Partition function of non-interacting gas

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Generally: $$Z = \int \mathcal{D}(\bar\psi,\psi)\, e^{-S[\bar\psi,\psi]} \equiv e^{-\beta F} \quad \text{(1a)}$$

free energy

$$S = \int_0^\beta d\tau \left[\bar\psi \partial_\tau \psi + H(\bar\psi,\psi) - \mu N(\bar\psi,\psi) \right] \quad \text{(1b)}$$

Consider noninteracting gas: $$H = H_0 = \sum_{ij} \bar\psi_i H_{0,ij} \psi_j \quad (2)$$

Diagonalize: $$H_0 = \mathcal{U} D \mathcal{U}^\dagger, \quad D_{ab} = \delta_{ab}\varepsilon_a \quad \text{(3a)}$$

eigenvalues

$$\mathcal{U}^\dagger \psi = \phi \quad \text{(3b)}$$

$$\Rightarrow \quad S = \sum_a \sum_n \bar\phi_{an}(-i\omega_n + \xi_a)\phi_{an} \qquad \xi_a = \varepsilon_a - \mu \quad (4)$$

$\phi_a(\tau)$ are independent variables: $$\Rightarrow \quad Z = \prod_a Z_a \quad (5)$$

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$$Z_a = \underbrace{\int \mathcal{D}(\bar\phi_a,\phi_a)}_{\prod_n d(\bar\phi_{an},\phi_{an})} e^{-\sum_n \bar\phi_{an}(-i\omega_n+\xi_a)\phi_{an}} \quad (6)$$

(45) of 6.12.06

Gaussian int. $$= \prod_n \left[\beta(-i\omega_n + \xi_a)\right]^{-\zeta} \qquad \zeta = \pm \text{ bosons / fermions} \quad (7)$$

$$\left(= \det\left[\beta(-i\hat\omega + \hat H - \mu\hat N)\right]^{-\zeta} \right) \quad (8)$$

Free energy: $$F = -\frac{1}{\beta}\ln Z = \sum_a F_a \quad (8)$$

$$F_a = \frac{1}{\beta}\zeta \sum_n \ln\left[\beta(-i\omega_n+\xi_a)\right] \quad (9)$$

Particle number: $$\bar N = \frac{\mathrm{Tr}\, \hat N e^{-\beta(\hat H - \mu\hat N)}}{Z} = -\frac{\partial F}{\partial\mu} = -\sum_a \partial_\mu F_a \quad (9)'$$

Matsubara summations

Notes, p. 12, 55.

General structure: $S = \sum_n h(i\omega_n)$, $\omega_n = \begin{cases} 2\pi n/\beta \\ 2\pi(n+1/2)/\beta \end{cases}$ (10)

Introduce auxiliary "counting function" $g(z)$ with simple poles at $z = i\omega_n$, and Res $= 1$.

Then $$S = \oint_C \frac{dz}{2\pi i}\, g(z)\, h(z) \qquad (11)$$

← contour surrounds all poles of $g(z)$

Typical choices:

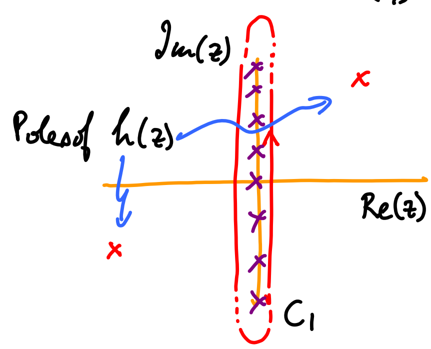
$$g_\pm(z) = \frac{\pm\xi\beta}{e^{\pm\beta z} - \xi} \qquad (12)$$

has desired poles, since $e^{\pm i\omega_n z} = \xi$

$$g_\pm(z \to i\omega_n + \delta) = \frac{\pm\xi\beta}{\cancel{\xi}(\cancel{1} \pm \beta\delta) - \cancel{\xi}} = \frac{1}{\delta} \Rightarrow \text{Res}\, g(i\omega_n) = 1 \qquad (13)$$

