

Local and global heat capacities of confined Bose gases: The impact of quantum migration

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(Received 14 June 2025; accepted 23 October 2025; published 18 November 2025)

The recently proposed macroscopic quantum phenomenon, Temperature-Induced Quantum Migration (TIQM), causes local heating and cooling and significantly affects the local heat capacity of a noninteracting confined Maxwell-Boltzmann gas. TIQM guarantees the non-negativity of local heat capacity at low temperatures, results in a substantial local heat-capacity overshoot, and provides a physical basis for global heat-capacity maxima and thermal confinement energy. We extend this framework here to Bose gases in three different rectangular domains, effectively providing three-dimensional (3D)/two-dimensional (2D)/one-dimensional (1D) confinement at high temperatures while transitioning to 2D/1D/zero-dimensional (0D) at low temperatures, thus inducing dimensional crossovers during temperature changes. We demonstrate that quantum degeneracy enhances the TIQM process, resulting in dimension-dependent effects on local and global heat capacities. For the 3D-2D crossover, TIQM leads to a giant excess local heat capacity and explains the mechanism for the enhancement of the global heat-capacity maximum, which surpasses the unconfined ideal Bose gas limit (1.93), reaching 1.97 at a finite density. Conversely, for the 2D-1D and 1D-0D crossovers, the excess local heat capacity diminishes with increasing quantum degeneracy (density), while it is TIQM alone that becomes responsible for excess global heat capacity. For the 1D-0D crossover, we find that only single-particle ergodic systems can have a global excess heat capacity; otherwise, the maximum behavior disappears completely. TIQM also provides a mechanism for the thermal confinement energy in Bose gases.

DOI: [10.1103/s72k-4vmx](https://doi.org/10.1103/s72k-4vmx)

I. INTRODUCTION

In the thermodynamic limit, the contributions of both quantum and classical size effects are completely negligible and all the local properties have a uniform distribution in equilibrium. In practice, this is true even in a finite system, as long as the particles are noninteracting and the system sizes are much larger than the thermal de Broglie wavelength of the particles, λ_{th} . Therefore, in a noninteracting macroscopic gas, the global properties are a function of volume, but not functions of the surface area, periphery, number of vertices or corners, curvature, etc., of the lower dimensional geometric parameters. Similarly, local properties are functions of the local volume, but not functions of position. In this way, the thermodynamic limit allows the use of the additivity rule and makes the solutions simple. In most of the problems of thermodynamics and statistical physics, the systems are considered in the thermodynamic limit.

On the other hand, this assumption breaks down at the nanoscale where λ_{th} is not negligible compared to system sizes. In such a case, quantum size effects make significant

contributions to thermodynamic properties and the system becomes inhomogeneous even for noninteracting particles at equilibrium [1–3]. Not only size, but also shape becomes a control parameter for thermodynamic state functions. Most of the simple relations of thermodynamics become invalid, and thermodynamics turns into a complicated analysis even for a simple system. This is why nanoscale thermodynamics has been one of the main hot topics in the last few decades [1–32]. Size and shape control extends the degree of freedom of the thermodynamic state space and opens up new possibilities for advanced energy conversion [23,26–28,33–35].

Quantum size and shape effects on the global heat capacity of confined and noninteracting gases constitute a unique problem as they suggest excess and adjustable heat capacity. For the heat capacity of noninteracting Maxwell-Boltzmann particles confined in a finite domain, plenty of work and discussion has been done in the literature starting from the 1960s [4,36–40]. These studies have showed that the global heat capacity per particle reaches the excess value of 0.56 over the corresponding classical value of 1/2 for each confined direction at a certain temperature (or size). The excess heat capacity is a direct consequence of the thermal part of the confinement energy [4–16,19,21,30]. Nanoscale heat capacity continues to be an important and active area of research, as quantum size effects suggest unusual and superior behavior in heat capacity [4,5,30,31,36–46].

As with the Maxwell-Boltzmann gases, finite-size effects in noninteracting Bose gases is also an active research topic [47–57]. The global heat capacity is one of the focused quantities in these studies [47,48,50–53,56,57]. New optical traps enable not only trapping the Bose gas in harmonic potentials

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but also in box potentials [54,58], which has revealed unusual behaviors [47,48,52,55–57]. Another recently studied problem is the quantum shape effect to control the Bose-Einstein condensation and its effect on the global heat capacity of a finite and noninteracting Bose gas confined in core-shell box potentials [59].

All the studies in the literature on the thermodynamics of confined systems focus on the global properties, while the local ones have been almost completely overlooked. The global heat capacity at constant sizes of a system is the temperature derivative of the exchanged heat of the entire system with its environment. Since there are no particle and work exchanges with the environment during this process, it is simply equal to the temperature derivative of the energy of the system. In the case of local heat capacity, however, in addition to the heat exchange across the external boundaries of the system, there are also particle, work, and heat exchanges between the local volume and the rest of the system as a result of the recently described Temperature-Induced Quantum Migration (TIQM) [60].

In a gas confined at nanoscale, even if the particles are noninteracting, the density is not homogeneous due to quantum size effects. Its distribution changes with temperature, even though the system sizes are kept constant [1–3,60]. Therefore, a change in the temperature causes the migration of particles from one local volume to another. This is a macroscopic quantum phenomenon caused by the variations in the occupancy number in each quantum mode and the corresponding quantum probability density due to temperature changes [60]. Particle migration within the system causes local work and heat exchanges, making the local heat capacity different from the global one and a complicated quantity to calculate.

For a confined noninteracting Maxwell-Boltzmann gas, the local heat capacity has recently been studied in detail by introducing TIQM [60]. It has been shown that TIQM causes a massive local heat capacity and also provides a physical macroscopic mechanism for the excess global heat capacity as well as the thermal part of the confinement energy. It has been declared that a stronger TIQM process is expected for a Bose gas under quantum degeneracy conditions.

Hence, in this study, we investigate the influence of the TIQM process on the *local* and *global* heat capacities of a noninteracting but confined (finite) Bose gas. We consider three different anisometric rectangular domains for the confinement, each with finite size in one, two, and three directions while practically infinite (much greater than λ_{th}) in the other directions, corresponding to three-dimensional (3D), two-dimensional (2D), and one-dimensional (1D) confinement at high-temperature limit, respectively. These distinct domains also allow us to study the effects of dimensional transitions from 3D to 2D, 2D to 1D, and 1D to zero-dimensional (0D) with decreasing temperature, i.e., increasing confinement in the finite-size directions. Section II is devoted to the investigation of temperature variations of the global heat capacity for these finite domains to provide benchmark results for the local heat capacity through their domain integrals. In addition to the benchmark results, we obtain an unusual single-particle condition that is necessary to observe the maximum heat-capacity behavior for a finite 1D ergodic system. To highlight the differences between the global heat-capacity predictions of finite

and infinite domain models, the results in the literature for an arbitrary integer-dimensional infinite rectangular domain (leading to a continuous energy spectrum) are also compared with those for the finite domain. In Sec. III, the local heat capacity and its conductive and quantum migration components are derived for the considered finite-size domains and their temperature and position variations are analyzed. The density dependencies of excess local and global heat capacities are also examined. Similarity between the local thermal confinement energy and the quantum migration contribution to the local heat capacity is observed. The conclusions are presented in Sec. IV.

II. GLOBAL HEAT CAPACITY IN FINITE-SIZE NANODOMAINS

The global heat capacity of a noninteracting and finite Bose gas has been extensively studied in harmonic traps and some regular geometries [47–57]. The studies of the confinement effect on the heat capacity for a rectangular domain can be traced back to 1964 [47,57]. In these studies, a D -dimensional Bose gas was studied by considering a box that is unconfined (unbounded) in the D directions while strongly confined in other directions. Therefore, the thermodynamic properties, based on infinite sums over the energy eigenvalues, have been calculated by using the continuum (integral) approach for the unconfined directions and the ground-state (the first state) approach for the strongly confined directions. Consequently, their results represent only the integer D -dimensional systems. In a relatively recent study [52], a finite-size 3D cubic confinement potential was considered and the size effects on the global heat capacity were analyzed. It has been seen that the maximum heat capacity goes beyond its conventional value (1.926) and the critical temperature shifts to the higher values. As the temperature decreases, the thermal de Broglie wavelength of particles becomes longer and the Bose gas in a finite cube undergoes a direct transition from 3D to 0D behavior since there is no preferred direction in an isometric cube.

On the other hand, considering an anisometric rectangular domain allows us to analyze the finite-size effects on the heat capacity behavior during the gradual transitions between the integer dimensions, such as 3D-2D, 2D-1D, and 1D-0D, which have not been studied yet. Therefore, with the aim of not only providing a benchmark for local heat-capacity calculations by their domain integrals but also investigating some of its yet unexplored behaviors, we consider the global heat capacity of a noninteracting Bose gas confined in three different rectangular domains shown in Fig. 1.

