Statistical physics cheat sheet

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1 Fock-states

$$|0\rangle = |0,0,0,\dots\rangle$$
$$\langle 0|0\rangle = \langle \dots,0,0,0|0,0,0,\dots\rangle = 1$$
$$\langle \dots, n_i', \dots, n_2', n_1'|n_1, n_2, \dots, n_i, \dots\rangle = \dots \times \delta_{n_1 n_1'} \times \delta_{n_2 n_2'} \times \dots \times \delta_{n_i n_i'} \times \dots$$

2 Creation and annihillation operators

2.1 Fermionic creation and annihillation operators

$$\hat{a}_k^\dagger |n_1, \dots, n_k, \dots\rangle = \sqrt{1-n_k}(-1)^{\Sigma_k} |n_1, \dots, 1+n_k, \dots\rangle$$
$$\hat{a}_k |n_1, \dots, n_k, \dots\rangle = \sqrt{n_k}(-1)^{\Sigma_k} |n_1, \dots, 1-n_k, \dots\rangle$$
$$n_k \in \{0,1\},\ \Sigma_k = \sum_{j=1}^{k-1} n_j$$
$$\hat{a}_k^\dagger |n_1, \dots, n_{k-1}, 1, n_{k+1}, \dots\rangle = 0$$
$$\hat{a}_k |n_1, \dots, n_{k-1}, 0, n_{k+1}, \dots\rangle = 0$$
$$\hat{a}_k = (\hat{a}_k^\dagger)^\dagger$$

Anticommutation relations:

$$\{\hat{a}_k, \hat{a}_l^\dagger\} = \hat{a}_k \hat{a}_l^\dagger + \hat{a}_l^\dagger \hat{a}_k = \delta_{kl}$$
$$\{\hat{a}_k, \hat{a}_l\} = \{\hat{a}_k^\dagger, \hat{a}_l^\dagger\} = 0$$

2.2 Bosonic creation and annihillation operators

$$\hat{a}_k^\dagger |n_1, \dots, n_k, \dots\rangle = \sqrt{1+n_k}\, |n_1, \dots, n_k+1, \dots\rangle$$
$$\hat{a}_k |n_1, \dots, n_k, \dots\rangle = \sqrt{n_k}\, |n_1, \dots, n_k-1, \dots\rangle$$
$$n_k \in \{0,1,\dots\}$$
$$\hat{a}_k^\dagger |n_1, \dots, n_{k-1}, 1, n_{k+1}, \dots\rangle = 0$$
$$\hat{a}_k |n_1, \dots, n_{k-1}, 0, n_{k+1}, \dots\rangle = 0$$

Commutation relations:

$$[\hat{a}_k, \hat{a}_l^\dagger] = \hat{a}_k \hat{a}_l^\dagger + \hat{a}_l^\dagger \hat{a}_k = \delta_{kl}$$
$$[\hat{a}_k, \hat{a}_l] = [\hat{a}_k^\dagger, \hat{a}_l^\dagger] = 0$$

For bosons only:

$$|n_1, \dots, n_k, \dots\rangle = \frac{1}{\sqrt{\prod_{i=1}^{\infty} n_i!}} (\hat{a}_1^\dagger)^{n_1} \times (\hat{a}_2^\dagger)^{n_2} \times \dots \times (\hat{a}_k^\dagger)^{n_k} \times \dots |0\rangle\,.$$

For both bosons and fermions:

- $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$ gives the number of particles in the k-th eigenstate:

$$\hat{n}_k |n_1, \dots, n_k, \dots\rangle = n_k |n_1, \dots, n_k, \dots\rangle\,.$$

- $\hat{N} = \sum_k \hat{n}_k$ gives the total number of particles:

$$\hat{N} \left| n_1, \ldots, n_k, \ldots \right\rangle = \sum_{j=1}^{\infty} n_j \left| n_1, \ldots, n_k, \ldots \right\rangle = N \left| n_1, \ldots, n_k, \ldots \right\rangle .$$

