Supplementary Materials for "Quantum Brayton refrigeration cycle with finite-size Bose-Einstein condensates"

Jiehong Yuan[1], Huilin Ruan[1], Dehua Liu[1], Jizhou He[1], and Jianhui Wang[1,2*]
[1] *Department of Physics, Nanchang University, Nanchang, 330031, China*
[2] *State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China*

I. DETAILED DERIVATION OF THE BOSE-EINSTEIN CONDENSATE

A. BEC thermodynamics

Let us consider an ideal Bose gas (with particle number N) confined in a three-dimensional harmonic trap, of which the frequencies along the x_1, x_2, and x_3 axes are ω_1, ω_2, ω_3, respectively. The single-particle energies are then given by ($\hbar \equiv 1$)

$$E_{n_1 n_2 n_3} = \omega_1 n_1 + \omega_2 n_2 + \omega_3 n_3 + \varepsilon_0, \tag{1}$$

where $n_i = 0, 1, 2, \ldots$. $(i = 1, 2, 3)$, and $\varepsilon_0 = \frac{1}{2}(\omega_1 + \omega_2 + \omega_3)$ is the ground state energy [1]. Within the context of grand canonical ensemble, the total particle number of the system can be written in terms of temperate T and chemical potential μ ($k_B \equiv 1$):

$$N = \sum_{n_1 n_2 n_3} \frac{1}{\exp\{[E'_{n_1 n_2 n_3} + (\varepsilon_0 - \mu)]/T\} - 1}, \tag{2}$$

where $E'_{n_1 n_2 n_3} = E_{n_1 n_2 n_3} - \varepsilon_0$.

Using $\Omega = (\omega_1 \omega_2 \omega_3)^{1/3}$ to denote the geometrically average harmonic frequency, the density of states [2] can be parameterized as

$$\rho(E) = \frac{1}{2}\frac{E^2}{\Omega^3} + \gamma \frac{E}{\Omega^2}, \tag{3}$$

where γ is the parameter associated with the frequency of the individual oscillators. For an isotropic harmonic system, i.e., $\omega_1 = \omega_2 = \omega_3 = \Omega$, γ =3/2; in the anisotropic case, the value of γ can be determined numerically [4]. Using integration $N = N_0 + \int \rho(E)/[e^{(E+\varepsilon_0-\mu)/T} - 1]dE$, we have

$$N = N_0 + \left(\frac{T}{\Omega}\right)^3 g_3(z) + \gamma \left(\frac{T}{\Omega}\right)^2 g_2(z), \tag{4}$$

where $N_0 = z/(1-z)$ with fugacity $z = \exp[(\mu - \varepsilon_0)/T]$ is the number of particles on the ground state. Here, $g_n(z)$ with $n = 2, 3$ represents the Bose-Einstein function, is given by

$$g_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{x^{n-1}}{z^{-1}e^x - 1} dx, \tag{5}$$

where $\Gamma(n)$ is the gamma function for integer n. The Bose-Einstein function can also be expressed in series as $g_n(z) = \sum_{l=1}^{\infty} z^l / l^n$. For given particle number N, the fugacity z can be numerically determined according to Eq. (4) when T, γ, Ω are given. Since the number of ground state particles is given by $N_0 = 1/(z^{-1} - 1)$, there is a result of $z = N_0/(N_0 + 1)$, hence $0 \leq z < 1$, so that the functions $g_n(z)$ are bounded by $g_n(1) = \zeta(n)$, with $\zeta(n)$ denoting the Riemannian zeta function.

For the system in the quantum condensed phase–Bose-Einstein condensation, the fugacity $z \approx 1$, and the particle number N_0 for the ground state is

$$N_0 = N - \left(\frac{T}{\Omega}\right)^3 \zeta(3) - \gamma \left(\frac{T}{\Omega}\right)^2 \zeta(2). \tag{6}$$

where we have introduced the Riemannian zeta function $\zeta(n) = g_n(1)$. The critical temperature for the finite Bose system can be calculated according to Eq. (6) to obtain

$$T_c^N \approx \Omega \left(\frac{N}{\zeta(3)}\right)^{1/3} \left[1 - \frac{\gamma\zeta(2)}{3\zeta(3)^{2/3}} \frac{1}{N^{1/3}}\right], \tag{7}$$

which reduces to the thermodynamic-limit one $T_0 = \Omega \left(N/\zeta(3)\right)^{1/3}$ when $N \to \infty$ as it should. Inserting the definition of T_0 into Eq. (6), the ground-state population below T_c can be written as