Due to the growing λ_{th} with decreasing temperature, the system illustrated in Fig. 1(a) becomes strongly confined in the direction of L_S in the low-temperature limit, thus representing a 2D system as $L_S < \lambda_{th}$. In the high-temperature limit, however, the system becomes practically unbounded (unconfined), as $L_S \gg \lambda_{th}$, and represents a 3D system. In other words, change of temperature induces a dimensional transition in the system. similar behavior appears also for the domains in Figs. 1(b) and 1(c) with lower dimensions. Therefore, such anisometric domains allow us to analyze not only finite-size effects on the global heat capacity but also the influence of dimensional transitions between different integer

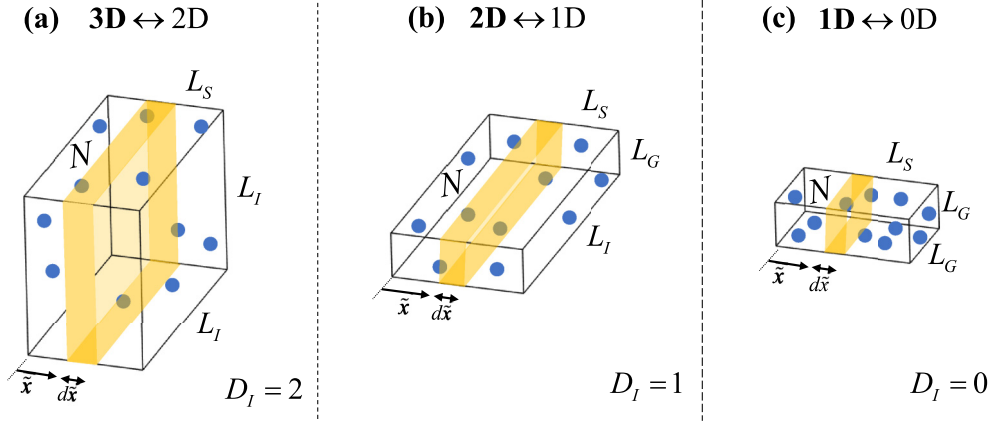


FIG. 1. The considered finite confinement domains. They are named according to the high temperature limit behavior of confined particles as (a) 3D, (b) 2D, and (c) 1D domains. D_I represents the integer dimension, which is equal to the number of unconfined (free) directions while D is the total dimension. Since the enlarging of λ_{th} with decreasing temperature reduces the dimension by one unit due to the finite size of L_S , the confinement dimension changes in between two consecutive integer dimensions (given above each subfigure) as the temperature changes. N denotes the total number of particles and the subscripts I , S , and G represent the sizes for which integral, summation, and ground-state approaches can be used, respectively, to calculate any summations over the energy components in that direction. For the maximum and the minimum temperatures of the investigation, T_{max} and T_{min} , the order of magnitude conditions of the domain sizes is $L_G \ll \lambda_{\text{th}}(T_{\text{max}}) \lesssim L_S \lesssim \lambda_{\text{th}}(T_{\text{min}}) \ll L_I$. The yellow regions refer to the local volume considered during the local heat-capacity calculations and $\tilde{x} = x/L_S$.

dimensions. In Fig. 1, the subscripts I , S , and G indicate that the sums over the energy components in the specified directions should be calculated by using the integral approach (I), by the sum itself (S), and by the ground-state approach (G), respectively. For a given temperature range, $T_{\text{min}} \leq T \leq T_{\text{max}}$, this requires that $L_G \ll \lambda_{\text{th}}(T_{\text{max}}) \lesssim L_S \lesssim \lambda_{\text{th}}(T_{\text{min}}) \ll L_I$.

In the direction of L_I , an effectively infinite number of momentum states are available for the occupation of particles and it means that each unconfined direction (I) contributes one integer dimension (1D) to the total dimension. In the direction of L_G , however, there is effectively only one available momentum state, the ground state, and each strongly confined direction has no contribution (0D) to the total dimension. On the other hand, for the direction of L_S , the confinement is neither too strong (0D) nor too weak (1D), but in between these two asymptotic limits. Therefore, its contribution to the total dimension is in between 1D and 0D, the fractional dimensional contribution [29]. At high temperatures, its contribution goes to 1D while it goes to 0D for low temperatures.

In a finite Bose gas, confined by a box potential, there is no phase transition as the ground-state occupation continuously increases when temperature decreases. There is also no discontinuity in the heat capacity [52]. As shown in this section, even the maximal behavior of heat capacity disappears for high-density conditions for a domain given in Fig. 1(c). Therefore, instead of Bose-Einstein Condensation (BEC) temperature, we use the ground-state temperature as a persistent temperature scale to define the dimensionless temperature.

For noninteracting particles confined in a rectangular domain, the energy eigenvalues in direction i are obtained from the Schrödinger equation as $\varepsilon_i = \pi^2 \hbar^2 k_i^2 / 2mL_i^2$, $k_i = 1, 2, 3, \dots$ with the particle mass m , the reduced Planck constant $\hbar$, and the domain sizes L_i . The dimensionless energy eigenvalues are then defined in the form of $\tilde{\varepsilon}_i = \varepsilon_i / k_B T = (\alpha_i k_i)^2$, where k_B is the Boltzmann constant, T is the temperature, $\alpha_i = \sqrt{T_{0,i}/T}$ is the confinement parameter, and

$T_{0,i} = \varepsilon_{0,i} / k_B$ is the ground-state temperature, which corresponds to the ground-state energy $\varepsilon_{0,i} = \pi^2 \hbar^2 / 2mL_i^2$ in direction i .

We choose $T_{0,S} = T_0$ as the reference temperature to define the *dimensionless temperature*, $\tilde{T} = T/T_0$. Therefore, $\alpha_S = 1/\sqrt{\tilde{T}}$ and considering the aspect ratios $r_I = L_I/L_S$ and $r_G = L_S/L_G$, the confinement parameters in the directions of L_I and L_G can be expressed in terms of α_S as $\alpha_I = \alpha_S/r_I$ and $\alpha_G = \alpha_S r_G$, respectively. The integral and ground-state approaches for the sums over the quantum state variables k_i require $\alpha_I = \alpha_S/r_I \ll 1$ and $\alpha_G = \alpha_S r_G \gg 1$, respectively. Thus, the aspect ratios of the box are determined by considering the following inequalities $r_I \gg 1/\sqrt{\tilde{T}_{\text{min}}}$ and $r_G \gg \sqrt{\tilde{T}_{\text{max}}}$ for a given temperature interval.

Similarly, we chose the quantum density at T_0 , as a temperature (T)-independent reference value, $n_q(T_0) = 1/\lambda_{\text{th}}^{D_I}(T_0)$, to define the *dimensionless density* as $\tilde{n}_0 = \tilde{n}/n_q(T_0)$. Here, $\lambda_{\text{th}}(T_0) = 2\pi \hbar / \sqrt{2\pi m k_B T_0} = 2L_S/\sqrt{\pi}$ is the thermal de Broglie wavelength of the particles at T_0 , and $\tilde{n} = N/V_f$ is the global density defined by the total number of particles, N , and the volume of the free domain, $V_f = L_I^{D_I}$, calculated by considering only the sizes in unconfined directions, L_I , and their number D_I , the integer (free) dimension. The total number of particles is related with $\tilde{n}_0$ by $N = \tilde{n}_0 * (\sqrt{\pi} r_I / 2)^{D_I}$. Therefore, as long as $r_I \gg 1/\tilde{n}_0^{1/D_I}$, it is possible to keep the number of particles much larger than one, $N \gg 1$, for any value of the density, $\tilde{n}_0$, when $D_I \neq 0$ [Figs. 1(a) and 1(b)]. The same condition holds, if $\tilde{n}_0 \gg 1$ when $D_I = 0$ [Fig. 1(c)].

By considering the Bose-Einstein distribution function and the equality $N = \tilde{n}_0 * (\sqrt{\pi} r_I / 2)^{D_I}$, as well as the integral and ground-state approaches for the directions of L_I and L_G , respectively, the following expression is obtained:

$$\tilde{n}_0(D_I) = \tilde{T}^{D_I/2} \sum_{k_S=1}^{\infty} \text{Li}_{D_I/2} \left[\exp \left(\Lambda_C - \frac{k_S^2}{\tilde{T}} \right) \right]. \quad (1)$$

where Li is the Polylogarithm function, $\Lambda_C = \mu_C/k_B T$ is the *dimensionless chemical potential*, modified by considering the ground-state energy in strongly confined directions, and it is defined as $\Lambda_C = \Lambda - (2 - D_I)r_G^2/\tilde{T}$. Appendix A provides the derivation of Eq. (1). To ensure that Eq. (1) yields real values, the parameter Λ_C must be constrained to the range $-\infty < \Lambda_C < 1/\tilde{T}$. For the domain in Fig. 1(a), $D_I = 2$ and the modified chemical potential is equal to the conventional one, $\Lambda_C = \Lambda$. For the ones in Figs. 1(b) and 1(c), $D_I = 1$ and $D_I = 0$, respectively, and chemical potential shifts by the dimensionless nonzero ground-state energy, $\alpha_G^2 = r_G^2/\tilde{T}$, in each strongly confined direction.

Note that spin states are not considered in this study. The summation over spin states yields a constant factor, g_s , representing the number of possible spin states. This factor can be readily incorporated into the quantum density expression as $n_q(T_0) = g_s/\lambda_{\text{th}}^{D_I}(T_0)$. Consequently, the exclusion of spin states as an explicit variable does not alter the results, provided that g_s is accounted for in the quantum density. Only the total number of particles changes if $g_s \neq 1$ as $N = g_s \tilde{n}_0 * (\sqrt{\pi} r_I/2)^{D_I}$. For simplicity, we assume $g_s = 1$ in this work.

In the high-temperature regime ($\tilde{T} \gg 1$), the factor of $1/\tilde{T}$ in Eq. (1) is small, which enables converting the sum to an integral, and thus reducing Eq. (1) to the conventional continuous form

$$\tilde{T} \gg 1 \Rightarrow \tilde{n}_0(D_I) = \tilde{T}^{(D_I+1)/2} \frac{\sqrt{\pi}}{2} \text{Li}_{(D_I+1)/2}[\exp(\Lambda_C)]. \quad (2)$$

In the strong degeneracy limit ($\Lambda_C \rightarrow -\Lambda_C^{\text{max}} = 0$), the asymptotic behavior of the Polylogarithm function causes distinct density behaviors depending on the dimensionality D_I . For $D_I = 2$, the maximum density is $\tilde{n}_0 = (\sqrt{\pi}/2)\tilde{T}^{3/2}\zeta(3/2)$, where ζ is the Riemann Zeta function. However, for $D_I = 1$ and $D_I = 0$, this limit predicts an infinite density ($\tilde{n}_0 \rightarrow \infty$).

The high-temperature regime, where $\lambda_{\text{th}} \ll L_S$, effectively causes the confinement to release in the L_S direction. Consequently, Fig. 1(a) corresponds to a 3D system in this regime. The maximum density predicted by Eq. (2) at a given temperature accounts only for particles in excited states. At higher densities, excess particles occupy the ground state and do not contribute to the heat capacity, the manifestation of BEC.

A similar phenomenon occurs in the temperature domain. In the high-density regime ($\tilde{n}_0 \gg 1$), Eq. (2) predicts a transition (BEC) temperature $\tilde{T}_C = \{2\tilde{n}_0/[\sqrt{\pi}\zeta(3/2)]\}^{2/3} \gg 1$ for $D_I = 2$. Below this temperature, the equation would predict a lower density, implying that the remaining particles condense into the ground state, thus we recover the standard theoretical treatment of BEC.

