Condensed Matter Theory I   WS 2022/2023

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Solutions to sheet 0

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1. Boson and fermion operators

Let $b^\dagger$ and $f^\dagger$ be the creation operators of a boson and a fermion, respectively. We write $[\dots]$ for the commutator and $\{\dots\}$ for the anti-commutator. Calculate the following expressions:

(a) $\left[b^\dagger b, b^\dagger\right]$ and $\left\{f^\dagger f, f^\dagger\right\}$

(b) $\left[b^\dagger b, b\right]$ and $\left\{f^\dagger f, f\right\}$

(c) $\left[e^{-b^\dagger b}, b\right]$ *(hint: expand exponential in power series)*

(d) $\left\{e^{-f^\dagger f}, f\right\}$

Solution:

(a) For the bosons, we use $\left[b^\dagger, b^\dagger\right] = 0$ and $\left[b, b^\dagger\right] = 1$:

$$\left[b^\dagger b, b^\dagger\right] = b^\dagger \left[b, b^\dagger\right] + \left[b^\dagger, b^\dagger\right] b = b^\dagger$$

For the fermions, we use the Pauli principle, i.e. $\left(f^\dagger\right)^2 = 0$, and $\left\{f, f^\dagger\right\} = 1$:

$$\left\{f^\dagger f, f^\dagger\right\} = f^\dagger f f^\dagger + \left(f^\dagger\right)^2 f = -\left(f^\dagger\right)^2 f + f^\dagger = f^\dagger$$

(b)

$$\left[b^\dagger b, b\right] = b^\dagger \left[b, b\right] + \left[b^\dagger, b\right] b = -b$$

$$\left\{f^\dagger f, f\right\} = f^\dagger f^2 + f f^\dagger f = -f^\dagger f^2 + f = f$$

(c) We express the exponential function as a power series:

$$\left[e^{-b^\dagger b}, b\right] = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left[\left(b^\dagger b\right)^n, b\right]$$

To evaluate $\left[\left(b^\dagger b\right)^n, b\right]$, we show that

$$\left(b^\dagger b\right)^n b = b \left(b^\dagger b - 1\right)^n \ . \tag{1}$$

This is true for $n = 0$. Going from n to $n+1$, we find

$$\left(b^\dagger b\right)^{n+1} b = b^\dagger b b \left(b^\dagger b - 1\right)^n = b \left(b^\dagger b - 1\right) \left(b^\dagger b - 1\right)^n = b \left(b^\dagger b - 1\right)^{n+1} \ , \tag{2}$$

which proves Eq. (1). Thus,

$$\left[\left(b^\dagger b\right)^n, b\right] = b \left(b^\dagger b - 1\right)^n - b \left(b^\dagger b\right)^n \ .$$

Inserting this in the series expansion, we find

$$\left[e^{-b^\dagger b}, b\right] = b e^{-b^\dagger b + 1} - b e^{-b^\dagger b} = (e-1) b e^{-b^\dagger b} \tag{3}$$

(d) We use the series expansion as in the previous task, but for fermions we use

$$\left(f^\dagger f\right)^2 = f^\dagger f f^\dagger f = -\left(f^\dagger\right)^2 f^2 + f^\dagger f = f^\dagger f$$

and thereby $\left(f^\dagger f\right)^n = f^\dagger f$. Recall that $f^\dagger f$ is the number operator, which can only yield 1 or 0 for fermions. We obtain

$$\begin{aligned}\left\{e^{-f^\dagger f}, f\right\} &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left\{\left(f^\dagger f\right)^n, f\right\} = \{1, f\} + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \left\{f^\dagger f, f\right\} \\ &= 2f + \frac{1-e}{e} f = \frac{e+1}{e} f\end{aligned}$$

2. Many-particle quantum states

We consider a system where the (normalized) single-particle orbitals $\phi_\lambda(\mathbf{r})$ are known, where $\mathbf{r}$ denotes the position coordinate.

(a) Let the system be populated by three identical spinless bosons in the states λ_1, λ_2, λ_3. Write down the normalized three-particle wave-function $\psi_{\lambda_1\lambda_2\lambda_3}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ with proper bosonic symmetry! Beware that $\lambda_1, \lambda_2, \lambda_3$ are not necessarily different and distinguish all possible cases.

Solution: There are three cases, depending on the number of *different* occupied single-particle states. In each case, the three-particle wavefunction must be constructed as a symmetric linear combination of all possible permutations of single-particle states, such that ψ is invariant under particle exchange.

