Exercise 1. ***Playing around with wave functions in second quantization.***

In the formalism of second quantization, a general state of N particles at positions $\vec{r}_1$, $\vec{r}_2$, ... is given by

$$|\vec{r}_1, \vec{r}_2, ..., \vec{r}_N\rangle = \frac{1}{\sqrt{N!}} \hat{\Psi}^\dagger (r_N) \cdots \hat{\Psi}^\dagger (r_1) |0\rangle \ , \tag{1}$$

where $|0\rangle$ is the vacuum state and the field operators $\hat{\Psi}(\vec{r})$ are defined as

$$\hat{\Psi}(\vec{r}) = \sum_k \phi_k(\vec{r}) \ \hat{a}_k \ , \tag{2}$$

with $\hat{a}_k$ the annihilator of mode k and $\phi_k(\vec{r})$ the one-particle wave function of mode k.

Consider a state $|\psi\rangle$ of three particles in modes k_1, k_2, and k_3. Consider its wave function

$$\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \langle \vec{r}_1, \vec{r}_2, \vec{r}_3 | \psi \rangle = \langle \vec{r}_1, \vec{r}_2, \vec{r}_3 | \hat{a}^\dagger_{k_3} \hat{a}^\dagger_{k_2} \hat{a}^\dagger_{k_1} |0\rangle \ . \tag{3}$$

(a) First calculate the vacuum expectation value

$$\langle 0 | \hat{a}_{\ell_1} \hat{a}_{\ell_2} \hat{a}_{\ell_3} \hat{a}^\dagger_{k_3} \hat{a}^\dagger_{k_2} \hat{a}^\dagger_{k_1} |0\rangle \ , \tag{4}$$

for bosons and for fermions.

Solution. Let's calculate using the usual (anti-)commutation relations (write for short $\hat{a}_3 = \hat{a}_{k_3}$, $\hat{a}_2 = \hat{a}_{k_2}$, $\hat{a}_1 = \hat{a}_{k_1}$):

$$\begin{aligned}
\hat{a}_l \hat{a}_m \hat{a}_n \hat{a}^\dagger_3 \hat{a}^\dagger_2 \hat{a}^\dagger_1 &= \hat{a}_l \hat{a}_m \left[\delta_{nk_3} \pm \hat{a}^\dagger_3 \hat{a}_n\right] \hat{a}^\dagger_2 \hat{a}^\dagger_1 = \hat{a}_l \left[\hat{a}_m \delta_{nk_3} \pm \left(\delta_{mk_3} \pm \hat{a}^\dagger_3 \hat{a}_m\right) \hat{a}_n\right] \hat{a}^\dagger_2 \hat{a}^\dagger_1 \\
&= \left[\hat{a}_l \hat{a}_m \delta_{nk_3} \pm \hat{a}_l \delta_{mk_3} \hat{a}_n + \delta_{lk_3} \hat{a}_m \hat{a}_n\right] \hat{a}^\dagger_2 \hat{a}^\dagger_1 + \hat{a}^\dagger(\ldots) \\
&= \left[\left(\hat{a}_l \delta_{mk_2} \pm \delta_{lk_2} \hat{a}_m\right) \delta_{nk_3} \pm \delta_{mk_3} \left(\hat{a}_l \delta_{nk_2} \pm \delta_{lk_2} \hat{a}_n\right) + \delta_{lk_3} \left(\hat{a}_m \delta_{nk_2} \pm \delta_{mk_2} \hat{a}_n\right)\right] \hat{a}^\dagger_1 + \hat{a}^\dagger(\ldots) \\
&= \delta_{lk_1} \delta_{mk_2} \delta_{nk_3} \pm \delta_{lk_2} \delta_{mk_1} \delta_{nk_3} \pm \delta_{lk_1} \delta_{mk_3} \delta_{nk_2} + \delta_{lk_2} \delta_{mk_3} \delta_{nk_1} + \delta_{lk_3} \delta_{mk_1} \delta_{nk_2} \pm \delta_{lk_3} \delta_{mk_2} \delta_{nk_1} + \hat{a}^\dagger(\ldots) \\
&= \sum_{ijk} f_{ijk} \delta_{lk_i} \delta_{mk_j} \delta_{nk_k} + \hat{a}^\dagger(\ldots) \ ,
\end{aligned} \tag{S.1}$$