In the high-temperature regime, the cases of $D_I = 1$ and $D_I = 0$ effectively correspond to 2D and 1D systems, respectively. In these lower dimensions, Eq. (2) predicts an infinite density for a given temperature (or zero temperature for a given density) as $\Lambda_C \rightarrow -0$, indicating the absence of a finite-density (or finite-temperature) phase transition. This aligns with conventional results for low-dimensional unconfined Bose gases.

In the opposite limit, $\tilde{T} \ll 1$, $1/\tilde{T}$ becomes big enough so that the sum can be represented by considering only the first

term,

$$\tilde{T} \ll 1 \Rightarrow \tilde{n}_0 = \tilde{T}^{D_I/2} \text{Li}_{D_I/2}\left[\exp\left(\Lambda_C - \frac{1}{\tilde{T}}\right)\right]. \quad (3)$$

In this temperature limit, as $\lambda_{\text{th}} \gg L_S$, confinement in the direction of L_S becomes too strong and the systems in Figs. 1(a)–1(c) reduce to 2D, 1D, and 0D systems, respectively. Therefore, in the strong degeneracy limit, $\Lambda_C \rightarrow -\Lambda_C^{\text{max}} = 1/\tilde{T}$, the Polylogarithm function goes to infinity for all the configurations in Fig. 1, confirming the nonexistence of BEC for $D < 2$ [47].

A general expression for the dimensionless global heat capacity of a noninteracting Bose gas confined in rectangular domains with constant sizes illustrated in Figs. 1(a)–1(c) is obtained as

$$\begin{aligned} \tilde{C} = \frac{C_L}{Nk_B} = & \left(\frac{{}_2A_{-1}}{{}_0A_0} - \frac{{}_1A_{-1}^2}{{}_0A_0{}_0A_{-1}} \right) \\ & + \frac{D_I}{2} \left[\frac{{}_0A_1}{{}_0A_0} + 2 \left(\frac{{}_1A_0}{{}_0A_0} - \frac{{}_1A_{-1}}{{}_0A_{-1}} \right) \right] \\ & - \left(\frac{D_I}{2} \right)^2 \left(\frac{{}_0A_0}{{}_0A_{-1}} - \frac{{}_0A_1}{{}_0A_0} \right), \end{aligned} \quad (4)$$

where ${}_xA_y$ is the energy moment function defined by

$$\begin{aligned} {}_xA_y = & {}_xA_y(\Lambda_C, \tilde{T}) \\ = & \sum_{k_S=1}^{\infty} \left(\frac{k_S^2}{\tilde{T}} \right)^x \text{Li}_{(D_I/2)+y} \left[\exp \left(\Lambda_C - \frac{k_S^2}{\tilde{T}} \right) \right]. \end{aligned} \quad (5)$$

Note that the subscript of L in $\tilde{C}$ is dropped for simplicity in later notations. The derivation, Eq. (4), can be found in Appendix A. The inverse solution of Eq. (1) gives the value of $\Lambda_C(\tilde{n}_0, \tilde{T})$ to be used in Eq. (4).

If the confinement in the direction of L_S is released, $L_S \gg \lambda_{\text{th}}(T_{\text{min}})$, then the reduced temperature $\tilde{T} \gg 1$ for any $T > T_{\text{min}}$. In this high-temperature regime, the summation in Eq. (5) can be approximated by an integral, resulting in the A functions reducing to B functions given by

$${}_xB_y = \left(\frac{\sqrt{\tilde{T}}}{2} \right) \Gamma \left(x + \frac{1}{2} \right) \text{Li}_{[(D_I+1)/2]+x+y}[\exp(\Lambda_C)]. \quad (6)$$

A relaxation of the confinement in the L_S direction, which corresponds to an additional degree of freedom, leads to an increase of 1 in the total dimension $D = D_I + 1$, thereby implying that D can only take integer values. Using the B functions, Eq. (6), instead of A functions in Eq. (4) leads to the following generalized piecewise heat-capacity expression for any integer dimension D :

$$\begin{aligned} D = 3 \quad \text{and} \quad \tilde{T} > \tilde{T}_C \quad \text{or} \quad D \leq 2 \Rightarrow \\ \tilde{C}_I = & \left(\frac{D}{2} \right) \left[\left(\frac{D+2}{2} \right) \frac{\text{Li}_{(D+2)/2}}{\text{Li}_{D/2}} - \frac{D}{2} \frac{\text{Li}_{D/2}}{\text{Li}_{(D-2)/2}} \right], \end{aligned} \quad (7)$$

$$D = 3 \quad \text{and} \quad \tilde{T} \leq \tilde{T}_C \Rightarrow$$

$$\tilde{C}_I = \tilde{C}_I^{\text{max}} \left(\frac{\tilde{T}}{\tilde{T}_C} \right)^{3/2}, \quad \tilde{C}_I^{\text{max}} = \left(\frac{15}{4} \right) \frac{\zeta[5/2]}{\zeta[3/2]} \approx 1.926, \quad (8)$$

where we use the subscript I in $\tilde{C}$ to stress that it applies solely to integer dimensions, Li is used for the compact representation, instead of $\text{Li}[\exp(\Lambda_C)]$. As the number of free dimensions increases 1 integer unit when $\tilde{T} \gg 1$, $n_q(T_0) = 1/\lambda_{\text{th}}^{D_I+1}(T_0)$ and $V_f = L_f^{D_I} L_S$, which leads to $\tilde{n}_0 = \tilde{n}_0(D_I) * (2/\sqrt{\pi})$. Therefore, we can write the BEC temperature by modifying the density as $\tilde{T}_C = [\tilde{n}_0/\zeta(3/2)]^{2/3}$ for $D = D_I + 1 = 3$. For other cases, $D = 2$ and $D = 1$, $\tilde{T}_C = 0$ since $\text{Li}_{D/2}[\exp(\Lambda_C)] \rightarrow \infty$ when $\Lambda_C \rightarrow -0$.

Finite systems exhibit fractional dimensions in their effective momentum space, and their global heat capacity is described by a single equation, Eq.(4). In contrast, infinite systems display integer-dimensional behavior and have a piecewise heat-capacity expression, represented by Eqs. (7) and (8). This piecewise behavior is a natural consequence of the phase transition (BEC) for $D = 3$ while the transition disappears for $D = 2$ and $D = 1$, as discussed in the paragraphs following Eq. (2).

For integer-dimensional systems, Eq. (8) dictates that the maximum global heat capacity appears only for $D = 3$ when $\tilde{T} = \tilde{T}_C$. Equations (7) and (8) are the expressions given in the literature for the global heat capacity of an ideal Bose gas confined in any integer-dimensional domain [47,57]. Therefore, the more general expression, Eq. (4), valid for any dimension, simplifies to Eqs. (7) and (8) specifically for integer-dimensional systems when confinement is very strong in some directions while negligible in others. If the confinement level is in between these two asymptotic conditions, the momentum space of the system is effectively fractional-dimensional and there is no sign of a phase transition in the heat capacity, but a continuous change including its maximum point. In other words, there is no BEC temperature if the confinement domain is finite. The temperature variation of heat capacity, Eq. (4), shows this behavior clearly in Fig. 2(a). This is in agreement with the nonexistence of phase transitions in small (finite) systems [53,61], and the studies in the literature about finite Bose gas in a box potential [47,48,52,55,57].

For the noninteracting Bose gas confined in the domains shown in Fig. 1, the global heat capacities and their integer-dimensional counterparts are seen in Figs. 2(a)–2(c). In Fig. 2(a), the conventional (unconfined) 3D heat capacities, calculated by Eqs. (7) and (8), are represented by the dashed curves for different densities. Their temperature derivatives are discontinuous at $\tilde{T}_C$ for which the heat capacities reach to their maximum, $\tilde{C}_{\text{max}}^{3D} = [15\zeta(5/2)]/[4\zeta(3/2)] \simeq 1.926$. The values of $\tilde{T}_C$ grow with increasing density, $\tilde{n}_0$. These results illustrated by the dashed curves represent the usual behavior of an unconfined Bose gas.

Their finite (confined) counterparts, calculated from Eq. (4) are indicated by the solid curves. They exhibit continuous variations, and their maximum values can be smaller than those of their conventional counterparts at low densities, but greater at high densities. The maximum heat-capacity temperatures are always higher than the BEC temperatures $\tilde{T}_C$, corresponding to the maximums of the dashed curves, as mentioned in the literature [48,52,55]. This temperature shift is more important for low densities while it becomes negligible for high densities. At high temperatures ($\tilde{T} \gg 1$), all of them converge the classical limit of $\tilde{C}_L^{\text{MB}} = 3/2$