- $\langle 0|0\rangle = 1$
- $\langle 0| \hat{a}_k^\dagger = 0$
- $\hat{a}_k |0\rangle = 0$

3 Field operators

$$\hat{\Psi}^\dagger(x) = \sum_{j=1}^{\infty} \varphi_j^*(x)\hat{a}_j^\dagger$$
$$\hat{\Psi}(x) = \sum_{j=1}^{\infty} \varphi_j(x)\hat{a}_j,$$

where $\varphi_j(x) = \langle x|j\rangle$ is the wavefunction of the j-th one-particle eigenstate.

The field operator satisfy the anticommutation relations for fermions:

$$\{\hat{\Psi}(x), \hat{\Psi}^\dagger(y)\} = \delta(x-y)$$
$$\{\hat{\Psi}^\dagger(x), \hat{\Psi}^\dagger(y)\} = \{\hat{\Psi}(x), \hat{\Psi}(y)\} = 0$$

And for bosons, the commutation relations:

$$[\hat{\Psi}(x), \hat{\Psi}^\dagger(y)] = \delta(x-y)$$
$$[\hat{\Psi}^\dagger(x), \hat{\Psi}^\dagger(y)] = [\hat{\Psi}(x), \hat{\Psi}(y)] = 0$$

The particle number operator is

$$\hat{N} = \int \mathrm{d}x \hat{\Psi}^\dagger(x)\hat{\Psi}(x) = \cdots = \sum_{k=1}^{\infty} \hat{a}_k^\dagger \hat{a}_k$$

Calculating the first-quantized wavefunction for an N-particle system: Let $|\Phi_N\rangle$ be a second quantized state for which

$$\hat{N} |\Phi_N\rangle = N |\Phi_N\rangle .$$

The first-quantized wavefunction for this state is

$$\Phi(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \left\langle 0 \left| \prod_{j=1}^{N} \hat{\Psi}(x_j) \right| \Phi_N \right\rangle .$$

4 Operators

5 Green function method

5.1 Grand canonical ensemble

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$
$$\hat{K} := \hat{H} - \mu\hat{N}$$
$$\hat{K} = \hat{K}_0 + \hat{K}_1$$
$$\hat{K}_0 = \hat{H}_0 - \mu\hat{N},\ \hat{K}_1 = \hat{H}_1$$

The trace of an operator:

$$\mathrm{Sp}\left(\hat{A}\right) = \mathrm{Tr}\left(\hat{A}\right) = \sum_{\{n_i\}} \langle \ldots, n_i, \ldots, n_1 | \hat{A} | n_1, \ldots, n_i, \ldots \rangle ,$$

where the sum is over the entire Fock-space, not just the N-particle subspace.

The grand canonical partition function is defined as

$$Z_G = e^{-\beta\Omega(T,V,\mu)} = \mathrm{Sp}\left(e^{-\beta\hat{K}}\right) = \sum_{\{n_i\}} \langle \ldots, n_i, \ldots, n_1 | e^{-\beta\hat{K}} | n_1, \ldots, n_i, \ldots \rangle ,$$

where $\beta = (1/k_B T)$.

The grand canonical density matrix is

$$\hat{\rho}_G = \frac{e^{-\beta\hat{K}}}{Z_G}.$$

The average of operator $\hat{O}$ *over the grand canonical ensemble* is

$$\langle\hat{O}\rangle = \mathrm{Sp}\left(\hat{\rho}_G\hat{O}\right).$$

6 Exercises

1. Find the eigenvalues and eigenvectors of $\hat{a}_k$ and $\hat{a}_k^\dagger$!
2. $\hat{\Psi}^\dagger(x)\,|0\rangle = ?$
3. $[\hat{\Psi}(x), \hat{N}] = ?$
4. Prove that

$$[\hat{a}_j, f(\hat{a}_j^\dagger)] = \frac{\partial f(\hat{a}_j^\dagger)}{\partial \hat{a}_j^\dagger}$$
$$[\hat{a}_j^\dagger, f(\hat{a}_j)] = -\frac{\partial f(\hat{a}_j)}{\partial \hat{a}_j}$$