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_0}\right)^3 - \frac{\gamma\zeta(2)}{\zeta(3)^{2/3}} \frac{1}{N^{1/3}} \left(\frac{T}{T_0}\right)^2. \tag{8}$$

The logarithm of the grand partition function can be obtained as [5]

$$\ln \Xi = \left(\frac{T}{\Omega}\right)^3 g_4(z) + \gamma \left(\frac{T}{\Omega}\right)^2 g_3(z) - \ln(1-z). \tag{9}$$

Using the identity $U = T^2 \left(\partial \ln \Xi / \partial T\right)_{z,\Omega}$, we obtain the internal energy U [i.e., main-text Eq. (2)] which reads

$$U = 3T \left(\frac{T}{\Omega}\right)^3 g_4(z) + 2\gamma T \left(\frac{T}{\Omega}\right)^2 g_3(z), \tag{10}$$

With the grand thermodynamic potential $\mathcal{G}(\Omega, T, \mu) = -T \ln \Xi$, the harmonic pressure for the confined system can be derived by introducing the harmonic volume as $\mathcal{V} = \Omega^{-3}$,

$$\mathcal{P} = -\left(\frac{\partial \mathcal{G}}{\partial \mathcal{V}}\right)_{T,\mu} = T^4 g_4(z) + \frac{2}{3}\gamma\Omega T^3 g_3(z), \tag{11}$$

which is main-text Eq. (3). For the system is in the condensed phase with $z \to 1$, the pressure (11) turns out to be

$$\mathcal{P} = T^4\zeta(4) + \frac{2}{3}\gamma\Omega T^3\zeta(3). \tag{12}$$

The pressure $\mathcal{P}$ turns out to be $\mathcal{P} = T^4\zeta(4)$ [3] in the thermodynamic limit, which indicates that the temperature remains constant during an isobaric process. By contrast, for the finite system the temperature is varied the isobaric process as the pressure depends not only T but also Ω.

Combining Eqs. (7) and (12), the critical temperature at constant pressure for the finite Bose system is obtained,

$$T_c^{\mathcal{P}} = \left[\frac{\mathcal{P}}{\zeta(4) + \frac{2}{3}\gamma \frac{\zeta(3)^{4/3}}{N^{1/3}} \left(1 - \frac{\gamma\zeta(2)}{3\zeta(3)^{2/3}} \frac{1}{N^{1/3}}\right)^{-1}}\right]^{1/4}. \tag{13}$$

B. The isobaric heat capacity

Combination of Eqs. (10) and (11) gives the relation: $U = 3\mathcal{P}\Omega^{-3}$, and we know that the harmonic volume $\mathcal{V} = \Omega^{-3}$, which yields $U = 3\mathcal{P}\mathcal{V}$. The enthalpy is then obtained as $\mathcal{H} = U + \mathcal{P}\mathcal{V} = 4\mathcal{P}\mathcal{V}$, or

$$\mathcal{H} = \frac{4\mathcal{P}}{\Omega^3}. \tag{14}$$

where $\mathcal{P}$ was given by Eq. (11) simplifying to Eq. (12) in the condensed phase. For constant pressure, inserting Eq. (12) into the relation $\partial\mathcal{P}/\partial T = 0$ leads to

$$\frac{\partial\Omega}{\partial T}\Big|_{T<T_c^{\mathcal{P}}} = -3\left(\frac{\Omega}{T} + \frac{2\zeta(4)}{\gamma\zeta(3)}\right), \tag{15}$$

where the ratio Ω/T can be derived from Eqs. (12) and (13) to obtain

$$\frac{\Omega}{T}\Big|_{T<T_c^{\mathcal{P}}} = \frac{3}{2\gamma\zeta(3)}\left[\frac{\Phi}{t^4} - \zeta(4)\right]. \tag{16}$$