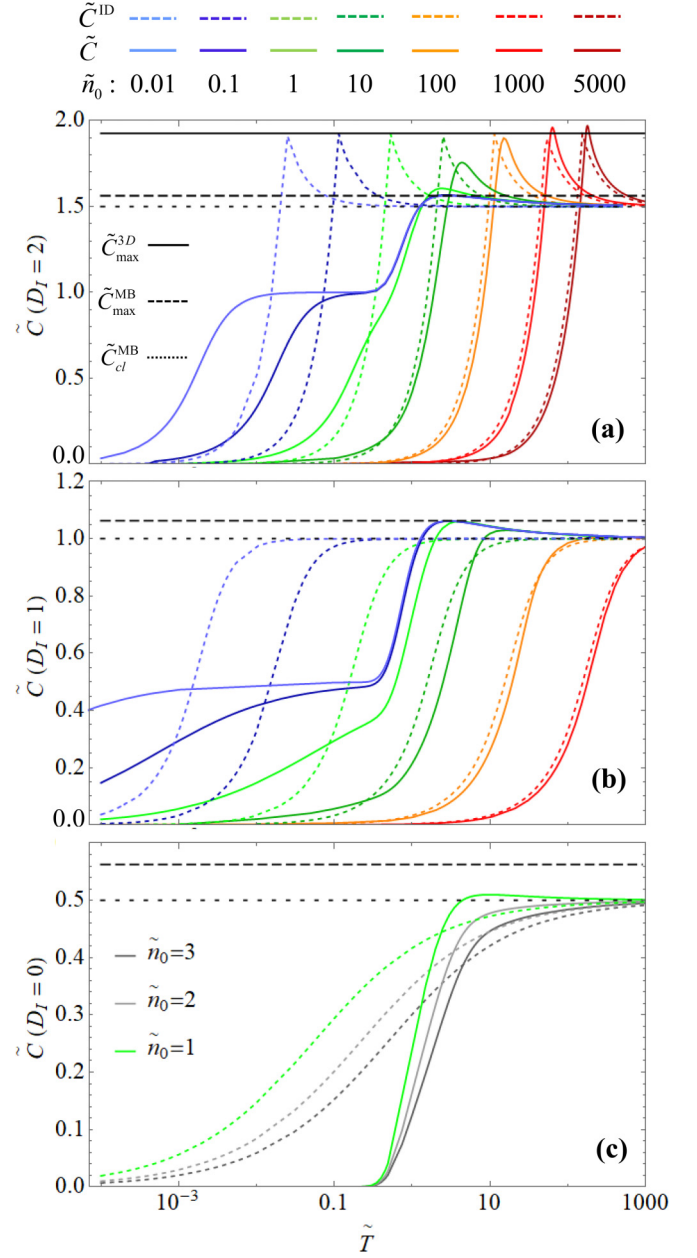


FIG. 2. Temperature variations of the global heat capacity of a confinement Bose gas at different densities for the domains in Fig. 1. Colored solid curves correspond to confined (finite) systems, and dashed curves to integer-dimensional (ID) systems, ID=3, 2, and 1 for (a), (b), and (c). The black dashed and dotted lines indicate the maximum and classical values of the global heat capacity for a Maxwell-Boltzmann (MB) gas, respectively. Given that $N = g_s \tilde{n}_0 = \tilde{n}_0$ when $D_I = 0$ as $g_s = 1$ in this study, we exclude cases where $\tilde{n}_0 < 1$, considering only a few integer values of $\tilde{n}_0$ around the critical value of $\sqrt{2}$ for $D_I = 0$.

while at low temperatures ($\tilde{T} \ll 1$), they approach zero as expected. Increasing density shifts the temperature range, in which the heat capacity takes noticeable values, to the higher temperatures. In the high-temperature region ($\tilde{T} \gg 1$), the confinement in the direction of L_S weakens and the system behavior approaches the unconfined one. This is why the dashed

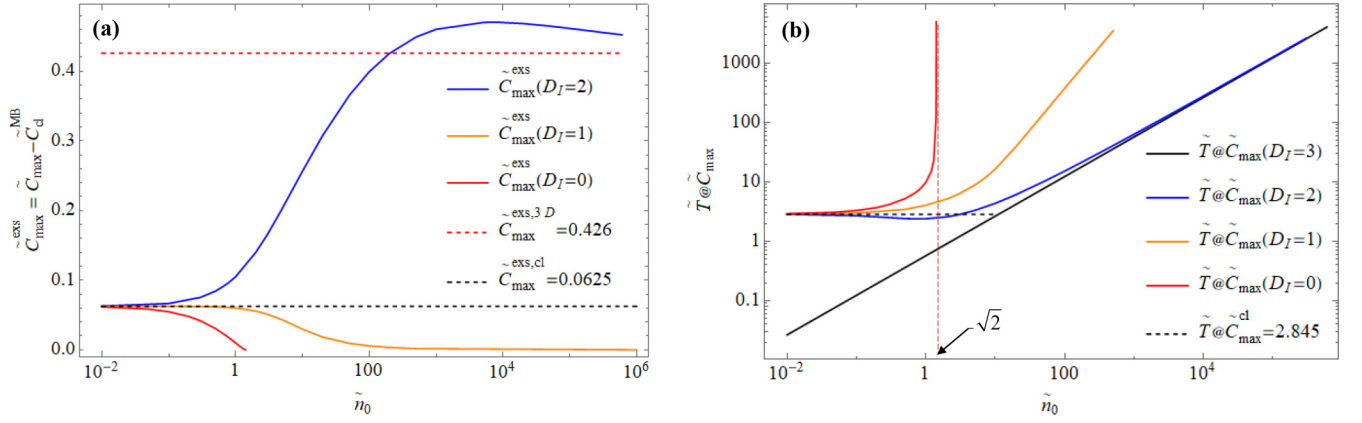


FIG. 3. (a) Variation of the maximum excess heat capacity with density for different confinement domains in Fig. 1. The red and black dashed lines represent the values for the conventional (unconfined) Bose gas and a Maxwell-Boltzmann gas confined in one direction, respectively. (b) The maximum heat-capacity temperature vs density for the domains in Fig. 1. The solid and dashed black lines represent the conventional BEC temperature and the temperature corresponding to the maximum heat capacity of a confined Maxwell-Boltzmann gas, respectively.

and solid curves become closer at higher densities while they are completely different at low densities.

At the low-density limit, e.g., ($\tilde{n}_0 = 0.01$), from high temperatures to low temperatures, the heat capacity first exhibits a maximum and takes the overcapacity value of $\tilde{C}_{\max}^{\text{MB}} = 1.562$ of an ideal Maxwell-Boltzmann gas [36–40,60], and then converges to the 2D classical limit of unity ($\tilde{C}_{\text{L}}^{\text{MB}} = 1$) forming a plateau region before it approaches zero at very low temperatures [the solid light-blue curve in Fig. 2(a)]. This is because the particles first occupy the low-lying momentum states in the L_S direction and cause an overheat capacity, and further decreasing temperature forces the particles to condensate on the ground-state momentum in the direction of L_S and forms a 2D gas. Lowering the temperature even more causes the particles to condensate on the ground-state momentum components in the direction of L_I as well, and thus the heat capacity goes to zero. At higher densities, this stepwise behavior disappears as the plateau region is getting narrower with increasing density. A comparison of the curves in Fig. 2(a) for $\tilde{n}_0 = 0.01$ and $\tilde{n}_0 = 0.1$ shows this narrowing process clearly. This is due to the stronger avalanche in the number of occupations of the momentum ground states in the directions of L_I for higher densities. In other words, the occupation of excited states becomes less likely and their contribution to the heat capacity decays more sharply at higher densities.

Another interesting behavior is that for some high-density values, the maximum heat capacity can even be slightly beyond the conventional (3D) value, 1.926. The blue curve in Fig. 3(a) illustrates the variation of the maximum excess global heat capacity, $\tilde{C}_{\max}^{\text{exs}} = \tilde{C}_{\max} - \tilde{C}_{\text{cl}}^{\text{MB}}$, with density for $D_I = 2$. $\tilde{C}_{\max}^{\text{exs}}$ reaches a peak value of 0.47 at $\tilde{n}_0 \approx 7000$ and approaches the conventional value of $1.926 - 1.5 = 0.426$ at higher densities. This exceeding of the conventional excess heat capacity aligns with findings reported in the literature [52].

Instead of the unidirectionally confined domain shown in Fig. 1(a), one may also consider a domain equally confined

along all directions, i.e., a cube, to determine the ultimate limit of the maximum global heat capacity of a finite noninteracting Bose gas. In such a cubic confinement, the particles undergo a dimensional transition directly from 3D to 0D as the temperature decreases. Evaluation of thermodynamic quantities in this case requires fully discrete triple-sum calculations, which lead to the strongest possible confinement effect on the global heat capacity. Our calculations show that the ultimate limit appears as $\tilde{C}_{\max}^{\text{cube}} \rightarrow 2.13$ for approximately $N \approx 1000$ particles at a dimensionless temperature of $\tilde{T} \approx 83$, corresponding to $T/T_c \approx 1.24$. These results are in very good agreement with those reported in the literature [52].

For the domains in Figs. 1(b) and 1(c), the heat-capacity behaviors are given in Figs. 2(b) and 2(c), respectively. A notable result is that the heat capacities of the lower-dimensional confined systems, $D_I = 1$ and $D_I = 0$, also exhibit maximum values, limited by the over heat capacity of a Maxwell-Boltzmann gas $\tilde{C}_{\max}^{\text{MB}} = 1.062$ for $D_I = 1$ and $\tilde{C}_{\max}^{\text{MB}} = 0.51$ for $D_I = 0$, respectively. In contrast, their unconfined counterparts show no maximum behavior at all, consistent with the conventional expectations in the literature.

For these lower dimensions, $D_I = 1$ and $D_I = 0$, the maximum excess heat capacity ($\tilde{C}_{\max}^{\text{exs}}$) consistently decays as density increases [Fig. 3(a) (orange and red curves)]. Note that, in the case of $D_I = 0$, the results for densities smaller than 1 ($\tilde{n}_0 < 1$) represent only the mathematical behavior of the heat-capacity function and do not correspond to a physically possible system, since $N = \tilde{n}_0$ for this specific case as $g_s = 1$ in this study. Furthermore, the maximum heat capacity disappears even when $\tilde{n}_0 > \sqrt{2}$, as shown in Figs. 3(a) and 2(c).

Therefore, for $D_I = 0$, depending on the value of g_s , the over heat capacity behavior can only be observed in an ergodic single-particle or a few-particle system as $N = g_s \tilde{n}_0$ in its general form. Figure 3(b) shows the density dependence of the temperature at the maximum heat capacity and supports this result as this temperature approaches infinity as $\tilde{n}_0 \rightarrow \sqrt{2}$ for $D_I = 0$. This unexpected finding is analytically proven

in Appendix B. In the low-density (nondegenerate) limit, all excess heat capacities approach the classical (MB) value of 0.0625, given by the studies in the literature [36–40,60].

At high temperatures ($\tilde{T} \gg 1$), the confinement in the L_S direction weakens and the maximum heat-capacity temperature for $D_I = 2$ approaches to the BEC temperature $\tilde{T}_C = \tilde{T} @ \tilde{C}_{\max}(D_I = 3)$ by taking higher values as expected [Fig. 3(b)]. This behavior agrees with the results in the literature for a cubic confinement domain [52]. On the other hand, the maximum heat-capacity temperature for $D_I = 2$ takes even slightly lower values than $\tilde{T} @ \tilde{C}_{\max}^{\text{cl}} = 2.845$ (the dashed black line) at the low-density region. The minimum value of $\tilde{T} @ \tilde{C}_{\max}(D_I = 2)$ is 2.4 and it appears when $\tilde{n}_0 = 0.8$. All the temperature curves approach to the classical value, $\tilde{T} @ \tilde{C}_{\max}^{\text{cl}} = 2.845$, when $\tilde{n}_0$ approaches zero.

