Statistical physics cheat sheet

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November 28, 2019

1 Fock-states

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

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:

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

Creating fermionic state from vacuum:

$$|n_1, \dots, n_k, \dots, n_N\rangle = (\hat{a}_1^\dagger)^{n_1} \times (\hat{a}_2^\dagger)^{n_2} \times \dots \times (\hat{a}_N^\dagger)^{n_N} |0\rangle\ ,$$

where $n_1, n_2, \dots, n_N \in \{0,1\}$.

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:

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

Creating bosonic state from vacuum:

$$|n_1, \dots, n_k, \dots, n_N\rangle = \frac{(\hat{a}_1^\dagger)^{n_1}}{\sqrt{n_1!}} \times \frac{(\hat{a}_2^\dagger)^{n_2}}{\sqrt{n_2!}} \times \dots \times \frac{(\hat{a}_N^\dagger)^{n_N}}{\sqrt{n_N!}} |0\rangle\ ,$$

where $n_1, n_2, \dots, n_N \in \{0,1,\dots\}$.

For both bosons and fermions:

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

3 Particle number operators

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

$$\hat{n}_k \left| n_1, \ldots, n_k, \ldots \right\rangle = n_k \left| n_1, \ldots, n_k, \ldots \right\rangle .$$

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

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

4 Field operators

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

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

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

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

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

The first-quantized wavefunction for this state is

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

5 Fock-space operators

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

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

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

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

6 Green function method

6.1 Grand canonical ensemble

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

The trace of an operator:

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

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

The grand canonical partition function is defined as

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

where $\beta = (1/k_BT)$, and

$$\Omega(T,V,\mu) = -k_BT\ln Z_G$$

is the grand potential.

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

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

6.2 Imaginary time and K-picture

The imaginary time is defined to be

$$\tau = -it.$$

The imaginary time dependendent 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 $\hat{K}(\tau) = \hat{K}$. First,

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

then, using the Baker-Campbell-Hausdorff formula:

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

Properties:

- $\frac{\mathrm{d}}{\mathrm{d}\tau}\hat{A}_K(\tau) = \frac{1}{\hbar}[\hat{K}, \hat{A}_K(\tau)] = \frac{1}{\hbar}[\hat{K}(\tau), \hat{A}_K(\tau)]$
- $e^{\frac{\hat{K}\tau}{\hbar}}\left[\prod_j \hat{A}_j\right]e^{-\frac{\hat{K}\tau}{\hbar}} = \prod_j \hat{A}_j(\tau)$ (proof is trivial)
- $e^{\frac{\hat{K}\tau}{\hbar}}\left[\sum_j \hat{A}_j\right]e^{-\frac{\hat{K}\tau}{\hbar}} = \sum_j \hat{A}_j(\tau)$ (proof using the Baker-Campbell-Hausdorff formula)
- $\hat{\Psi}(x,\tau) = e^{\frac{\hat{K}\tau}{\hbar}}\hat{\Psi}(x)e^{-\frac{\hat{K}\tau}{\hbar}} = \sum_k \varphi_k(x)\hat{a}_k(\tau)$
- $\hat{\Psi}^\dagger(x,\tau) = e^{\frac{\hat{K}\tau}{\hbar}}\hat{\Psi}^\dagger(x)e^{-\frac{\hat{K}\tau}{\hbar}} = \sum_k \varphi_k(x)\hat{a}_k^\dagger(\tau)$
- $[\hat{A}(\tau), \hat{B}(\tau)] = e^{\frac{\hat{K}\tau}{\hbar}}[\hat{A}, \hat{B}]e^{-\frac{\hat{K}\tau}{\hbar}}$

6.3 Definition of the Green function

$$\begin{aligned}\mathcal{G}(x,\tau;x',\tau') &= -\left\langle T[\hat{\Psi}(x,\tau)\hat{\Psi}^\dagger(x',\tau')]\right\rangle \\ &= -\mathrm{Tr}\left[\hat{\rho}_G T[\hat{\Psi}(x,\tau)\hat{\Psi}^\dagger(x',\tau')]\right],\end{aligned}$$

where T is the time-ordering operator:

$$T[\hat{\Psi}(x,\tau)\hat{\Psi}^\dagger(x',\tau')] = \begin{cases}\hat{\Psi}(x,\tau)\hat{\Psi}^\dagger(x',\tau'), & \text{if } \tau > \tau' \\ \hat{\Psi}^\dagger(x',\tau')\hat{\Psi}(x,\tau), & \text{if } \tau \le \tau'\end{cases}$$

$$\begin{aligned}\mathcal{G}(x,x';\tau) &= \frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty}\mathcal{G}(x,x';i\omega_n)e^{-i\omega_n\tau} \\ \mathcal{G}(x,x';i\omega_n) &= \int_0^{\beta\hbar}\mathcal{G}(x,x';\tau)e^{i\omega_n\tau},\end{aligned}$$

where ω_n are called Matsubara-frequencies:

$$\omega_n = \begin{cases}\frac{2n\pi}{\beta\hbar}, & \text{for bosons} \\ \frac{(2n+1)\pi}{\beta\hbar}, & \text{for fermions}\end{cases}$$

7 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.

