [\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')]_- = 0 \qquad [\hat{\psi}(x), \hat{\psi}^\dagger(x')]_- = \delta(x - x')$$

(2 Points)

(ii) Single-particle operators can be written in the form of Eq.(6.8) of the lecture notes, i.e. $\hat{O} = \sum_{i=1}^N \hat{o}(i)$, where $\hat{o}(i)$ is an operator that acts only on the i-th particle (N is the total number of particles in the system). The argument i just tells us on which particle the operator $\hat{o}$ acts.

In second quantization, using annihilation/creation operators of a generic basis $\{|\alpha\rangle\}$, single-particle operators $\hat{O}$ are expressed as

$$\hat{O} = \sum_{\alpha,\alpha'} \langle\alpha|\hat{o}|\alpha'\rangle \hat{b}_\alpha^\dagger \hat{b}_{\alpha'} \tag{3}$$

Using this formula, express the position operator (i.e., take $\hat{o} = \hat{x}$) in terms of the annihilation/creation operators of the basis $\{|x\rangle\}$ (i.e., the field operators $\hat{\psi}(x)$ and $\hat{\psi}^\dagger(x)$).

(2 Points)

(iii) Express the density operator $\hat{N}_r = \sum_{i=1}^N \hat{n}_r(i)$ in terms of the annihilation/creation operators of the basis $\{|x\rangle\}$ (i.e., the field operators $\hat{\psi}(x)$ and $\hat{\psi}^\dagger(x)$). You should use Eq. (3) with

$$\hat{o} = \hat{n}_r = \delta(\hat{x} - r), \tag{4}$$

where r is a certain position in space. *(2 Points)*

(iv) We now introduce the basis of plane waves $\{|k\rangle\}$, where $\langle x|k\rangle = \frac{1}{\sqrt{V}} e^{ikx}$ (V being the volume of the system). Express the density operator in terms of creation and annihilation operators of the $\{|k\rangle\}$ basis. Use Eq. (3) with $\hat{o} = \hat{n}_r = \delta(\hat{x} - r)$. Compare the result to the one of the previous point. *(2 Points)*