

Statistical physics cheat sheet

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1 Fock-states

$$\begin{aligned}
|0\rangle &= |0, 0, 0, \dots\rangle \\
\langle 0|0\rangle &= \langle \dots, 0, 0, 0|0, 0, 0, \dots\rangle = 1 \\
\langle \dots, n'_i, \dots, n'_2, n'_1|n_1, n_2, \dots, n_i, \dots\rangle &= \dots \times \delta_{n_1 n'_1} \times \delta_{n_2 n'_2} \times \dots \times \delta_{n_i n'_i} \times \dots
\end{aligned}$$

2 Creation and annihilation operators

2.1 Fermionic creation and annihilation operators

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

Anticommutation relations:

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

2.2 Bosonic creation and annihilation 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:

$$\begin{aligned}
[\hat{a}_k, \hat{a}_l^\dagger] &= \hat{a}_k \hat{a}_l^\dagger - \hat{a}_l^\dagger \hat{a}_k = \delta_{kl} \\
[\hat{a}_k, \hat{a}_l] &= [\hat{a}_k^\dagger, \hat{a}_l^\dagger] = 0
\end{aligned}$$

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:

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

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

3 Field operators

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

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:

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

And for bosons, the commutation relations:

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

The particle number operator is

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

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

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

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

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

5 Green function method

5.1 Grand canonical ensemble

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

The trace of an operator:

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

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

The grand canonical partition function is defined as

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

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

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

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

5.2 Imaginary time and K -picture

The imaginary time is defined to be

$$\tau = -it.$$

The imaginary time dependent form of an operator is defined as

$$\hat{A}_K(\tau) = e^{\frac{\hat{K}\tau}{\hbar}} \hat{A} e^{-\frac{\hat{K}\tau}{\hbar}}$$

This is also called the K -picture of the operator. It can be shown that $\hat{K}(\tau) = \hat{K}$:

$$[f(\hat{K}), \hat{K}] = 0 \implies [e^{\frac{\hat{K}\tau}{\hbar}}, \hat{K}] = 0$$

Using the Baker-Campbell-Hausdorff formula:

$$\hat{K}(\tau) = e^{\frac{\hat{K}\tau}{\hbar}} \hat{K} e^{-\frac{\hat{K}\tau}{\hbar}} = \hat{K} + [e^{\frac{\hat{K}\tau}{\hbar}}, \hat{K}] + \frac{1}{2!} [e^{\frac{\hat{K}\tau}{\hbar}}, [e^{\frac{\hat{K}\tau}{\hbar}}, \hat{K}]] + \frac{1}{3!} [e^{\frac{\hat{K}\tau}{\hbar}}, [e^{\frac{\hat{K}\tau}{\hbar}}, [e^{\frac{\hat{K}\tau}{\hbar}}, \hat{K}]]] + \dots = \hat{K}$$

Properties:

- $\frac{d}{d\tau} \hat{A}_K(\tau) = \frac{1}{\hbar} [\hat{K}, \hat{A}_K(\tau)]$
- If $\hat{C} = \hat{A}\hat{B}$, then $\hat{C}(\tau) = \hat{A}(\tau)\hat{B}(\tau)$
- $\hat{\Psi}(x, \tau) = e^{\frac{\hat{K}\tau}{\hbar}} \hat{\Psi}(x) e^{-\frac{\hat{K}\tau}{\hbar}} = \sum_k \varphi_k(x) \hat{a}_k(\tau)$
- $\hat{\Psi}^\dagger(x, \tau) = e^{\frac{\hat{K}\tau}{\hbar}} \hat{\Psi}^\dagger(x) e^{-\frac{\hat{K}\tau}{\hbar}} = \sum_k \varphi_k(x) \hat{a}_k^\dagger(\tau)$
- $[\hat{A}(\tau), \hat{B}(\tau)] = e^{\frac{\hat{K}\tau}{\hbar}} [\hat{A}, \hat{B}] e^{-\frac{\hat{K}\tau}{\hbar}}$

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

$$\begin{aligned}\psi_1(x_1) &= \sum_k b_k \varphi_k(x_1) \\ \psi_2(x_2) &= \sum_l c_l \varphi_l(x_2).\end{aligned}$$

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.

$$\begin{aligned}\psi_1(x_1) &= \sum_k b_k \varphi_k(x_1) \rightarrow \sum_k b_k \hat{a}_k^\dagger |0\rangle \\ \psi_2(x_2) &= \sum_l c_l \varphi_l(x_2) \rightarrow \sum_l c_l \hat{a}_l^\dagger |0\rangle \\ \Phi(x_1, x_2) &= \sum_{k,l} b_k c_l \frac{1}{\sqrt{2}} [\varphi_k(x_1)\varphi_l(x_2) - \varphi_k(x_2)\varphi_l(x_1)] \rightarrow \sum_{k,l} b_k c_l \hat{a}_k^\dagger \hat{a}_l^\dagger |0\rangle\end{aligned}$$

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 $|2, 0, 1, 0, 0, \dots\rangle$.
8. Prove that

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

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 $\text{Tr} [\hat{N}]$ for bosonic particles!

Solution.