Or: $$\tilde{g}_\pm(z) = \left(\frac{\xi\beta}{2}\right)\frac{e^{\pm\beta z} + \xi}{e^{\pm\beta z} - \xi} = \left(\xi\frac{\beta}{2}\right)\begin{cases}\coth\beta z/2 \\ \tanh\beta z/2\end{cases} \text{ for } \xi = \begin{cases} +1 \\ -1\end{cases} \qquad (14)$$

$$\xrightarrow{z = i\omega_n + \delta} \left(\frac{\xi\beta}{2}\right)\frac{\xi(1 \pm \beta\delta) + \xi}{\xi(1 \pm \beta\delta) - \xi} = \frac{1}{\delta}$$

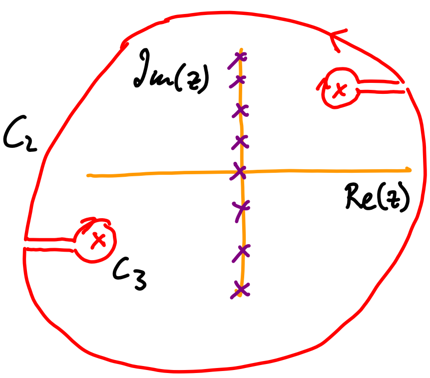


But $$\oint_{C_1} dz = \oint_{C_2} dz + \oint_{C_3} dz \qquad (15)$$

← surrounds all poles of h_z

$$= 0, \text{ if } \lim_{z \to \pm\infty} \left(z\, g(z)\, h(z)\right) = 0 \qquad (16)$$

(this condition dictates the sign choice to be made in (11))



$$S \overset{(11)}{=} \oint_{C_3} \frac{dz}{2\pi i}\, g_\pm(z)\, h(z)$$

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(17)

If $g(z)$ has isolated poles at $\{z_k\}$ (all enclosed by C_3):

$$S = - \sum_k \mathrm{Res}\left\{ g_\pm(z)\, h(z) \right\}_{z=z_k} \qquad (18)$$

due to change of direction of C_3 from ↻ to ↺

Sum over finite number of poles ⇒ doable!!

Example: Calculate average particle number:

$$\bar{N} = \frac{\mathrm{Tr}\{\hat{N} e^{-\beta(\hat{H}-\mu\hat{N})}\}}{Z} \overset{(9)'}{=} -\partial_\mu \sum_a F_a \qquad (19)$$

$$F_a = -\frac{1}{\beta}\, \zeta \sum_n \ln\left[\beta(-i\omega_n + \xi_a)\right] \quad \xi_a = \varepsilon_a - \mu \qquad (20)$$

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$$\bar{N} = \frac{1}{\beta} \sum_{an} \zeta \frac{1 \times e^{i\omega_n \delta}}{(-i\omega_n + \xi_a)}$$

convergence factor, from $\bar{\psi}\psi = \bar{\psi}(\tau+\delta)\psi(\tau)$ (where $\delta = 0^+$)

(22)

[More precisely:

$$\bar{N} = \mathrm{Tr} \sum_a c_a^\dagger c_a\, e^{-\beta(\hat{H}-\mu\hat{N})}$$

$$= \int \prod D(\bar{\psi}_a \psi_a)\, \bar{\psi}_a(\tau+\delta)\, \psi(\tau)\, e^{-S(\bar{\psi}_a, \psi_a)}$$]

$\bar{N}$ of (22) has form of (10)

$$\bar{N} = \sum_n h(i\omega_n) \quad \text{with:} \quad h(i\omega_n) = \frac{-\zeta e^{i\omega_n \delta}}{i\omega_n - \xi_a} \qquad (23)$$

[typical for Green's function]

$$\text{Then} \lim_{z=\pm\infty} z\, g_\pm(z)\, h(z) \overset{(12)}{=} \left(\frac{\pm\zeta\beta}{e^{\pm\beta z} - \zeta}\right)\left(\frac{-\zeta z e^{z\delta}}{z - \xi_a}\right) \qquad (24)$$

$= 0$ if we choose the + sign [this choice is dictated by convergence factor]

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So: $$\bar N \overset{(22)}{=} \frac{1}{\beta}\sum_{an} \frac{-\zeta\, e^{i\omega_n\delta}}{i\omega_n - \xi_a} \qquad (25)$$

$$\overset{(18)}{=} \cancel{+}\frac{1}{\cancel{\beta}}\sum_{ak} \mathrm{Res}\left[\left(\frac{+\cancel{\zeta}\cancel{\beta}}{e^{\beta z}-\zeta}\right)\left(\frac{\cancel{-}\,\cancel{\zeta}\, e^{z\delta}}{z-\xi_a}\right)\right]_{z=z_k} \qquad (26)$$