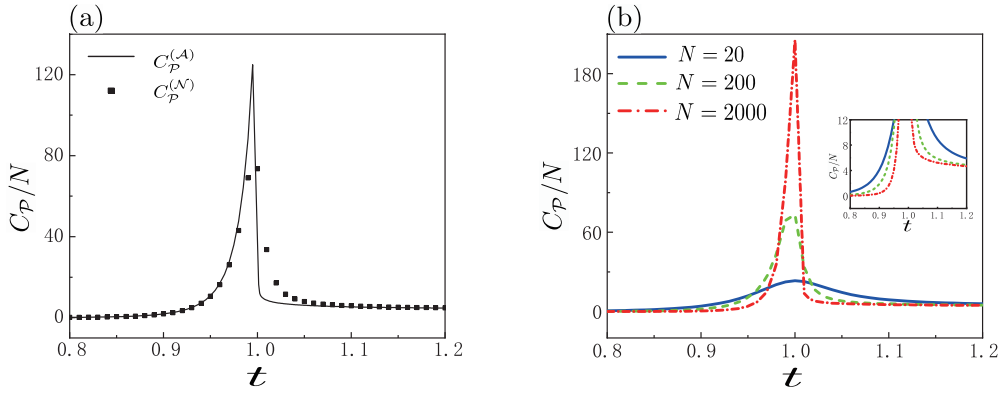

FIG. 1: Isobaric heat capacity $C_{\mathcal{P}}$ of the non-interacting bosonic system as a function of reduced temperature t. (a) Analytical and numerical solutions of the isobaric heat capacity for $N = 200$ particles in the isotropic harmonic oscillator potential, $C_{\mathcal{P}}^{\mathcal{A}}$ and $C_{\mathcal{P}}^{\mathcal{N}}$, are denoted by the solid black line and the small square, respectively. (b) Numerical solutions of the isobaric heat capacity for isotropic harmonic potentials with different numbers of particles. $N = 20$, 200, and 2000 are represented by a blue solid line, a green dash line, and a red dotted dash line, respectively.

Here, we have defined $\Phi = \zeta(4) + \frac{2}{3}\gamma\frac{\zeta(3)^{4/3}}{N^{1/3}}\left(1 - \frac{\gamma\zeta(2)}{3\zeta(3)^{2/3}}\frac{1}{N^{1/3}}\right)^{-1}$ and $t = T/T_c^{\mathcal{P}}$. With consideration Eq. (14), (15), and (16), the specific heat at constant pressure $C_{\mathcal{P}} = \left(\frac{\partial\mathcal{H}}{\partial T}\right)_{N,\mathcal{P}}$ in the condensed phase can be given by

$$\frac{C_{\mathcal{P}}}{N}\Big|_{T<T_c^{\mathcal{P}}} = \frac{32\Phi\gamma^3\zeta(3)^3t^8\left[3\Phi + t^4\zeta(4)\right]}{9N\left[\Phi - t^4\zeta(4)\right]^4}. \tag{17}$$

By using the same approach as in the case of condensed phase, for the non-condensed phase with $T > T_c^{\mathcal{P}}$, we have

$$\frac{\partial\Omega}{\partial T}\Big|_{T>T_c^{\mathcal{P}}} = \frac{\left(\frac{\Omega}{T}\right)^3\gamma^2\Sigma_1 + \left(\frac{\Omega}{T}\right)^2\gamma\Psi_1 + \left(\frac{\Omega}{T}\right)\Upsilon_1}{\left(\frac{\Omega}{T}\right)^2\gamma^2\Sigma_2 + \left(\frac{\Omega}{T}\right)\gamma\Psi_2 + \Upsilon_2}, \tag{18}$$

and

$$\frac{\Omega}{T}\Big|_{T>T_c^{\mathcal{P}}} = \frac{3}{2\gamma g_3(z)}\left[\frac{\Phi}{t^4} - g_4(z)\right]. \tag{19}$$

