Statistical physics cheat sheet

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1 Fock-states

$$\begin{aligned} |0\rangle &= |0,0,0,\ldots\rangle \\ \langle 0|0\rangle &= \langle \ldots,0,0,0|0,0,0,\ldots\rangle = 1 \\ \langle \ldots,n_i',\ldots,n_2',n_1'|n_1,n_2,\ldots,n_i,\ldots\rangle &= \cdots \times \delta_{n_1n_1'} \times \delta_{n_2n_2'} \times \cdots \times \delta_{n_in_i'} \times \cdots \end{aligned}$$

2 Creation and annihillation operators

2.1 Fermionic creation and annihillation operators

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

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

$$\begin{aligned} \hat{a}_{k}^{\dagger} & | n_{1}, \dots, n_{k}, \dots \rangle = \sqrt{1 + n_{k}} & | n_{1}, \dots, n_{k} + 1, \dots \rangle \\ \hat{a}_{k} & | n_{1}, \dots, n_{k}, \dots \rangle = \sqrt{n_{k}} & | n_{1}, \dots, n_{k} - 1, \dots \rangle \\ n_{k} & \in \{0, 1, \dots\} \\ \hat{a}_{k}^{\dagger} & | n_{1}, \dots, n_{k-1}, 1, n_{k+1}, \dots \rangle = 0 \\ \hat{a}_{k} & | n_{1}, \dots, n_{k-1}, 0, n_{k+1}, \dots \rangle = 0 \end{aligned}$$

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:

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

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:

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

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

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:

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

The particle number operator is

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

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

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

4 Fock-space operators

If \hat{o} is a single-particle operator in first-quantization, then its second quantized form is

$$\hat{O} = \int dx \hat{\Psi}^{\dagger}(x) \hat{o} \hat{\Psi}(x)$$
$$= \sum_{j,k} \int dx \varphi_j^*(x) \hat{o} \varphi_k(x) \hat{a}_j^{\dagger} \hat{a}_k.$$

If \hat{o} is a two-particle operator in first-quantization, then its second-quantized form is

$$\hat{O} = \frac{1}{2} \int dx dx' \hat{\Psi}^{\dagger}(x) \hat{\Psi}^{\dagger}(x') \hat{o} \hat{\Psi}(x') \hat{\Psi}(x)$$

$$= \frac{1}{2} \sum_{i,j,k,l} \int dx dx' \varphi_i^*(x) \varphi_j^*(x') \hat{o} \varphi_k(x') \varphi_l(x) \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l.$$

5 Green function method

5.1 Grand canonical ensemble

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

The trace of an operator:

$$\operatorname{Tr}\left[\hat{A}\right] = \operatorname{Tr}\left[\hat{A}\right] = \sum_{\{n_i\}} \langle \dots, n_i, \dots, n_1 | \hat{A} | n_1, \dots, n_i, \dots \rangle,$$

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

The grand canonical partition function is defined as

$$Z_G = e^{-\beta\Omega(T,V,\mu)} = \operatorname{Tr}\left[e^{-\beta\hat{K}}\right] = \sum_{\{n_i\}} \langle \dots, n_i, \dots, n_1|e^{-\beta\hat{K}}|n_1, \dots, n_i, \dots \rangle,$$

where $\beta = (1/k_BT)$.

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

$$\langle \hat{O} \rangle = \text{Tr} \left[\hat{\rho}_G \hat{O} \right] = \frac{1}{Z_G} \text{Tr} \left[e^{-\beta \hat{K}} \hat{O} \right].$$

6 Exercises

- 1. What is the first quantized wavefunction of $\sum_{k} c_k \hat{a}_k^{\dagger} |0\rangle$, where \hat{a}_k^{\dagger} is a fermionic creation operator?
- 2. Calculate the first-quantized wavefunction for $\hat{a}_k^{\dagger}\hat{a}_l^{\dagger}|0\rangle$ for both fermionic and bosonic operators!
- 3. Consider 2 fermionic particles prepared in states

$$\Psi_1(x_1) = \sum_k b_k \varphi_k(x_1)$$

$$\Psi_2(x_2) = \sum_l c_l \varphi_l(x_2).$$

The state of the joint system in first quantization is

$$\Phi(x_1, x_2) = \frac{1}{\sqrt{2}} [\Psi_1(x_1)\Psi_2(x_2) - \Psi_1(x_2)\Psi_2(x_1)]$$

What is the Fock-space representation of $\Phi(x_1, x_2)$? Verify Your result by converting it back to first-quantization using the formula!

Solution.

$$\begin{split} &\Psi_1(x_1) = \sum_k b_k \varphi_k(x_1) \to \sum_k b_k \hat{a}_k^\dagger \, |0\rangle \\ &\Psi_2(x_2) = \sum_l c_l \varphi_l(x_2) \to \sum_l c_l \hat{a}_k^\dagger \, |0\rangle \\ &\Phi(x_1, x_2) = \sum_{k,l} b_k c_l \frac{1}{\sqrt{2}} [\varphi_k(x_1) \varphi_l(x_2) - \varphi_k(x_2) \varphi_l(x_1)] \to \sum_{k,l} b_k c_l \hat{a}_k^\dagger a_l^\dagger \, |0\rangle \end{split}$$

4. Find the eigenvalues and eigenvectors of \hat{a}_k and \hat{a}_k^{\dagger} !

- 5. $\hat{\Psi}^{\dagger}(x)|0\rangle = ?$
- 6. $[\hat{\Psi}(x), \hat{N}] = ?$
- 7. Calculate the first-quantized wavefunction $\Phi(x_1, x_2, x_3)$ for bosonic three-particle system prepared in state $|2, 0, 1, 0, 0, \cdots\rangle$.
- 8. 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

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

- 9. Consider a fermionic system. What is the Fock-space representation of \hat{S}_z and what is the meaning of this operator? What are the eigenstates of \hat{S}_z ?
- 10. Calculate Tr $\left[\hat{N}\right]$ for bosonic particles!

Solution.

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

11. Calculate Tr $\left[\hat{H}_{0}\right]$, where

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

12. Calculate $\langle \hat{n}_k \rangle$ for free non-interacting bosons! Solution.

$$\langle \hat{n}_k \rangle = \langle \hat{a}_k^{\dagger} \hat{a}_k \rangle = \frac{1}{Z_G} \operatorname{Tr} \left[e^{-\beta \hat{K}} \hat{a}_k^{\dagger} \hat{a}_k \right]$$
$$= \frac{1}{Z_G} \sum_{\{n_i\}} \langle \dots, n_i, \dots, n_1 | e^{-\beta \hat{K}} \hat{a}_k^{\dagger} \hat{a}_k | n_1, \dots, n_i, \dots \rangle$$

- 13. Calculate $\langle \hat{N} \rangle$ for bosonic particles!
- 14. Do something
- 15. asdfghjk