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

11. Calculate $\text{Tr} [\hat{H}_0]$, where

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

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

Solution. For non-interacting particles,

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

$$\langle \hat{n}_k \rangle = \langle \hat{a}_k^\dagger \hat{a}_k \rangle = \frac{1}{Z_G} \text{Tr} \left[e^{-\beta \hat{K}_0} \hat{a}_k^\dagger \hat{a}_k \right] = \frac{1}{Z_G} \text{Tr} \left[\hat{a}_k e^{-\beta \hat{K}_0} \hat{a}_k^\dagger \right] = \frac{1}{Z_G} \text{Tr} \left[e^{-\beta \hat{K}_0} e^{\beta \hat{K}_0} \hat{a}_k e^{-\beta \hat{K}_0} \hat{a}_k^\dagger \right].$$

We can use the imaginary time-dependence of operators (K -picture):

$$\begin{aligned} \hat{a}_k(\tau) &= e^{\frac{\hat{K}\tau}{\hbar}} \hat{a}_k e^{-\frac{\hat{K}\tau}{\hbar}} \implies \hat{a}_k(\beta\hbar) = e^{\beta \hat{K}_0} \hat{a}_k e^{-\beta \hat{K}_0} \\ \frac{d}{d\tau} \hat{a}_k(\tau) &= \frac{1}{\hbar} [\hat{K}_0, \hat{a}_k(\tau)] \end{aligned}$$

Using the identity $K_0 = K_0(\tau)$:

$$\begin{aligned} \frac{d}{d\tau} \hat{a}_k(\tau) &= \frac{1}{\hbar} [\hat{K}_0(\tau), \hat{a}_k(\tau)] \\ &= \frac{1}{\hbar} \left[\sum_{l,m} \int dx \varphi_l^*(x) \left(-\frac{\hbar^2}{2M} \nabla^2 + U(x) - \mu \right) \varphi_m(x) \hat{a}_l^\dagger(\tau) \hat{a}_m(\tau), \hat{a}_k(\tau) \right] \\ &= \frac{1}{\hbar} \left[\sum_l a_l^\dagger(\tau) \hat{a}_l(\tau) (e_l - \mu), \hat{a}_k(\tau) \right] = \frac{1}{\hbar} \sum_l (e_l - \mu) \left[a_l^\dagger(\tau) \hat{a}_l(\tau), \hat{a}_k(\tau) \right]. \end{aligned}$$

$$\begin{aligned} [\hat{a}_l^\dagger(\tau) \hat{a}_l(\tau), \hat{a}_k(\tau)] &= \hat{a}_l^\dagger(\tau) \hat{a}_l(\tau) \hat{a}_k(\tau) - \hat{a}_k(\tau) \hat{a}_l^\dagger(\tau) \hat{a}_l(\tau) \\ &= e^{\frac{\hat{K}\tau}{\hbar}} \hat{a}_l^\dagger \hat{a}_l \hat{a}_k e^{-\frac{\hat{K}\tau}{\hbar}} - e^{\frac{\hat{K}\tau}{\hbar}} \hat{a}_k \hat{a}_l^\dagger \hat{a}_l e^{-\frac{\hat{K}\tau}{\hbar}} \\ &= e^{\frac{\hat{K}\tau}{\hbar}} \hat{a}_l^\dagger \hat{a}_l \hat{a}_k e^{-\frac{\hat{K}\tau}{\hbar}} - e^{\frac{\hat{K}\tau}{\hbar}} (\delta_{kl} - \hat{a}_l^\dagger \hat{a}_k) \hat{a}_l e^{-\frac{\hat{K}\tau}{\hbar}} \\ &= e^{\frac{\hat{K}\tau}{\hbar}} \hat{a}_l^\dagger \hat{a}_l \hat{a}_k e^{-\frac{\hat{K}\tau}{\hbar}} - e^{\frac{\hat{K}\tau}{\hbar}} (\delta_{kl} \hat{a}_l - \hat{a}_l^\dagger \hat{a}_l \hat{a}_k) e^{-\frac{\hat{K}\tau}{\hbar}} \\ &= -e^{\frac{\hat{K}\tau}{\hbar}} \delta_{kl} \hat{a}_l e^{-\frac{\hat{K}\tau}{\hbar}}. \end{aligned}$$

Using this result, we get

$$\begin{aligned} \frac{d}{d\tau} \hat{a}_k(\tau) &= -\frac{1}{\hbar} \sum_l (e_l - \mu) \hat{a}_k(\tau) \\ \implies \hat{a}_k(\tau) &= \hat{a}_k e^{-\frac{(e_l - \mu)}{\hbar} \tau} \end{aligned}$$

$$\begin{aligned} \langle \hat{n}_k \rangle &= \frac{1}{Z_G} \text{Tr} \left[e^{-\beta \hat{K}_0} e^{\beta \hat{K}_0} \hat{a}_k e^{-\beta \hat{K}_0} \hat{a}_k^\dagger \right] = \frac{1}{Z_G} \text{Tr} \left[e^{-\beta \hat{K}_0} \hat{a}_k(\beta\hbar) \hat{a}_k^\dagger \right] \\ &= \frac{1}{Z_G} \text{Tr} \left[e^{-\beta \hat{K}_0} (1 \pm \hat{a}_k^\dagger \hat{a}_k(\beta\hbar)) \right] \\ &= \frac{1}{Z_G} \text{Tr} \left[e^{-\beta \hat{K}_0} \right] \pm \frac{1}{Z_G} \text{Tr} \left[e^{-\beta \hat{K}_0} \hat{a}_k^\dagger \hat{a}_k(\beta\hbar) \right] \\ &= \frac{1}{Z_G} \text{Tr} \left[e^{-\beta \hat{K}_0} \right] \pm \frac{1}{Z_G} \text{Tr} \left[e^{-\beta \hat{K}_0} \hat{a}_k^\dagger \hat{a}_k e^{-\beta(e_l - \mu)} \right] \\ &= 1 \pm \langle \hat{n}_k \rangle e^{-\beta(e_l - \mu)} \\ \implies \langle \hat{n}_k \rangle &= \frac{1}{1 \mp e^{-\beta(e_l - \mu)}}. \end{aligned}$$

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

14. Do something

15. asdfghjk

$$(\circledast), (\nabla), \mathcal{G}(x, \tau, x', \tau')$$