where the sum ranges over all sets of indices ijk which are all different, and where $f_{ijk} = \epsilon_{ijk}$ is the fully antisymmetric tensor (Levi-Civita) for fermions and $f_{ijk} = 1$ for bosons. We do not care about the terms which start by a creation operator (all symbolized above by $\hat{a}^\dagger(\ldots)$), because they will vanish once sandwiched between vacuum states. The vacuum expectation value is then

$$\langle 0 | \hat{a}_l \hat{a}_m \hat{a}_n \hat{a}^\dagger_3 \hat{a}^\dagger_2 \hat{a}^\dagger_1 |0\rangle = \sum_{ijk} f_{ijk} \delta_{lk_i} \delta_{mk_j} \delta_{nk_k} \ . \tag{S.2}$$

For N particles, by similar procedure the expression generalizes to

$$\langle 0 | \hat{a}_{\ell_1} \ldots \hat{a}_{\ell_N} \hat{a}^\dagger_{k_N} \ldots \hat{a}^\dagger_{k_1} |0\rangle = \sum_{i_1 \ldots i_N} f_{i_1 \ldots i_N} \delta_{\ell_1 k_{i_1}} \ldots \delta_{\ell_N k_{i_N}} \ . \tag{S.3}$$

(b) Determine $\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ for bosons and for fermions. What symmetries does the wave function possess?

Solution. The wave function is

$$\psi(\vec{r}_1,\vec{r}_2,\vec{r}_3) = \frac{1}{\sqrt{N!}}\langle 0|\hat{\Psi}_1\hat{\Psi}_2\hat{\Psi}_3\hat{a}_3^\dagger\hat{a}_2^\dagger\hat{a}_1^\dagger|0\rangle = \frac{1}{\sqrt{N!}}\sum_{lmn}\phi_l^*(\vec{r}_1)\phi_m^*(\vec{r}_2)\phi_n^*(\vec{r}_3)\,\langle 0|\hat{a}_l\hat{a}_m\hat{a}_n\hat{a}_3^\dagger\hat{a}_2^\dagger\hat{a}_1^\dagger|0\rangle$$
$$= \frac{1}{\sqrt{N!}}\sum f_{ijk}\,\delta_{lk_i}\delta_{mk_j}\delta_{nk_k}\phi_l^*(\vec{r}_1)\phi_m^*(\vec{r}_2)\phi_n^*(\vec{r}_3) = \frac{1}{\sqrt{N!}}\sum f_{ijk}\,\phi_{k_i}^*(\vec{r}_1)\phi_{k_j}^*(\vec{r}_2)\phi_{k_k}^*(\vec{r}_3)\ . \quad \text{(S.4)}$$

Thus, the wave function is an explicit symmetrization (antisymmetrization) of $\phi_{k_1}^*(\vec{r}_1)\phi_{k_2}^*(\vec{r}_2)\phi_{k_3}^*(\vec{r}_3)$ for bosons (fermions).

(c) Determine the normalization of the wave function for fermions and for bosons. First consider the case where k_1, k_2 and k_3 are all different, and then study the case where two or more modes are the same. What do you observe?