Here, $\Sigma_1 = 4g_2(z)^2 - 6g_1(z)g_3(z)$, $\Psi_1 = 6g_2(z)g_3(z) - 12g_1(z)g_4(4)$, $\Upsilon_1 = 9g_3(z)^2 - 12g_2(z)g_4(z)$, $\Sigma_2 = 4g_2(z)^2 + 2g_1(z)g_3(z)$, $\Psi_2 = 14g_2(z)g_3(z)$, $\Upsilon_2 = 9g_3(z)^2$. From Eqs. (14), (18), and (19), we can obtain the specific heat by simple algebra to arrive at

$$\frac{C_{\mathcal{P}}}{N}\Big|_{T>T_c^{\mathcal{P}}} = \frac{-24\Phi g_3(z)}{2t^4g_3(z)^2 + 3g_2(z)\Lambda}\frac{4\Upsilon_1t^8g_3(z)^2 + 6\Psi_1t^4g_3(z)\Lambda + 9\Sigma_1\Lambda^2}{4\Upsilon_2t^8g_3(z)^2 + 6\Psi_2t^4g_3(z)\Lambda + 9\Sigma_2\Lambda^2}, \tag{20}$$

with $\Lambda \equiv \Phi - t^4g_4(z)$. In the thermodynamic limit Eq. (20) becomes

$$\frac{C_{\mathcal{P}}^{N\to\infty}}{N}\Big|_{T>T_c^{\mathcal{P}}} = 4\left[\frac{4g_4(z)^2g_2(z)}{g_3(z)^3} - \frac{3g_4(z)}{g_3(z)}\right]. \tag{21}$$

In the high temperature limit where the fugacity z is particularly small, $g_n(z) = \sum_{l=1}^{\infty} z^l/l^n$ can be simply approximated by $g_n(z) \approx z$, leading to $C_{\mathcal{P}>}^{N\to\infty} = 4N$ as it should [5], which can be clearly observed in the inset of Fig. 1(b).

We should keep in mind that, the analytical expressions of the specific heat [cf. Eqs. (17) and (20)] are not exact owing to the two approximations, $z = 1$ for $T < T_c^{\mathcal{P}}$, and $N_0 = 0$ for $T > T_c^{\mathcal{P}}$. Therefore, a more accurate numerical calculation for the specific heat at constant pressure is required, in which z is calculated exactly from Eq. (2) for given N , T and ω_i with $i = 1, 2, 3$. However, when determining the heat capacity $C_{\mathcal{P}}$ analytically expressed as Eqs. (17) and (20), we use Eq. (4) to determine z for given N and Ω/T. For comparison, we plot the analytical and numerical solutions corresponding to $C_{\mathcal{P}<}/N$ and $C_{\mathcal{P}>}/N$ in Fig. 1(a). We observe that our analytical solution is

in nice agreement with the exact numerical calculation, supporting in favor of our analytical approach. Fig. 1 (b) shows the specific heat as a function of reduced temperature t. It can be seen that this specific heat is smooth at the critical point for N, while it becomes sharper with increasing N. The larger system with larger particle number N, the smaller the width of the transition zone near the critical point, as also shown in Fig. 1(b).

C. The equation of state at finite-size

We now explore the equation of state for the finite-size Bose system. For the condensed case, using Eqs (6) and (12), we have

$$\begin{aligned}\mathcal{PV} &= (N-N_0)T\frac{\zeta(4)+(2\gamma\Omega/3T)\,\zeta(3)}{\zeta(3)+(\gamma\Omega/T)\,\zeta(2)} \\ &= NT\frac{\zeta(4)+(2\gamma\Omega/3T)\,\zeta(3)}{\zeta(3)+(\gamma\Omega/T)\,\zeta(2)}\left[\left(\frac{T}{\Omega}\right)^3\frac{\zeta(3)}{N}+\left(\frac{T}{\Omega}\right)^2\frac{\gamma\zeta(2)}{N}\right].\end{aligned} \tag{22}$$