III. LOCAL HEAT CAPACITY AT NANOSCALE

In our recent study [60], we derived a fundamental equation for local heat capacity in a general framework, independent of specific statistical assumptions. This equation incorporates the contributions of both conduction and quantum migration heat exchanges, and was subsequently applied to Maxwell-Boltzmann particles. The dimensionless local heat capacity, $\tilde{c} = \tilde{c}_{\text{cnd}} + \tilde{c}_{\text{qmh}}$, is the sum of contributions from local heat conduction, $\tilde{c}_{\text{cnd}} = c_{\text{cnd}}/\tilde{n}k_B$, and local heat of quantum migration $\tilde{c}_{\text{qmh}} = c_{\text{qmh}}/\tilde{n}k_B$, and they are expressed in the energy representation as

$$\tilde{c}_{\text{cnd}} = \tilde{c}_0 + \hat{\omega}\tilde{\gamma}_L, \quad (9a)$$

$$\tilde{c}_{\text{qmh}} = (\hat{\Omega} - \hat{\omega})\tilde{\gamma}_L, \quad (9b)$$

$$\tilde{c} = \tilde{c}_0 + \hat{\Omega}\tilde{\gamma}_L = \tilde{c}_0 + \tilde{c}_{\text{QC}}. \quad (9c)$$

Here, $\tilde{c}_0 = (1/\tilde{n}k_B)(\partial u/\partial T)_L = \tilde{n}(\partial \hat{u}\tilde{T}/\partial \tilde{T})_L - \hat{u}\tilde{\gamma}_L$ denotes the dimensionless apparent local heat capacity, derived from the temperature derivative of local energy u . Using the position-independent global density $\tilde{n}$, dimensionless local energy is defined by $\hat{u} = u/(\tilde{n}k_B T)$. Dimensionless local energy per particle, however, is expressed as $\hat{u} = u/(nk_B T)$ by considering the local density n , instead of $\tilde{n}$. By defining dimensionless density $\tilde{n} = n/\tilde{n}$, the relationship between these two quantities is written as $\tilde{u} = \hat{u}\tilde{n}$. Similarly, the dimensionless state functions per particle $\hat{\omega} = \omega/(nk_B T)$ and $\hat{\Omega} = \Omega/(Nk_B T)$ in Eq. (9) are defined in terms of local (φ) and global (Φ) grand potentials (Landau free energies) and the corresponding energies (u and U) through $\omega = u - \varphi$ and $\Omega = U - \Phi$. The fundamental linear relationship between pressure and grand potential holds at the local scale, $p = -\varphi$, but breaks down globally $P \neq -\Phi/V$ as highlighted in Ref. [60]. This allows us to consider ω equivalent to the local enthalpy, a positive quantity, $h = u + p = \omega$, and thus $\hat{\omega} = \hat{h}$. $\tilde{\gamma}_L = -T(\partial \tilde{n}/\partial T)_L$ is the isometric (constant size) local thermal expansion coefficient of (dimensionless) density. The term $\tilde{c}_{\text{QC}}$ accounts for the quantum correction to $\tilde{c}_0$.

The decomposition of the local heat capacity given in Eq. (9) is a direct consequence of thermodynamics applied to an open local control volume. Due to the wave nature of particles, the number of particles in a local volume is not a conserved quantity. Therefore, the conductive heat exchange through local boundaries is not simply Tds

but $\delta q_{\text{cnd}} = nTd(s/n) = Tds - T(s/n)dn$, as discussed in Ref. [60]. When particles migrate between the local and global volumes, there is a jump in entropy per particle, resulting in a quantum migration-induced local heat exchange given by $\delta q_{\text{qmh}} = T[(s/n) - (S/N)]dn$. In the energy representation, thermodynamics allows us to express these heat exchange components as $\delta q_{\text{cnd}} = du - (\omega/n)dn$ and $\delta q_{\text{qmh}} = [(\omega/n) - (\Omega/N)]dn$, which correspond directly to Eqs. (9a) and (9b), respectively.

We emphasize that additive shifts in the local and global thermodynamic potentials (e.g., due to external fields) cancel in the differences that define the heat contributions. In particular, $\hat{\Omega} - \hat{\omega}$ in Eq. (9b), $\hat{u}$ in $\tilde{c}_0$, and $\hat{\omega}$ in Eq. (9a) do not contain such additive shifts and therefore cannot flip the signs of the individual components. Thus, the total local heat exchange and total local heat capacity remain invariant and the decomposition is free from any gauge-like ambiguity.

The thermodynamic quantities in Eq. (9) are determined by considering their fundamental definitions based on infinite summations over the quantum state variable, k values. The integral and ground-state approximations are applied, respectively, for the sums over the k numbers associated with the directions of L_I and L_G , while keeping the summation operation over the k_S values. These local quantities are then expressed in terms of the local version of A functions, LA , which are defined below.

The quantum probability density of a particle within the yellow regions shown in Fig. 1 is $|\psi_{k_S}(\tilde{x})|^2 = (2/L_S)\sin^2 \pi k_S \tilde{x}$ where $\psi_{k_S}(\tilde{x})$ is the eigenfunctions obtained from the Schrödinger equation for state k_S and $\tilde{x} = x/L_S$. Using the quantum probability density in the A functions in Eq. (5), leads the local A functions defined as

$$\begin{aligned} xLA_y &= 2 \sum_{k_S=1}^{\infty} \left(\frac{k_S^2}{\tilde{T}} \right)^x \text{Li}_{(D_I/2)+y} \left[\exp \left(\Lambda_C - \frac{k_S^2}{\tilde{T}} \right) \right] \sin^2(\pi k_S \tilde{x}). \end{aligned} \quad (10)$$

Dimensionless density is first given in its general form and then determined for the yellow local regions in Fig. 1 as follows:

$$\tilde{n} = \frac{n}{\tilde{n}} = \frac{\sum_k f_k |\psi_k|^2}{\frac{1}{V} \sum_k f_k} = \frac{0LA_0}{0A_0}, \quad (11)$$

where f_k and ψ_k represent the generic forms of Bose-Einstein distribution function and eigenfunction of a translational quantum state k , respectively. Note that k is a generic symbol representing $\{k_S, k_G, k_I\}$ corresponding to the momentum components of a particle confined in the domains shown in Fig. 1. $V = L_I L_S L_G$ is the geometric volume of the confinement domain.

Similarly, dimensionless local energy $\tilde{u} = u/\tilde{n}k_B T$ is defined and given by LA functions as

$$\begin{aligned} \tilde{u} &= \frac{\sum_k \tilde{e}_k f_k |\psi_k|^2}{\frac{1}{V} \sum_k f_k} \\ &= \frac{1LA_0}{0A_0} + \frac{(2-D_I)r_G^2}{\tilde{T}} \frac{0LA_0}{0A_0} + \frac{D_I}{2} \frac{0LA_1}{0A_0}, \end{aligned} \quad (12)$$

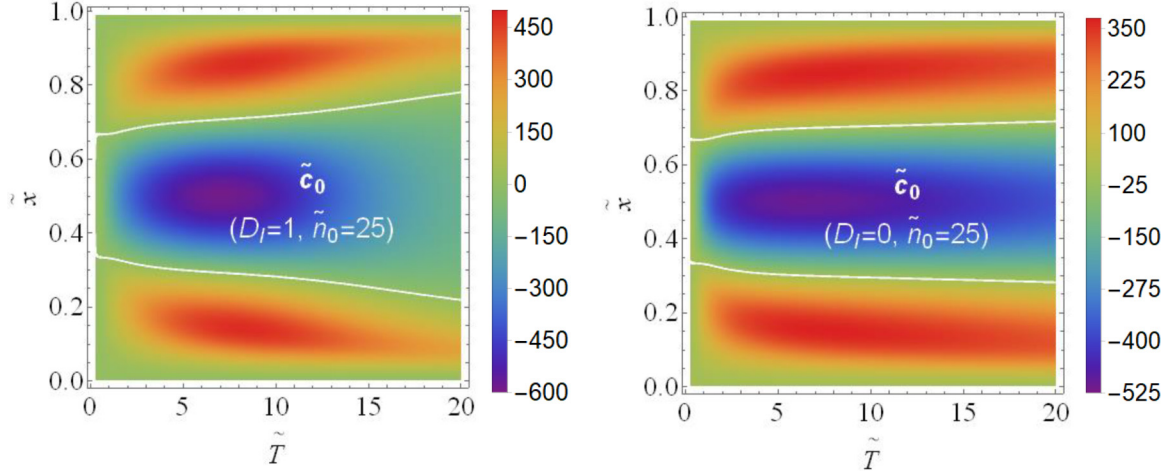


FIG. 4. Position and temperature dependence of the apparent local heat capacity for $D_I = 1$ and $D_I = 0$. The white curves denote the zero-crossing zones.

where the right-hand side terms of Eq. (12) represent the directional components of local energy, $\tilde{u} = \tilde{u}_S + \tilde{u}_G + \tilde{u}_I$, respectively.

Although the numerical temperature derivative of density is sufficient to determine $\hat{\gamma}_L$, an analytical derivative reveals the following useful expression for $\hat{\gamma}_L = \hat{\gamma}_L / \tilde{n}$, allowing a physical interpretation:

$$\begin{aligned} \hat{\gamma}_L &= -\frac{\tilde{T}}{\tilde{n}} \left(\frac{\partial \tilde{n}}{\partial \tilde{T}} \right)_L \\ &= \frac{\sum_k \sigma_k |\psi_k|^2}{\sum_k f_k |\psi_k|^2} \left[\frac{\sum_k \tilde{\epsilon}_k \sigma_k}{\sum_k \sigma_k} - \frac{\sum_k \tilde{\epsilon}_k \sigma_k |\psi_k|^2}{\sum_k \sigma_k |\psi_k|^2} \right] \\ &= \hat{\sigma}_I (\hat{U}_\sigma - \hat{u}_\sigma), \end{aligned} \quad (13)$$

where $\sigma_k = \partial f_k / \partial (\mu / k_B T) = f_k (1 + f_k)$ is the variance of the number of Bose particles in state k . The terms $\hat{\sigma}_I$, $\hat{U}_\sigma$, and $\hat{u}_\sigma$ represent the local occupancy variance per particle and the dimensionless global and local variance-weighted energy averages, respectively. For the yellow local regions in Fig. 1, $\hat{\gamma}_L$ is given in terms of LA functions as

$$\begin{aligned} \hat{\gamma}_L &= \frac{{}_0LA_{-1}}{{}_0LA_0} \left[\frac{{}_1A_{-1}}{{}_0A_{-1}} + \frac{D_I}{2} \frac{{}_0A_0}}{{}_0A_{-1}} \right] \\ &\quad - \left[\frac{{}_1LA_{-1}}{{}_0LA_0} + \frac{D_I}{2} \right]. \end{aligned} \quad (14)$$

In the Maxwell-Boltzmann limit (high-temperature or low-density conditions), where the degeneracy is negligible ($f_k \ll 1$ and $\sigma_k \rightarrow f_k$), Eq. (13) simplifies as $\hat{\sigma}_I \rightarrow 1$, $\hat{U}_\sigma \rightarrow \hat{U}$ and $\hat{u}_\sigma \rightarrow \hat{u}$ and $\hat{\gamma} \rightarrow \hat{U} - \hat{u}$. This represents the deviation of the global energy per particle from its local value, as given in [60]. Note that this interpretation of $\hat{\gamma}_L$ is not valid in its general form since Eqs. (13) and (14) involve multiplication of different types of averages: the products of local and global averages, the terms with and without the $|\psi_k|^2$ term, respectively. In the opposite limit (low-temperature or high-density conditions), where the degeneracy completely dominates the system, particles occupy only the ground state, summation operations drop in Eq. (13), and we obtain $\hat{\gamma} \rightarrow 0$.