Solution. Recall the wave function is given by

$$\psi(\vec{r}_1,\vec{r}_2,\vec{r}_3) = \frac{1}{\sqrt{3!}}\sum_{ijk} f_{ijk}\,\phi_{k_i}^*(\vec{r}_1)\phi_{k_j}^*(\vec{r}_2)\phi_{k_k}^*(\vec{r}_3)\ , \quad \text{(S.5)}$$

and thus its normalization is

$$\int d^3\vec{r}_1 d^3\vec{r}_2 d^3\vec{r}_3\ \psi^*(\vec{r}_1,\vec{r}_2,\vec{r}_3)\,\psi(\vec{r}_1,\vec{r}_2,\vec{r}_3)$$
$$= \frac{1}{3!}\sum f_{ijk}f_{i'j'k'}\int d^3\vec{r}_1 d^3\vec{r}_2 d^3\vec{r}_3\ \phi_{k_i}^*(\vec{r}_1)\phi_{k_{i'}}(\vec{r}_1)\ \phi_{k_j}^*(\vec{r}_2)\phi_{k_{j'}}(\vec{r}_2)\ \phi_{k_k}^*(\vec{r}_3)\phi_{k_{k'}}(\vec{r}_3)$$
$$= \frac{1}{3!}\sum f_{ijk}f_{i'j'k'}\int d^3\vec{r}_1\,\phi_{k_i}^*(\vec{r}_1)\phi_{k_{i'}}(\vec{r}_1)\int d^3\vec{r}_2\,\phi_{k_j}^*(\vec{r}_2)\phi_{k_{j'}}(\vec{r}_2)\int d^3\vec{r}_3\,\phi_{k_k}^*(\vec{r}_3)\phi_{k_{k'}}(\vec{r}_3)$$
$$= \frac{1}{3!}\sum f_{ijk}f_{i'j'k'}\ \delta_{k_ik_{i'}}\ \delta_{k_jk_{j'}}\ \delta_{k_kk_{k'}}\ . \quad \text{(S.6)}$$

This expression obviously generalizes to N particles as

$$\langle\psi|\psi\rangle = \frac{1}{N!}\sum_{\substack{i_1\ldots i_N,\\ i'_1\ldots i'_N}} f_{i_1\ldots i_N}f_{i'_1\ldots i'_N}\ \delta_{k_{i_1}k_{i'_1}}\cdots\delta_{k_{i_N}k_{i'_N}}\ . \quad \text{(S.7)}$$

Assuming that k_1, k_2, k_3 are all different in (S.6), then all terms in the sum that don't satisfy $i = i', j = j', k = k'$ vanish because of the orthgonality of the single-particle states, and thus

$$\langle\psi|\psi\rangle = \frac{1}{3!}\sum f_{ijk}^2\,\delta_{k_ik_{i'}}\delta_{k_jk_{j'}}\delta_{k_kk_{k'}} = \frac{1}{3!}\sum f_{ijk}^2 = 1\ . \quad \text{(S.8)}$$

Additionally, if two or more modes are equal (e.g., $k_1 = k_2$), then all possible permutations of matching modes must be included (e.g., if $k_1 = k_2$, then the term $i = j', j = i', k = k'$ also needs to be counted in the above), multiplying the result by an additional factor $N_n!$ for each repeated mode n (N_n then being the number of particles in mode n):

$$\langle\psi|\psi\rangle = N_1!\cdots = \prod_{\text{modes}} N_n! \quad \text{(S.9)}$$

Of course, for fermions N_n is either zero or one, such that these factors do not contribute. However they must be included for bosons.

Note: for the lazy, it is also possible to do the whole exercise with two particles only. For the motivated, calculate it for N particles.

Exercise 2. ***Correlation functions in 1D***

Consider particles of mass m in 1 dimension that sit on a ring of (very large) length L (this is a system with periodic boundary conditions).

(a) Calculate the pair correlation function for fermions in the cases $T = 0$ and in the limit of high temperature. How do the resulting functions differ from the 3 dimensional case? Try to give a physical interpretation and explanation for what you find.

