Statistical physics cheat sheet

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1   Fock-states

$$|0\rangle = |0, 0, 0, \ldots\rangle$$

$$\langle 0|0\rangle = \langle \ldots, 0, 0, 0|0, 0, 0, \ldots\rangle = 1$$

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

2   Creation and annihillation operators

2.1   Fermionic creation and annihillation operators

$$\hat{a}_k^\dagger |n_1, \ldots, n_k, \ldots\rangle = \sqrt{1 - n_k}(-1)^{\Sigma_k} |n_1, \ldots, 1 + n_k, \ldots\rangle$$

$$\hat{a}_k |n_1, \ldots, n_k, \ldots\rangle = \sqrt{n_k}(-1)^{\Sigma_k} |n_1, \ldots, 1 - n_k, \ldots\rangle$$

$$n_k \in \{0, 1\}, \ \Sigma_k = \sum_{j=1}^{k-1} n_j$$

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

$$\hat{a}_k |n_1, \ldots, n_{k-1}, 0, n_{k+1}, \ldots\rangle = 0$$

$$\hat{a}_k = (\hat{a}_k^\dagger)^\dagger$$

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

$$\hat{a}_k^\dagger |n_1, \ldots, n_k, \ldots\rangle = \sqrt{1 + n_k} |n_1, \ldots, n_k + 1, \ldots\rangle$$

$$\hat{a}_k |n_1, \ldots, n_k, \ldots\rangle = \sqrt{n_k} |n_1, \ldots, n_k - 1, \ldots\rangle$$

$$n_k \in \{0, 1, \ldots\}$$

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

$$\hat{a}_k |n_1, \ldots, n_{k-1}, 0, n_{k+1}, \ldots\rangle = 0$$

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:

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

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:

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

- $\hat{N} = \sum_k \hat{n}_k$ 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 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

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

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

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:

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

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

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

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

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.

$$\Psi_1(x_1) = \sum_k b_k \varphi_k(x_1) \rightarrow \sum_k b_k \hat{a}_k^\dagger \lvert 0 \rangle$$

$$\Psi_2(x_2) = \sum_l c_l \varphi_l(x_2) \rightarrow \sum_l c_l \hat{a}_k^\dagger \lvert 0 \rangle$$

$$\Phi(x_1, x_2) = \sum_{k,l} b_k c_l \frac{1}{\sqrt{2}} [\varphi_k(x_1)\varphi_l(x_2) - \varphi_k(x_2)\varphi_l(x_1)] \rightarrow \sum_{k,l} b_k c_l \hat{a}_k^\dagger \hat{a}_l^\dagger \lvert 0 \rangle$$

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

5. $\hat{\Psi}^\dagger(x) \lvert 0 \rangle = ?$

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 $\lvert 2, 0, 1, 0, 0, \cdots \rangle$.

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

Solution.

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

$$= \sum_{\{n_i\}} \left\langle \ldots, n_i, \ldots, n_1 \left| \int \mathrm{d}x \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \right| n_1, \ldots, n_i, \ldots \right\rangle$$

$$= \sum_{\{n_i\}} \left\langle \ldots, n_i, \ldots, n_1 \left| \int \mathrm{d}x \sum_{k,l} \varphi_k^*(x)\varphi_l(x) \hat{a}_k^\dagger \hat{a}_l \right| n_1, \ldots, n_i, \ldots \right\rangle$$

$$= \sum_{\{n_i\}} \sum_{k,l} \int \mathrm{d}x \varphi_k^*(x)\varphi_l(x) \langle \ldots, n_i, \ldots, n_1 | \hat{a}_k^\dagger \hat{a}_l | n_1, \ldots, n_i, \ldots \rangle$$

$$= \sum_{\{n_i\}} \sum_{k,l} \int \mathrm{d}x \varphi_k^*(x)\varphi_l(x) \langle \ldots, n_i, \ldots, n_1 | \hat{a}_k^\dagger \sqrt{n_l} | n_1, \ldots, n_l - 1, \ldots \rangle$$

$$= \sum_{\{n_i\}} \sum_{k,l} \int \mathrm{d}x \varphi_k^*(x)\varphi_l(x) \langle \ldots, n_i, \ldots, n_1 | \sqrt{n_k + 1}\sqrt{n_l} | n_1, \ldots, n_k + 1, \ldots, n_l - 1, \ldots \rangle$$

$$= \sum_{\{n_i\}} \sum_{k,l} \sqrt{n_k + 1}\sqrt{n_l} \int \mathrm{d}x \varphi_k^*(x)\varphi_l(x) \langle \ldots, n_i, \ldots, n_1 | n_1, \ldots, n_k + 1, \ldots, n_l - 1, \ldots \rangle$$

$$= \sum_{\{n_i\}} \sum_{k,l} \sqrt{n_k + 1}\sqrt{n_l} \int \mathrm{d}x \varphi_k^*(x)\varphi_l(x) \delta_{kl}$$

$$= \sum_{\{n_i\}} \sum_{k} n_k \underbrace{\int \mathrm{d}x \varphi_k^*(x)\varphi_k(x)}_{=1}$$

$$= \sum_{\{n_i\}} \sum_{k} n_k$$

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):

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

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\hat{O}_K(\tau) = \frac{1}{\hbar}[\hat{K}, \hat{O}_K(\tau)]$$

we also know, that

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

Using the Baker-Campbell-Hausdorff formula:

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

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

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

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

$$= \frac{1}{\hbar} \left[\sum_l a_l^\dagger \hat{a}_l (e_l - \mu), \hat{a}_k(\tau) \right] = \frac{1}{\hbar} \sum_l (e_l - \mu) \left[a_l^\dagger \hat{a}_l, \hat{a}_k(\tau) \right].$$

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

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

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

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

$$=$$

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

14. Do something

15. asdfghjk

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