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

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

$$e^{-\beta \sum_k (\varepsilon_k - \mu)\hat{a}_k^\dagger \hat{a}_k} |n_1, \ldots, n_k, \ldots\rangle = e^{-\beta \sum_k (\varepsilon_k - \mu) n_k} |n_1, \ldots, n_k, \ldots\rangle$$

9. 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

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

10. Prove that if $\hat{B} = e^{\hat{A}}$, then $\hat{B}(\tau) = e^{\hat{A}(\tau)}$!

11. 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 $\hat{S}_z$?

12. Calculate $\mathrm{Tr}\left[\hat{N}\right]$ for bosonic particles!

    Solution.

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

13. Consider a system, for which the second-quantized Hamiltonian is $\hat{H} = \sum_j \varepsilon_j \hat{a}_j^\dagger \hat{a}_j$. Calculate $\hat{a}_k(\tau)$!

    Solution 1

    By definition,

$$\hat{a}_k(\tau) = e^{\frac{\hat{K}\tau}{\hbar}} \hat{a}_k e^{-\frac{\hat{K}\tau}{\hbar}}.$$

where $\hat{K} = \hat{H} - \mu\hat{N} = \sum_j (\varepsilon_j - \mu) \hat{a}_j^\dagger \hat{a}_j$. Applying the Baker-Campbell-Hausdorff formula,

$$\hat{a}_k(\tau) = \hat{a}_k + \left[e^{\frac{\hat{K}\tau}{\hbar}}, \hat{a}_k\right] + \frac{1}{2!}\left[e^{\frac{\hat{K}\tau}{\hbar}}, \left[e^{\frac{\hat{K}\tau}{\hbar}}, \hat{a}_k\right]\right] + \frac{1}{3!}\left[e^{\frac{\hat{K}\tau}{\hbar}}, \left[e^{\frac{\hat{K}\tau}{\hbar}}, \left[e^{\frac{\hat{K}\tau}{\hbar}}, \hat{a}_k\right]\right]\right] + \ldots$$

Substituting

$$e^{\frac{\hat{K}\tau}{\hbar}} = \sum_l \frac{1}{l!} \left(\frac{\tau}{\hbar}\right)^l \hat{K}^l$$

$$
\begin{aligned}
\hat{a}_k(\tau) &= \hat{a}_k + \left[\sum_l \frac{1}{l!}\left(\frac{\tau}{\hbar}\right)^l \hat{K}^l, \hat{a}_k\right] + \frac{1}{2!}\left[\sum_l \frac{1}{l!}\left(\frac{\tau}{\hbar}\right)^l \hat{K}^l, \left[\sum_n \frac{1}{n!}\left(\frac{\tau}{\hbar}\right)^n \hat{K}^n, \hat{a}_k\right]\right] + \dots \\
&= \hat{a}_k + \sum_l \frac{1}{l!}\left(\frac{\tau}{\hbar}\right)^l \left[\hat{K}^l, \hat{a}_k\right] + \frac{1}{2!}\sum_l\sum_n \frac{1}{l!}\frac{1}{n!}\left(\frac{\tau}{\hbar}\right)^{l+n} \left[\hat{K}^l, \left[\hat{K}^n, \hat{a}_k\right]\right] + \dots \\
&= \hat{a}_k + \sum_l \frac{1}{l!}\left(\frac{\tau}{\hbar}\right)^l \left[\left(\sum_j (\varepsilon_j - \mu)\hat{a}_j^\dagger \hat{a}_j\right)^l, \hat{a}_k\right] + \dots
\end{aligned}
$$