Solution. Similarly to what is done in the lectures, we have for fermions for equal spin that

$$(\frac{n}{2})^2 g_2(r-r') = (1/L)^2 \sum_{k,k',q,q'} e^{-i(k-k')r} e^{-i(q-q')r'} \langle a_k^\dagger a_q^\dagger a_{q'} a_{k'} \rangle \tag{S.10}$$

$$= (1/L)^2 \sum_{k,k',q,q'} \langle n_k \rangle \langle n_q \rangle (1 - e^{-i(k-q)(r-r')}) \tag{S.11}$$

$$= \left(\frac{n}{2}\right)^2 (1 - g_1(r-r')^2). \tag{S.12}$$

Now we calculate g_1 for the $T = 0$ as

$$\frac{n}{2} g_1(r-r') = (1/L) \int_{-k_F}^{k_F} \frac{L}{2\pi} e^{-ik(r-r')} \tag{S.13}$$

$$= \frac{1}{\pi} \sin(k_F(r-r'))/(r-r') \tag{S.14}$$

$$= \frac{n}{2k_F} \sin(k_F(r-r'))/(r-r'), \tag{S.15}$$

and thus

$$g_2(r-r') = \left(1 - \frac{1}{k_F^2} \frac{\sin^2(k_F(r-r'))}{(r-r')^2}\right). \tag{S.16}$$

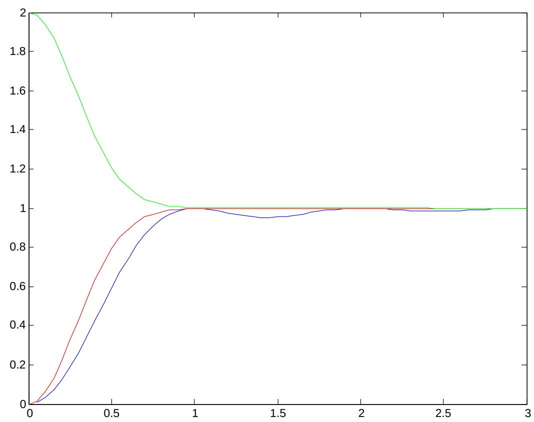

Figure 1: 1D pair correlation functions for fermions (blue: T=0, red: T large) and bosons (green: T large).

This, as in the 3 dimensional case, exhibits fluctuations that drop with the distance between the particles. In 1 D, however, they are much stronger than for 3 dimensions: the particles are much more likely to localise among the ring with equal spacing (see Figure 1). The reason for this is that in 1D in k-space there are less available modes for a particular distance dk than in 3 D (for a particular dk the modes are points on a line instead of densely occupying a shell in 3 D). The impact of occupied modes is hence much stronger than in 3D.

For large temperatures, we can take the Maxwell-Boltzmann distribution $\langle n_k \rangle = n\sqrt{\pi}Ae^{-k^2/A^2}$ with $A^2 = \frac{2mk_BT}{\hbar^2} = \frac{4\pi}{\lambda^2}$

$$\frac{n}{2}g_s(r-r') \approx \int dk \frac{1}{2\pi} e^{-ik(r-r')} \langle n_k \rangle \tag{S.17}$$

$$= \frac{n}{2} e^{-(r-r')^2\pi/\lambda^2} \tag{S.18}$$

Hence

$$g_2(r-r') = (1 - e^{-2(r-r')^2\pi/\lambda^2}), \tag{S.19}$$

which is the same result as in 3D.

(b) Do the same for bosons, distinguishing the low temperature case (condensate) and the high temperature limit. Again, comment on the differences to the corresponding results in $3D$ and their relations to the fermionic case.

Solution. The result for $T = 0$ is exactly the same as in the lecture notes, namely

$$g_2(r-r') = \frac{N(N-1)}{V^2}. \tag{S.20}$$

In the high temperature limit, we get

$$n^2 g_2(r-r') \approx n^2 + \left| \int dk \frac{1}{2\pi} e^{-ik(r-r')} \langle n_k \rangle \right|^2 \tag{S.21}$$

$$= n^2(1 + e^{-2\pi(r-r')^2/\lambda^2}), \tag{S.22}$$

which is again the same as in 3D.