By introducing the correction factor

$$F(z=1)\Big|_{T<T_c^{\mathcal{P}}} = \frac{\zeta(4)+(2\gamma\Omega/3T)\,\zeta(3)}{\zeta(3)+(\gamma\Omega/T)\,\zeta(2)}\left[\left(\frac{T}{\Omega}\right)^3\frac{\zeta(3)}{N}+\left(\frac{T}{\Omega}\right)^2\frac{\gamma\zeta(2)}{N}\right], \tag{23}$$

which, together with Eq. (16), can be re-expressed as

$$F(z)\Big|_{T<T_c^{P}} = \frac{1}{9N\Phi_t^2}\frac{\Phi_t+\zeta(4)}{\zeta(3)+3\zeta(2)/2\zeta(3)\Phi_t}\left[\frac{8\gamma^3\zeta(3)^4}{3\Phi_t}+4\gamma^3\zeta(2)\zeta(3)^2\right], \tag{24}$$

where Φ has been defined below Eq. (16) and use of $\Phi_t \equiv \Phi/t^4-\zeta(4)$ has been made. When the system temperature is larger than the critical value $T_c^{\mathcal{P}}$, the particle number N_0 on the ground state is vanishing, and the state function for the system can be derived via use of Eqs (4) and (12), yielding

$$\mathcal{PV} = NT\frac{g_4(z)+(2\gamma\Omega/3T)g_3(z)}{g_3(z)+(\gamma\Omega/T)g_2(z)}. \tag{25}$$

When we define $F(z)\Big|_{T>T_c^{P}} = \frac{g_4(z)+(2\gamma\Omega/3T)g_3(z)}{g_3(z)+(\gamma\Omega/T)g_2(z)}$ and use Eq, (19), we get

$$F(z)\Big|_{T>T_c^{P}} = \frac{\Phi/t^4}{g_3(z)+3g_2(z)/2g_3(z)\,[\Phi/t^4-g_4(z)]}. \tag{26}$$

With these, the equation of state for the finite-size Bose system can be given by main-text Eq. (4), namely

$$\mathcal{PV} = NTF(z), \tag{27}$$

where

$$F(z) = \begin{cases} \frac{\Phi/t^4}{g_3(z)+3g_2(z)/2g_3(z)[\Phi/t^4-g_4(z)]}, & T \geq T_c^{\mathcal{P}} \\ \frac{1}{9N\Phi_t^2}\frac{\Phi_t+\zeta(4)}{\zeta(3)+3\zeta(2)/2\zeta(3)\Phi_t}\left[\frac{8\gamma^3\zeta(3)^4}{3\Phi_t}+4\gamma^3\zeta(2)\zeta(3)^2\right]. & T < T_c^{\mathcal{P}} \end{cases} \tag{28}$$

When $T > T_c^{\mathcal{P}}$, we reproduce $F(z)^{N\to\infty} = g_4(z)/g_3(z)$ in the thermodynamic limit. Additionally, the classical limit where $F(z) \approx 1$ leads to the state function $\mathcal{PV} = NT$[5] for the classical gas as expected.

II. THE ISENTROPIC CONDITION

The thermodynamic entropy S can determined by using the grand thermodynamic potential $\mathcal{G} = -T\ln\Xi$ to obtain

$$S = -\left(\frac{\partial\mathcal{G}}{\partial T}\right)_{\mu,\Omega} = \left(\frac{T}{\Omega}\right)^3[4g_4(z)-g_3(z)\ln z]+\gamma\left(\frac{T}{\Omega}\right)^2[3g_3(z)-g_2(z)\ln z]. \tag{29}$$

During an isentropic, adiabatic process, we have

$$dS = \left(\frac{\partial S}{\partial T}\right)_\Omega dT + \left(\frac{\partial S}{\partial \Omega}\right)_T d\Omega = 0, \tag{30}$$

or

$$\frac{d\Omega}{dT} = -\frac{\left(\frac{\partial S}{\partial T}\right)_\Omega}{\left(\frac{\partial S}{\partial \Omega}\right)_T}. \tag{31}$$