Solution 2

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\tau}\hat{a}_k(\tau) &= \frac{1}{\hbar}[\hat{K}(\tau), \hat{a}_k(\tau)] \\
&= \frac{1}{\hbar}\left[\sum_j (\varepsilon_j - \mu)\hat{a}_j^\dagger(\tau)\hat{a}_j(\tau), \hat{a}_k(\tau)\right] \\
&= \frac{1}{\hbar}\sum_j (\varepsilon_j - \mu)\left[\hat{a}_j^\dagger(\tau)\hat{a}_j(\tau), \hat{a}_k(\tau)\right] \\
&= \frac{1}{\hbar}\sum_j (\varepsilon_j - \mu)\left(\hat{a}_j^\dagger(\tau)\hat{a}_j(\tau)\hat{a}_k(\tau) - \hat{a}_k(\tau)\hat{a}_j^\dagger(\tau)\hat{a}_j(\tau)\right) \\
&= \frac{1}{\hbar}\sum_j (\varepsilon_j - \mu)\left(e^{\frac{\hat{K}\tau}{\hbar}}\hat{a}_j^\dagger\hat{a}_j\hat{a}_k e^{-\frac{\hat{K}\tau}{\hbar}} - e^{\frac{\hat{K}\tau}{\hbar}}\hat{a}_k\hat{a}_j^\dagger\hat{a}_j e^{-\frac{\hat{K}\tau}{\hbar}}\right) \\
&= \frac{1}{\hbar}\sum_j (\varepsilon_j - \mu)\left(e^{\frac{\hat{K}\tau}{\hbar}}\hat{a}_j^\dagger\hat{a}_j\hat{a}_k e^{-\frac{\hat{K}\tau}{\hbar}} - e^{\frac{\hat{K}\tau}{\hbar}}(\delta_{kj} - \hat{a}_j^\dagger\hat{a}_k)\hat{a}_j e^{-\frac{\hat{K}\tau}{\hbar}}\right) \\
&= \frac{1}{\hbar}\sum_j (\varepsilon_j - \mu)\left(e^{\frac{\hat{K}\tau}{\hbar}}\hat{a}_j^\dagger\hat{a}_j\hat{a}_k e^{-\frac{\hat{K}\tau}{\hbar}} - e^{\frac{\hat{K}\tau}{\hbar}}(\delta_{kj}\hat{a}_j - \hat{a}_j^\dagger\hat{a}_j\hat{a}_k) e^{-\frac{\hat{K}\tau}{\hbar}}\right) \\
&= \frac{1}{\hbar}\sum_j (\varepsilon_j - \mu)\left(-e^{\frac{\hat{K}\tau}{\hbar}}\delta_{kj}\hat{a}_j e^{-\frac{\hat{K}\tau}{\hbar}}\right) \\
&= -\frac{1}{\hbar}(\varepsilon_k - \mu)\hat{a}_k(\tau) \\
\Longrightarrow \hat{a}_k(\tau) &= e^{-\frac{\tau}{\hbar}(\varepsilon_k - \mu)}\hat{a}_k
\end{aligned}
$$

14. Calculate the second quantized Hamiltonian for a homogeneous, non-interacting system with periodic boundary conditions!

    Solution. The periodic boundary condition means that the single-particle wavefunctions are the solutions of the 3D particle in a box problem. These are:

$$
\langle \mathbf{r}|n\rangle = \varphi_n(\mathbf{r}) = \frac{1}{\sqrt{L^3}}e^{i\mathbf{k}_n\mathbf{r}},\ \mathbf{k}_n = \frac{2\pi n}{L}\begin{pmatrix}1\\1\\1\end{pmatrix}.
$$

The homogeneous non-interacting Hamiltonian is simply the kinetic energy:

$$
\hat{H} = \sum_{j=1}^{N}\left[-\frac{\hbar^2}{2M}\triangle_j\right] \Longrightarrow \hat{H}\varphi_n(\mathbf{r}_l) = \frac{3}{L^2}\frac{4\pi^2\hbar^2}{2M}n^2\varphi_n(\mathbf{r}_l).
$$

The second quantized Hamiltonian is

$$\begin{aligned}
\hat{H} &= \sum_{k,l} \int \mathrm{d}^3 r \varphi_k^*(\mathbf{r}) \hat{H} \varphi_l(\mathbf{r}) \hat{a}_k^\dagger \hat{a}_l \\
&= \sum_{k,l} \int \mathrm{d}^3 r \varphi_k^*(\mathbf{r}) \frac{3}{L^2} \frac{4\pi^2\hbar^2}{2M} l^2 \varphi_l(\mathbf{r}) \hat{a}_k^\dagger \hat{a}_l \\
&= \frac{3}{L^2} \frac{4\pi^2\hbar^2}{2M} \sum_{k,l} \int \mathrm{d}^3 r \varphi_k^*(\mathbf{r}) l^2 \varphi_l(\mathbf{r}) \hat{a}_k^\dagger \hat{a}_l \\
&= \frac{3}{L^2} \frac{4\pi^2\hbar^2}{2M} \sum_{k,l} \delta_{kl} l^2 \hat{a}_k^\dagger \hat{a}_l \\
&= \frac{3}{L^2} \frac{4\pi^2\hbar^2}{2M} \sum_{k} k^2 \hat{a}_k^\dagger \hat{a}_k
\end{aligned}$$

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

Solution. For non-interacting particles,

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

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

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

$$\hat{a}_k(\tau) = e^{\frac{\hat{K}\tau}{\hbar}} \hat{a}_k e^{-\frac{\hat{K}\tau}{\hbar}} \implies \hat{a}_k(\beta\hbar) = e^{\beta \hat{K}_0} \hat{a}_k e^{-\beta \hat{K}_0}$$

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \hat{a}_k(\tau) = \frac{1}{\hbar} [\hat{K}_0, \hat{a}_k(\tau)]$$

Using the identity $\hat{K}_0 = \hat{K}_0(\tau)$:

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

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

Using this result, we get

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \hat{a}_k(\tau) = -\frac{1}{\hbar} \sum_l (e_l - \mu) \hat{a}_k(\tau)$$

$$\implies \hat{a}_k(\tau) = \hat{a}_k e^{-\frac{(e_l - \mu)}{\hbar} \tau}$$

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

$$
\implies \langle \hat{n}_k \rangle = \frac{1}{1 \mp e^{-\beta(e_l - \mu)}}.
$$

16. Calculate $\langle \hat{N} \rangle$ for bosonic particles!
17. Do something
18. asdfghjk

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