(i) three different states, $\lambda_1 \neq \lambda_2 \neq \lambda_3 \neq \lambda_1$

$$\begin{aligned}\psi_{\lambda_1,\lambda_2,\lambda_3}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \frac{1}{\sqrt{6}} \Big[&\phi_{\lambda_1}(\mathbf{r}_1)\phi_{\lambda_2}(\mathbf{r}_2)\phi_{\lambda_3}(\mathbf{r}_3) + \phi_{\lambda_1}(\mathbf{r}_1)\phi_{\lambda_2}(\mathbf{r}_3)\phi_{\lambda_3}(\mathbf{r}_2) \\ &+\phi_{\lambda_1}(\mathbf{r}_2)\phi_{\lambda_2}(\mathbf{r}_1)\phi_{\lambda_3}(\mathbf{r}_3) + \phi_{\lambda_1}(\mathbf{r}_2)\phi_{\lambda_2}(\mathbf{r}_3)\phi_{\lambda_3}(\mathbf{r}_1) \\ &+\phi_{\lambda_1}(\mathbf{r}_3)\phi_{\lambda_2}(\mathbf{r}_1)\phi_{\lambda_3}(\mathbf{r}_2) + \phi_{\lambda_1}(\mathbf{r}_3)\phi_{\lambda_2}(\mathbf{r}_2)\phi_{\lambda_3}(\mathbf{r}_1)\Big]\end{aligned}$$

(ii) two different states (two particles in the same state), w.l.o.g. $\lambda_1 = \lambda_2 \neq \lambda_3$

$$\begin{aligned}\psi_{\lambda_1,\lambda_1,\lambda_3}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \frac{1}{\sqrt{3}} \Big[&\phi_{\lambda_1}(\mathbf{r}_1)\phi_{\lambda_1}(\mathbf{r}_2)\phi_{\lambda_3}(\mathbf{r}_3) + \phi_{\lambda_1}(\mathbf{r}_1)\phi_{\lambda_1}(\mathbf{r}_3)\phi_{\lambda_3}(\mathbf{r}_2) \\ &+\phi_{\lambda_1}(\mathbf{r}_2)\phi_{\lambda_1}(\mathbf{r}_3)\phi_{\lambda_3}(\mathbf{r}_1)\Big]\end{aligned}$$

(ii) all particles occupy the same state, $\lambda_1 = \lambda_2 = \lambda_3$

$$\psi_{\lambda_1,\lambda_1,\lambda_1}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \phi_{\lambda_1}(\mathbf{r}_1)\phi_{\lambda_1}(\mathbf{r}_2)\phi_{\lambda_1}(\mathbf{r}_3)$$

(b) Now assume that there is only one spatial orbital $\phi(\mathbf{r})$, but we fill the system with three bosons of spin $S = 2$. How many independent three-particle states exist in this system?

Solution: Now the single-particle states gain a spin quantum number, namely $\sigma \in \{-2, -1, 0, 1, 2\}$. Thus, one spatial orbital yields 5 distinct states. There are three cases depending on how many of the bosons have the same σ:

(i) $\sigma_1 \neq \sigma_2 \neq \sigma_3 \neq \sigma_1$: There are $\binom{5}{3} = 10$ possibilities to distribute the bosons on the different spin states. This equals the amount of independent three-particle states.

(ii) $\sigma_1 = \sigma_2 \neq \sigma_3$: 5 possibilities for σ_1 times 4 possibilities to pick a different σ_3, thus 20 independent three-particle states.

(iii) $\sigma_1 = \sigma_2 = \sigma_3$: 5 distinct states.

In total, there are 35 independent three-boson wavefunctions.

(c) How many spin-$\frac{1}{2}$ fermions or spin-$\frac{3}{2}$ fermions could one place in one spatial orbital $\phi(\mathbf{r})$? Write down the Slater determinant for the second case. State explicitly the normalization factor.

Solution: Only two spin-$\frac{1}{2}$ fermions (e.g., electrons) fit in one orbital with $\sigma_1 =\uparrow$ and $\sigma_2 =\downarrow$, respectively. For spin-$\frac{3}{2}$ fermions, $\sigma \in \{-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}\}$. Thus, up to 4 such fermions can exist in the system without violation of the Pauli principle. Indicating the spin part of the single-particle states by χ_σ, the corresponding four-fermion wavefunction can be expressed in terms of the Slater determinant

$$\begin{aligned}\psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \mathbf{r}_3\sigma_3, \mathbf{r}_4\sigma_4) &= \phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\phi(\mathbf{r}_3)\phi(\mathbf{r}_4) \times \\ & C \begin{vmatrix} \chi_{-\frac{3}{2}}(\sigma_1) & \chi_{-\frac{1}{2}}(\sigma_1) & \chi_{\frac{1}{2}}(\sigma_1) & \chi_{\frac{3}{2}}(\sigma_1) \\ \chi_{-\frac{3}{2}}(\sigma_2) & \chi_{-\frac{1}{2}}(\sigma_2) & \chi_{\frac{1}{2}}(\sigma_2) & \chi_{\frac{3}{2}}(\sigma_2) \\ \chi_{-\frac{3}{2}}(\sigma_3) & \chi_{-\frac{1}{2}}(\sigma_3) & \chi_{\frac{1}{2}}(\sigma_3) & \chi_{\frac{3}{2}}(\sigma_3) \\ \chi_{-\frac{3}{2}}(\sigma_4) & \chi_{-\frac{1}{2}}(\sigma_4) & \chi_{\frac{1}{2}}(\sigma_4) & \chi_{\frac{3}{2}}(\sigma_4) \end{vmatrix}\end{aligned}$$

with the normalization factor $C = \dfrac{1}{\sqrt{4!}}$.