Employing the identity $\frac{d}{dz}g_n(z) = \frac{1}{z}g_{n-1}(z)$, Eq. (29) gives rise to

$$\begin{aligned}\left(\frac{\partial S}{\partial T}\right)_\Omega &= \frac{3T^2}{\Omega^3}\left[4g_4(z) - \ln z g_3(z)\right] + \frac{2\gamma T}{\Omega^2}\left[3g_3(z) - \ln z g_2(z)\right] \\ &+ \frac{\partial z}{\partial T}\frac{T^2}{\Omega^2}\left[\frac{T}{\Omega}\frac{3g_3(z) - \ln z g_2(z)}{z} + \gamma\frac{2g_2(z) - \ln z g_1(z)}{z}\right],\end{aligned} \tag{32}$$

and

$$\begin{aligned}\left(\frac{\partial S}{\partial \Omega}\right)_T &= -\frac{3T^3}{\Omega^4}[4g_4(z) - \ln z g_3(z)] - \frac{2\gamma T^2}{\Omega^3}[3g_3(z) - \ln z g_2(z)] \\ &+ \frac{\partial z}{\partial \Omega}\frac{T^2}{\Omega^2}\left[\frac{T}{\Omega}\frac{3g_3(z) - \ln z g_2(z)}{z} + \gamma\frac{2g_2(z) - \ln z g_1(z)}{z}\right].\end{aligned} \tag{33}$$

We assume that the temperature-frequency relation under the isotropic condition is the same as that of the harmonic systems [6], i.e., T/Ω =Const. Under this condition, we find from Eqs. (33) and (32) that the relation

$$T\frac{\partial z}{\partial T} = -\Omega\frac{\partial z}{\partial \Omega}. \tag{34}$$

By applying this to Eq. (4), we get

$$\frac{\partial z}{\partial T} = -\frac{3z}{T}\frac{g_3(z) + (2\gamma\Omega/3T)g_2(z)}{g_2(z) + (\gamma\Omega/T)g_1(z)}, \tag{35}$$

and

$$\frac{\partial z}{\partial \Omega} = \frac{3z}{\Omega}\frac{g_3(z) + (2\gamma\Omega/3T)g_2(z)}{g_2(z) + (\gamma\Omega/T)g_1(z)}. \tag{36}$$

By comparing Eqs. (35) and (36), we confirm that Eq. (34) holds for arbitrary z throughout the isentropic process.

Since for an isentropic process $S = S(\Omega/T, z) =$ const with $\Omega/T =$ const, z is kept constant. That is, for the machine cycle sketched in main-text Fig. 1, there exists a relation of $z_1 = z_2$ and $z_3 = z_4$. The correction factor $F(z)$ in Eq. (27) is therefore kept constant during the adiabatic process, yielding

$$\frac{\mathcal{V}_l}{\mathcal{V}_2} = \left(\frac{\mathcal{P}_h}{\mathcal{P}_l}\right)^{3/4} = \left(\frac{T_2}{T_l}\right)^3, \ \frac{\mathcal{V}_h}{\mathcal{V}_4} = \left(\frac{\mathcal{P}_l}{\mathcal{P}_h}\right)^{3/4} = \left(\frac{T_4}{T_h}\right)^3. \tag{37}$$

Using Eq. (37) and main-text Eq. (7), we can obtain

$$\varepsilon = \frac{Q_l}{W} = \frac{4\mathcal{P}_l\left(\mathcal{V}_l - \mathcal{V}_4\right)}{4\mathcal{P}_h\left(\mathcal{V}_2 - \mathcal{V}_h\right) - 4\mathcal{P}_l\left(\mathcal{V}_l - \mathcal{V}_4\right)} = \frac{1}{\left(\mathcal{P}_h/\mathcal{P}_l\right)^{1/4} - 1}. \tag{38}$$

* Electronic address: wangjianhui@ncu.edu.cn

[1] S. Grossmann and M. Holthaus, λ-transition to the Bose-Einstein condensate, Z. Naturforsch. A **50**, 921 (1995).
[2] K. Kirsten and D. J. Toms, Density of states for Bose-Einstein condensation in harmonic oscillator potentials, Phys. Lett. A **222**, 148 (1996).
[3] V. Romero-Rochín, Equation of state of an interacting Bose gas confined by a harmonic trap: The role of the "harmonic" pressure, Phys. Rev. Lett. **94**, 130601 (2005).
[4] S. Grossmann and M. Holthaus, On Bose-Einstein condensation in harmonic traps, Phys. Lett. A **208**, 188 (1995).
[5] R. K. Pathria, Statistical Mechanics (Butterworth-Heinemann, Washington, DC, 1996).
[6] S. Deffner, Efficiency of harmonic quantum Otto engines at maximal power, Entropy **20**, 875 (2018).