Dimensionless local ($\hat{\phi}$) and global ($\hat{\Phi}$) grand potentials are also defined and calculated, respectively, as

$$\hat{\phi} = \frac{\varphi}{nk_B T} = -\frac{\sum_k \ln(1 + f_k) |\psi_k|^2}{\sum_k f_k |\psi_k|^2} = -\frac{{}_0LA_1}{{}_0LA_0} \leq 0, \quad (15a)$$

$$\hat{\Phi} = \frac{\Phi}{Nk_B T} = -\frac{\sum_k \ln(1 + f_k)}{\sum_k f_k} = -\frac{{}_0A_1}{{}_0A_0} \leq 0. \quad (15b)$$

In the nondegenerate (MB) limit ($\tilde{n}_0 \rightarrow 0$ or $\tilde{T} \rightarrow \infty$), ($\hat{\phi} \rightarrow -1$, $\hat{\Phi} \rightarrow -1$), whereas in the completely degenerate limit ($\tilde{n}_0 \rightarrow \infty$ or $\tilde{T} \rightarrow 0$), $\hat{\phi} \rightarrow \hat{\Phi} \rightarrow 0$. Observe that, in the MB limit, $(\hat{\Omega} - \hat{\omega}) \rightarrow (\hat{U} - \hat{u})$ and $\hat{\gamma}_L \rightarrow (\hat{U} - \hat{u})$, yielding $\tilde{c}_{\text{qmh}} \rightarrow (\hat{U} - \hat{u})^2 \tilde{n} \geq 0$. Conversely, in the fully degenerate limit, $\tilde{c}_{\text{qmh}} \rightarrow 0$, since $\hat{U} \rightarrow \hat{u}$, $\hat{\phi} \rightarrow \hat{\Phi}$, and $\hat{U}_\sigma \rightarrow \hat{u}_\sigma$, leading to $\hat{\gamma}_L \rightarrow 0$.

Figure 4 illustrates the position and temperature variations of $\tilde{c}_0$ for two distinct cases: $D_I = 1$ and $D_I = 0$. These calculations are performed for the dimensionless density of $\tilde{n}_0 = 25$ to ensure significant quantum degeneracy effects. The white curves indicate regions where the heat capacity crosses zero. Notably, the behavior of the *apparent local heat capacity* is entirely unphysical, exhibiting both strongly negative and positive values as a result of the substantial confinement energy, $(2 - D_I)r_G^2/\tilde{T}$, carried by the migrated particles. The magnitude of these values depends on the strength of r_G , and it is set to $r_G = 100$ during the calculations of Fig. 4 to prevent infinitely large positive and negative values. Note that the ground-state approximation remains safe even for $r_G = 100$ as long as $\tilde{T} \ll r_G^2 = 10^4$.

Thermodynamic stability requires the non-negativity of the local heat capacity. Otherwise, even a small local energy fluctuation that transfers energy from a positive heat-capacity region to a negative one, for example, would destroy the temperature homogeneity within the system. This could lead to a catastrophic collapse of the equilibrium condition as the temperature decreases towards absolute zero in both regions, or increases towards infinity in the case of the opposite energy transfer. Consequently, negative and positive local

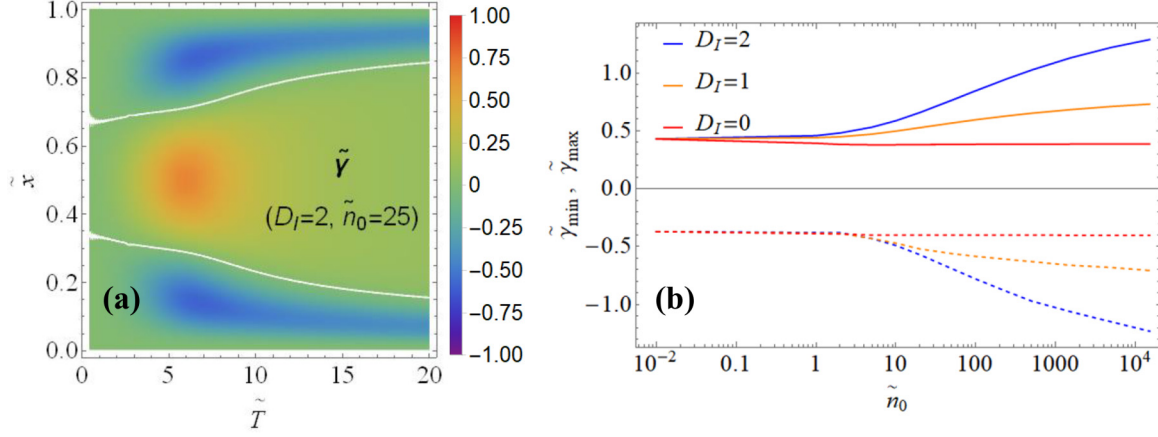


FIG. 5. (a) The thermal expansion coefficient as a function of position and temperature for $D_I = 2$ and $\tilde{n} = 25$. Zero-crossing zones are marked by the white curve. (b) Maximum and minimum $\tilde{\gamma}_L$ values vs density for various confinement domains shown in Fig. 1.

heat-capacity regions cannot coexist in the same system. As a result, the negative local heat capacities observed in the central regions of the domain, Fig. 4, are nonphysical results, as we discussed for Maxwell-Boltzmann gas in our recent study [60].

Negative predictions clearly indicate that $\tilde{c}_0$ cannot represent the correct local heat capacity but rather an apparent one requiring the correction given by Eq. (9c). The misprediction of $\tilde{c}_0$ arises from two misapproaches: (i) incorrect consideration of local energy transferred by quantum migration as if it results from local boundary heat exchange and (ii) neglecting the cooling and heating effects of quantum migration.

By considering $\tilde{c}_0 = \tilde{n}(\partial \hat{u} \tilde{T} / \partial \tilde{T})_L - \hat{u} \tilde{\gamma}_L$ together with $\hat{u}_G = (2 - D_I) r_G^2 / \tilde{T}$, as implied by Eqs. (11) and the second term on the right-hand side of Eq. (12), the component of $\tilde{c}_0$ in the strongly confined direction can be written as $\tilde{c}_{G,0} = -\tilde{\gamma}_L (2 - D_I) r_G^2 / \tilde{T}$. Note that although $\tilde{c}_{G,0}$ is zero for $D_I = 2$, it dominates $\tilde{c}_0$ for $D_I = 1$ and $D_I = 0$, taking large negative values proportional to r_G^2 in the central region where $\tilde{\gamma}_L > 0$. This anomalous prediction originates from the fact that $\tilde{c}_0$ misinterprets energy changes due to particle migration as boundary heat exchange. Therefore, not only $\tilde{c}_{G,0}$ but even $\tilde{c}_0$ itself acquires nonphysical negative values for $D_I = 1$ and $D_I = 0$. Section IV A further discusses why the apparent heat capacity is negative in the central region and positive near the boundaries of any finite domain. These results demonstrate that the quantum migration process and its corresponding correction to the local heat capacity, as defined in Eqs. (9), must be considered. Therefore, analyzing the predictions of these equations for a finite Bose gas provides detailed insights into the effect of quantum degeneracy on quantum migration and its importance for local heat capacity of a confined Bose gas.

Given the significant role of $\tilde{\gamma}_L$ in Eqs. (9), understanding its behavior is essential for comprehending the quantum migration process. Figure 5(a) illustrates the variation of $\tilde{\gamma}_L$ with position and temperature for $D_I = 2$, $\tilde{n} = 25$, whereas (b) provides detailed information about the variation of its maximum and minimum values with density for different D_I values. The white curve in (a) represents the zero values, separating regions of positive (expansion) and negative

(contraction) $\tilde{\gamma}_L$. The maximum value consistently appears at the center, while the minimum emerges near the boundaries. This general behavior of $\tilde{\gamma}_L$ aligns with recent findings for Maxwell-Boltzmann gas in the literature [60]. As exposed in Fig. 5(b), the extremum values exhibit an increase with increasing density for $D_I = 2$ and $D_I = 1$ while maintaining a constant level for $D_I = 0$. This indicates that quantum degeneracy in a Bose gas enhances the quantum migration process except for $D_I = 0$. Additionally, a further analysis shows that the temperatures at which these extrema occur shift to higher values with increasing densities.

