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 annihillation operators

2.1 Fermionic creation and annihillation operators

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

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 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:

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

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:

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

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

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 Fock-space operators

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

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

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

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

5 Green function method

5.1 Grand canonical ensemble

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

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

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

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

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

$$\begin{aligned}\Psi_1(x_1) &= \sum_k b_k\varphi_k(x_1) \\ \Psi_2(x_2) &= \sum_l c_l\varphi_l(x_2).\end{aligned}$$

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.

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

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 $|2, 0, 1, 0, 0, \cdots\rangle$.
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 $\mathrm{Tr}\left[\hat{N}\right]$ for bosonic particles!

Solution.

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

11. Calculate $\mathrm{Tr}\left[\hat{H}_0\right]$, 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 particles!

Solution.

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

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

$$\begin{aligned}
\hat{O}_K(\tau) &= e^{\frac{\hat{K}\tau}{\hbar}} \hat{O} e^{-\frac{\hat{K}\tau}{\hbar}} \\
\frac{\mathrm{d}}{\mathrm{d}\tau}\hat{O}_K(\tau) &= \frac{1}{\hbar}[\hat{K}, \hat{O}_K(\tau)]
\end{aligned}$$

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

therefore,

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

Using the Baker-Campbell-Hausdorff formula:

$$e^{\beta \hat{K}_0} \hat{a}_k e^{-\beta \hat{K}_0} = \hat{a}_k + [e^{\beta \hat{K}_0}, \hat{a}_k] + \frac{1}{2!}[e^{\beta \hat{K}_0}, [e^{\beta \hat{K}_0}, \hat{a}_k]] + \frac{1}{3!}[e^{\beta \hat{K}_0}, [e^{\beta \hat{K}_0}, [e^{\beta \hat{K}_0}, \hat{a}_k]]] + \cdots$$

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

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