Hint: Use the Taylor-expansion formula:

$$f(\hat{A}) = \sum_{k=1}^{\infty} \frac{1}{k!} f^{(k)}(0)\hat{A}^k$$

And the derivative is

$$\frac{\partial f(\hat{A})}{\partial A} = \sum_{k=1}^{\infty} \frac{1}{(k-1)!} f^{(k)}(0)\hat{A}^{k-1}$$

5. Calculate $\mathrm{Sp}\left(\hat{N}\right)$ for bosonic particles!

Solution.

$$
\begin{aligned}
\mathrm{Sp}\left(\hat{N}\right) &= \sum_{\{n_i\}} \langle \ldots, n_i, \ldots, n_1 | \hat{N} | n_1, \ldots, n_i, \ldots \rangle \\
&= \sum_{\{n_i\}} \left\langle \ldots, n_i, \ldots, n_1 \left| \int \mathrm{d}x \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \right| n_1, \ldots, n_i, \ldots \right\rangle \\
&= \sum_{\{n_i\}} \left\langle \ldots, n_i, \ldots, n_1 \left| \int \mathrm{d}x \sum_{k,l} \varphi_k^*(x) \varphi_l(x) \hat{a}_k^\dagger \hat{a}_l \right| n_1, \ldots, n_i, \ldots \right\rangle \\
&= \sum_{\{n_i\}} \sum_{k,l} \int \mathrm{d}x \varphi_k^*(x) \varphi_l(x) \langle \ldots, n_i, \ldots, n_1 | \hat{a}_k^\dagger \hat{a}_l | n_1, \ldots, n_i, \ldots \rangle \\
&= \sum_{\{n_i\}} \sum_{k,l} \int \mathrm{d}x \varphi_k^*(x) \varphi_l(x) \langle \ldots, n_i, \ldots, n_1 | \hat{a}_k^\dagger \sqrt{n_l} | n_1, \ldots, n_l - 1, \ldots \rangle \\
&= \sum_{\{n_i\}} \sum_{k,l} \int \mathrm{d}x \varphi_k^*(x) \varphi_l(x) \langle \ldots, n_i, \ldots, n_1 | \sqrt{n_k + 1} \sqrt{n_l} | n_1, \ldots, n_k + 1, \ldots, n_l - 1, \ldots \rangle \\
&= \sum_{\{n_i\}} \sum_{k,l} \sqrt{n_k + 1} \sqrt{n_l} \int \mathrm{d}x \varphi_k^*(x) \varphi_l(x) \langle \ldots, n_i, \ldots, n_1 | n_1, \ldots, n_k + 1, \ldots, n_l - 1, \ldots \rangle \\
&= \sum_{\{n_i\}} \sum_{k,l} \sqrt{n_k + 1} \sqrt{n_l} \int \mathrm{d}x \varphi_k^*(x) \varphi_l(x) \delta_{kl} \\
&= \sum_{\{n_i\}} \sum_{k} n_k \underbrace{\int \mathrm{d}x \varphi_k^*(x) \varphi_k(x)}_{=1} \\
&= \sum_{\{n_i\}} \sum_{k} n_k
\end{aligned}
$$

6. Calculate $\mathrm{Sp}\left(\hat{H}_0\right)$, where
$$\hat{H}_0 = \int \mathrm{d}x \hat{\Psi}^\dagger(x) \left[-\frac{\hbar^2}{2M} \nabla^2 + U(x) \right] \hat{\Psi}(x)$$

7. Calculate $\langle \hat{N} \rangle$ for bosonic particles!