Figure 6 demonstrates the predictions for the local heat capacity for $\tilde{n}_0 = 25$ with quantum migration correction, Eq. (9c), along with its conductive and migration parts, Eqs. (9a) and (9b), for the confinement configurations shown in Fig. 1, corresponding to different D_I values. Despite that the quantum migration component takes practically zero negative values ($\approx -10^{-3}$) in a narrow (white colored) region across all configurations, the conductive component exhibits negative values ($\approx -10^{-2}$) only for $D_I = 0$ and near boundary regions. Conversely, the total local heat capacity consistently remains non-negative, $\tilde{c}_{\text{tot}} \geq 0$ [see Figs. 6(c), 6(f), and 6(i)], thus satisfying the thermodynamic stability criterion. It is essential to recognize that the negativity of the conductive and quantum migration components does not induce instability, as stability is governed by the (total) local heat capacity. Furthermore, since $\tilde{\gamma}_L$ appears in both Eqs. (9a) and (9b), these components respond simultaneously to the migration process. Therefore, this corrected framework of the (total) local heat-capacity formulation successfully addresses the negativity problem previously encountered with $\tilde{c}_0$ shown in Fig. 4, guaranteeing its positivity and thus the stability of thermodynamic equilibrium. Figure 6 also reveals that the maximum conductive contribution is consistently observed at the domain's center, whereas the maximum quantum migration contribution emerges near the boundaries.

Negative values of $\tilde{c}_{\text{cnd}}$ are observed exclusively in systems strongly confined in two directions, ($D_I = 0$), as illustrated in Fig. 6(g). Upon the addition of heat energy to a finite system, the temperature rises, leading to the expansion of the higher-density gas in the central region. This expansion,

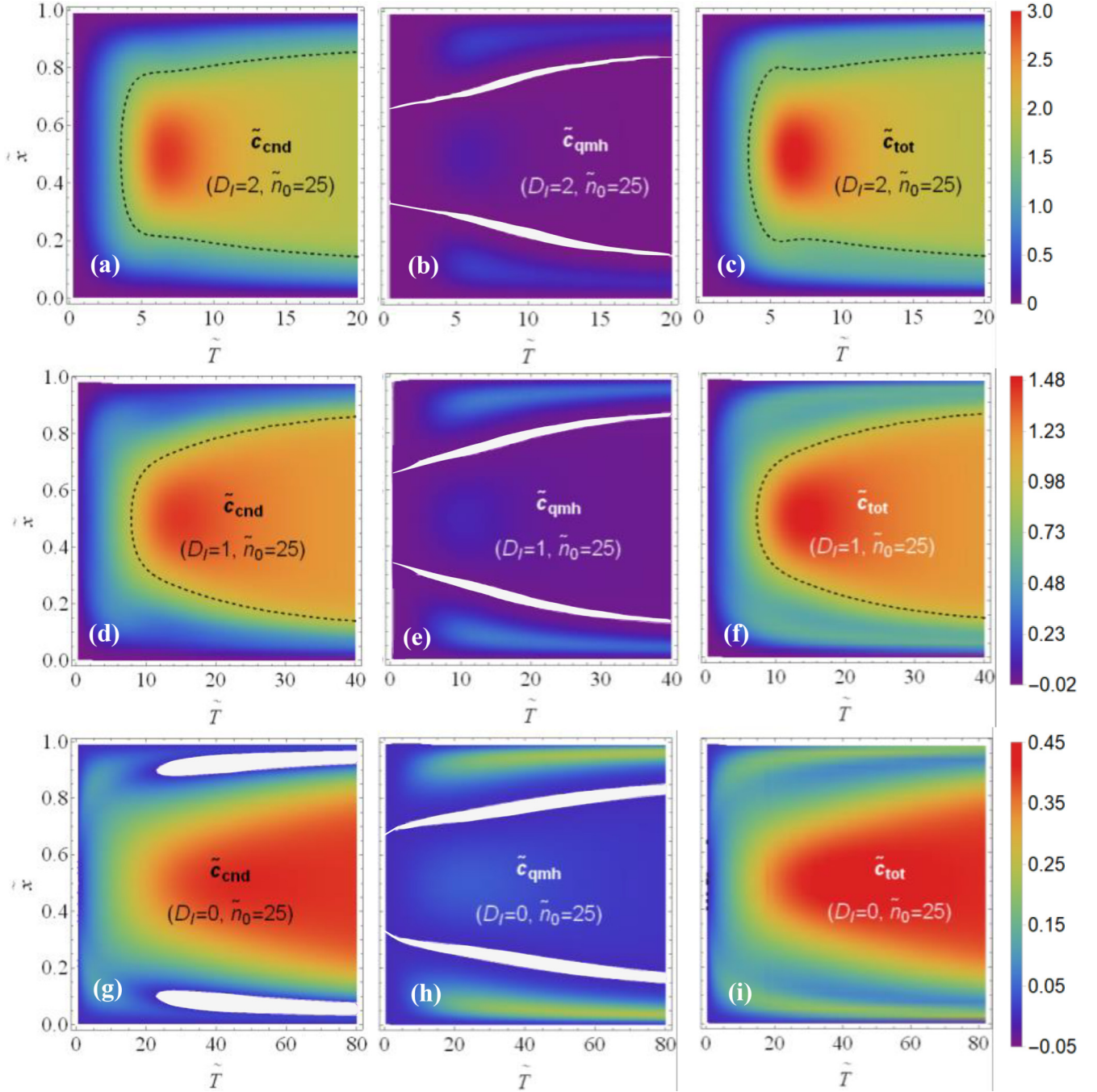


FIG. 6. Position and temperature dependencies of local heat-capacity contributions for $\tilde{n} = 25$. Panels (a), (d), and (g) display the conductive contribution ($\tilde{c}_{\text{cnd}}$), while (b), (e), and (h) show the quantum migration contribution ($\tilde{c}_{\text{qmh}}$). The total local heat capacity ($\tilde{c}_{\text{tot}}$) is presented in (c), (f), and (i). Each row corresponds to a different confinement domain, as illustrated in Fig. 1. White regions highlight zones of negative values, and dashed black curves indicate classical heat-capacity values, calculated as $(1 + D_I)/2$.

in turn, compresses the lower-density gas near boundaries. The expansion in the central region facilitates further heat absorption, whereas the compression near the boundaries results in a local temperature increase. In a system with $D_I = 0$, strong confinement in two directions lowers the heat capacity significantly. Consequently, local compression near the boundaries supplies even more energy than required to equalize the local temperature with the system's overall temperature. Therefore, to maintain thermal equilibrium, heat energy must be released from these local boundary regions.

This explains the observation of $\tilde{c}_{\text{cnd}} < 0$ near the boundaries when $D_I = 0$. Considering $\tilde{c}_0 = \tilde{u} - \tilde{\gamma}\hat{u} + \tilde{n}\tilde{T}(\partial\hat{u}/\partial\tilde{T})_L$ and $\hat{\omega} = \hat{u} + \hat{p}$ in Eq. (9a), it is possible to express $\tilde{c}_{\text{cnd}} = \tilde{u} + \tilde{n}\tilde{T}(\partial\hat{u}/\partial\tilde{T})_L + \hat{p}\tilde{\gamma}_L$. While the first two terms are inherently positive, the last term ($\hat{p}\tilde{\gamma}_L$) can be either positive or negative, depending on the sign of $\tilde{\gamma}_L$. However, for the configurations of $D_I = 1$ and $D_I = 2$, the sum of the first two terms consistently outweighs the magnitude of the last term and consequently, $\tilde{c}_{\text{cnd}}$ is positive for these configurations [Figs. 6(a) and 6(d)].

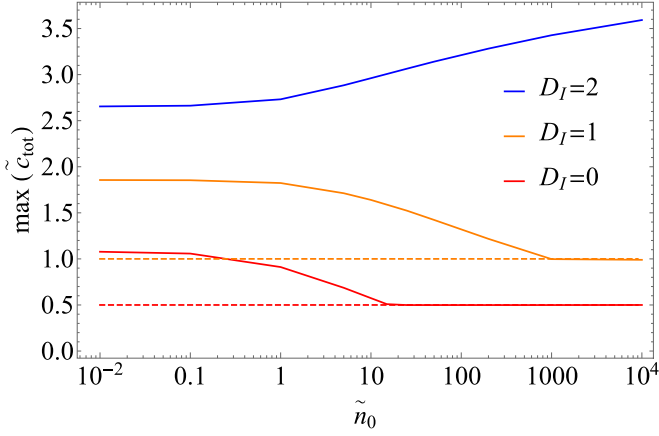


FIG. 7. Variation of maximum local heat capacity with density for different confinement domains in Fig. 1.

In contrast, negative values of $\tilde{c}_{\text{qmh}}$ are observed not only for $D_I = 0$ but also across all D_I configurations, as shown in Figs. 6(b), 6(e), and 6(h). The negative sign regions of $\tilde{c}_{\text{qmh}}$ arise from the differing spatial locations where $\tilde{\gamma}_L$, and $(\hat{\Omega} - \hat{\omega})$ in Eq. (9b) change sign. Both $\tilde{\gamma}_L$ and $(\hat{\Omega} - \hat{\omega})$ are positive in the central region and negative near the boundaries. Consequently, their product, $\tilde{c}_{\text{qmh}}$, is positive in these areas. However, between the central and boundary regions, $\tilde{\gamma}_L$ and $(\hat{\Omega} - \hat{\omega})$ change signs at slightly different spatial locations. This mismatch in zero-crossing points leads to tiny negative values of $\tilde{c}_{\text{qmh}}$ within a narrow intermediate region. As discussed following Eq. (15b), in the high-temperature or low-density limit (nondegeneracy limit), $\hat{\Omega} - \hat{\omega} \rightarrow \hat{\gamma}$ making $\tilde{c}_{\text{qmh}}$ a positive-definite quantity and eliminating negative values. Conversely, the low-temperature or high-density limit, where both $\hat{\Omega} - \hat{\omega}$ and $\tilde{\gamma}_L$ approach zero, also leads to the vanishing of the negative regions' width. These behaviors are clearly evident in Figs. 6(b), 6(e), and 6(h).

The results also show that the conductive component ($\tilde{c}_{\text{cnd}}$) is dominant in the central regions, while the quantum migration component ($\tilde{c}_{\text{qmh}}$) prevails near the boundaries.

A massive (total) local heat capacity appears at the center of the domain and its variation with density is given in Fig. 7 for different D_I values. Unlike the trend observed for $\tilde{\gamma}_L$ in Fig. 5(b), the central $\tilde{c}_{\text{tot}}$ increases with density only for $D_I = 2$, surpassing twice the classical value of 1.5. For $D_I = 1$ and

$D_I = 0$, however, the central $\tilde{c}_{\text{tot}}$ decreases as density rises. The peak values of $\tilde{c}_{\text{tot}}$ for $D_I = 1$ and $D_I = 0$ are found in the low-density (nondegenerate) limit, approaching double the classical values of 1 and 1/2, respectively.