$h(z)$ has only one pole: $z_k = \xi_a$

(27)

$$\boxed{\bar N = \frac{1}{\beta}\sum_{an}\frac{-\zeta}{i\omega_n-\xi_a} = \sum_a \frac{1}{e^{\beta\xi_a}-\zeta} = \begin{cases}\sum_a n_B(\xi_a) & \text{for bosons}\\ \sum_a n_F(\xi_a) & \text{fermions}\end{cases}}$$

$n_{B/F}$ = Bose/Fermi function!

Sometimes it's more complicated, e.g. when $h(z)$ has branch cuts or worse singularities!

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Back to partition function/free energy: inserted to ensure that $N = -\partial_\mu \sum_a F_a$ has conv. factor.

$$F_a \overset{(9)}{=} \frac{1}{\beta}\,\zeta \sum_n e^{i\omega_n\delta} \ln\left[\beta(-i\omega_n+\xi_a)\right] \qquad (28)$$

$$= \frac{1}{\beta}\,\zeta\sum_n \Big\{\underbrace{e^{i\omega_n\delta}\big(\ln\beta(i\omega_n-\xi_a) + \underbrace{\ln(-1)}_{=c}\big)}_{h(i\omega_n)}\Big\} \qquad (29)$$

forget about this constant

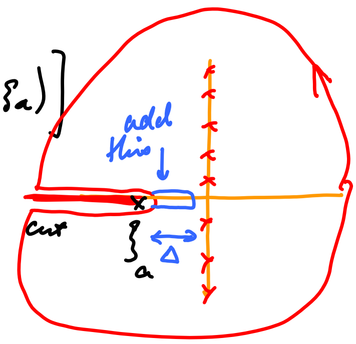
$$\left\{\frac{\zeta\beta}{e^{\beta z}-\zeta} \to \begin{cases} e^{-\beta z} & \text{for } z\to\infty \\ -\beta & -\infty\end{cases}\right.$$

Choose $g_+(z)$, then (16) is satisfied: $$\lim_{z\to\pm\infty} z\, g(z)\, h(z) = 0 \qquad (30)$$

So: $$F_a = \frac{\zeta}{\beta}\int_{C_1} dz\, g(z)\, h(z)$$

$$= \zeta\frac{1}{\beta}\int_{-\infty}^{\xi_a+\Delta}\frac{d\varepsilon}{2\pi i}\, g_+(\varepsilon)\left[\ln(\varepsilon^+-\xi_a) - \ln(\varepsilon^- - \xi_a)\right]$$

$$\varepsilon^\pm = \varepsilon \pm i0^+$$



(Since [ ] = 0 for $\varepsilon > \xi$, we enlarged integration interval from $[-\infty, \xi_a]$ to $[-\infty, \xi_a+\Delta]$)

Integrate by parts, using

$$g_+ = \frac{\xi\beta}{e^{\beta z}-\xi} = \partial_z \ln(1-\xi e^{-\beta z}) \quad \text{check} = \frac{\xi\beta e^{-\beta z}}{1-\xi e^{-\beta z}} = \frac{\xi\beta}{e^{\beta z}-\xi} \checkmark$$

FFIH

$$F_a = -\frac{\xi}{\beta}\int_{-\infty}^{\xi_a+\Delta}\frac{d\varepsilon}{2\pi i}\ln(1-\xi e^{-\beta z})\underbrace{\left[\frac{1}{\varepsilon^+-\xi_a}-\frac{1}{\varepsilon^--\xi_a}\right]}_{-i2\pi\delta(\varepsilon-\xi_a)}$$

$$= \frac{\xi}{\beta}\ln(1-\xi e^{-\beta\xi_a})$$

$\xi_a = \varepsilon_a - \mu$

which is well-known free energy of Bose/Fermi gas.

check: $N_a = -\partial_\mu \sum_a F_a = \frac{\cancel{\xi}}{\cancel{\beta}}\frac{+\cancel{\xi\beta}\, e^{-\beta\xi_a}}{1-\xi e^{-\beta\xi_a}}$

$$= \frac{1}{e^{\beta\xi_a}-\xi} \checkmark.$$