The global heat capacity ($\tilde{C}_{\text{tot}}$), as well as its conductive ($\tilde{C}_{\text{cnd}}$) and migration ($\tilde{C}_{\text{qmh}}$) contributions, are obtained by integrating their local counterparts over the domain. Figure 8 illustrates the temperature dependence of these global quantities for the domains shown in Fig. 1, revealing that quantum migration enhances the global heat capacity for $D_I = 2$. In the case of $D_I = 1$, quantum migration is the only reason for the overheat capacity as the conductive component approaches its classical value from below. However, when $D_I = 0$, the migration contribution is insufficient to induce a global overheat capacity. Given that a large number of particles ($N \gg 1$) necessitates $\tilde{n} \gg 1$ for $D_I = 0$, global overheat capacity never appears in such a system. Only in the case of a single-particle ergodic system does migration lead to an overheat capacity for $D_I = 0$ as discussed in the explanations of Fig. 3.

Figure 9 shows the results of further analyses, illustrating the maximum contributions of conduction ($\tilde{C}_{\text{cnd}}^{\text{max}}$) and quantum migration ($\tilde{C}_{\text{qmh}}^{\text{max}}$) to the global heat capacity as a function of density for the domain configurations shown in Fig. 1. For $D_I = 2$, the maximum conductive contribution to the global heat capacity increases with density. In contrast, for $D_I = 1$ and $D_I = 0$, $\tilde{C}_{\text{cnd}}^{\text{max}}$ remains constant at the classical value, independent of density. The maximum quantum migration contribution, $\tilde{C}_{\text{qmh}}^{\text{max}}$, exhibits a peak at $\tilde{n} \approx 1000$ for $D_I = 2$ and at $\tilde{n} \approx 100$ for $D_I = 1$, but continuously diminishes with density for $D_I = 0$. Notably, $\tilde{C}_{\text{cnd}}$ reaches its maximum at a finite temperature for $D_I = 2$ as evident in Fig. 8(a). For $D_I = 1$, Fig. 8(b), the $\tilde{C}_{\text{cnd}}$ curve approaches the classical limit asymptotically as its maximum value. For $D_I = 0$ [Fig. 8(c)], the $\tilde{C}_{\text{cnd}}$ curve also exhibits an asymptotic trend towards its classical value as a maximum value, but this behavior is less pronounced within the considered temperature range, suggesting saturation occurs at significantly higher temperatures. Briefly, $\tilde{C}_{\text{cnd}}^{\text{max}}$ appears at a finite temperature for $D_I = 2$, but is only asymptotically approached at infinite temperature for $D_I = 1$ and for $D_I = 0$, tending towards the classical heat capacity.

Conversely, $\tilde{C}_{\text{qmh}}^{\text{max}}$ is always achieved at a finite temperature [Figs. 8(a)–8(c)]. Consequently, for $D_I = 1$ and $D_I = 0$, $\tilde{C}_{\text{qmh}}^{\text{max}}$ is the only source of global excess heat capacity since

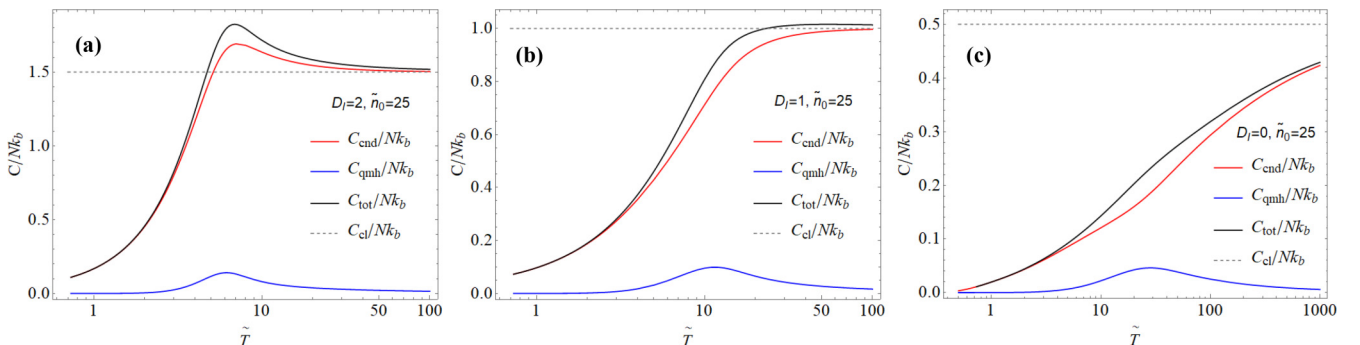


FIG. 8. Temperature dependencies of global heat capacity and contributions from conductive and migration processes for $\tilde{n} = 25$ and (a) $D_I = 2$, (b) $D_I = 1$, and (c) $D_I = 0$. The black dotted lines indicate the classical values.

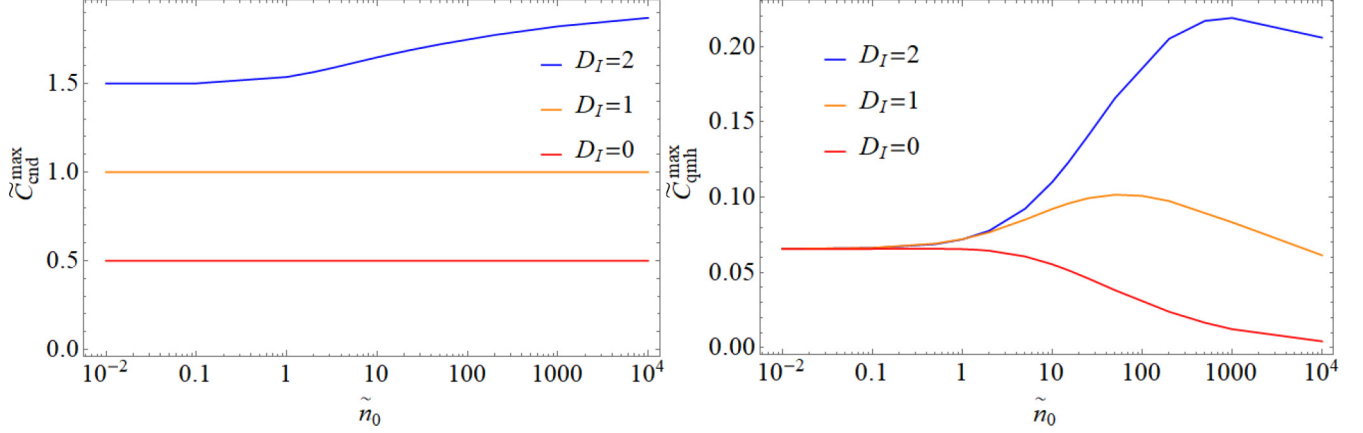


FIG. 9. Density dependencies of the (a) conductive and (b) migration contributions to the global heat capacity for different confinement conditions.

$\tilde{C}_{\text{cnd}}^{\text{max}} \leq \tilde{C}_{\text{cl}}^{\text{MB}}$. However, for $D_I = 2$, both $\tilde{C}_{\text{cnd}}^{\text{max}}$ and $\tilde{C}_{\text{qmh}}^{\text{max}}$ contribute to this excess capacity. It is important to note that these maximum contributions occur at different temperatures. Specifically, for $D_I = 0$, the global heat capacity does not exhibit an excess value if $\tilde{n} > \sqrt{2}$ because $\tilde{C}_{\text{cnd}}^{\text{max}}$ only approaches $1/2$ asymptotically as $\tilde{T} \rightarrow \infty$, although $\tilde{C}_{\text{qmh}}^{\text{max}} > 0$ appears at a finite temperature. Nevertheless, when $D_I = 0$ and $\tilde{n} = 1$, $\tilde{C}_{\text{cnd}}$ reaches values close to $1/2$ at a finite temperature where also $\tilde{C}_{\text{qmh}}$ approaches its maximum. As a result, the global heat capacity does exhibit an overcapacity for $D_I = 0$ if $\tilde{n} = 1$. On the other hand, as previously mentioned, this condition is meaningful only if we consider a single-particle ergodic system, where the ensemble averages equal to the time averages.

It is insightful to analyze the similarity between $\tilde{C}_{\text{qmh}}$ and the thermal part of confinement energy, $\hat{u}_c^{\text{th}}$, defined by

$$\hat{u}_c^{\text{th}} = \hat{u} - \frac{1}{\tilde{T}} - \hat{u}_{\text{uc}}. \quad (16)$$

Here, $\hat{u}_{\text{uc}}$ is the per-particle local energy in the absence of confinement along L_S and is determined by using the integral approach for the summations in Eqs. (11) and (12) as

$$\hat{u}_{\text{uc}} = \frac{1 + D_I}{2} \frac{\text{Li}_{(3+D_I)/2}}{\text{Li}_{(1+D_I)/2}} + \frac{2 - D_I}{\tilde{T}} r_g^2. \quad (17)$$

Notice that when the integral approach is used we replace LA functions with their classical counterparts, ${}_x\text{LA}_y \rightarrow (1/V)_x B_y$. The definition of $\hat{u}_c^{\text{th}}$ isolates the excess thermal energy resulting solely from the confinement by subtracting the per-particle ground-state energy component along L_S (which is $1/\tilde{T}$) and $\hat{u}_{\text{uc}}$ from the total energy $\hat{u}$. Figure 10 illustrates the distribution of this confinement-induced excess thermal energy, normalized by the total local energy per particle excluding the ground-state energy in the L_G direction ($\hat{u} - \hat{u}_G$) for different configurations shown in Fig. 1. Note that $(\hat{u} - \hat{u}_G)$ represents the total local energy per particle, including the confinement energy along L_S but excluding that along L_G , which is irrelevant here.

Thermal confinement energy is the primary driver of the unusual behavior observed in the thermal state functions of confined systems. Generally, thermal components of state functions approach zero as temperature tends to absolute zero. In contrast, nonthermal parts retain finite values even at zero

temperature, such as zero-point energy ($N\epsilon_0$) and zero-point pressure. Figure 10 illustrates that thermal confinement energy accumulates near the system boundaries due to quantum migration. This quantum migration acts as an energy-filtering transport process, carrying higher-energy particles from the central regions to the boundaries as temperature increases. The lower the dimension D_I , the more pronounced this accumulation of thermal confinement energy becomes. Similar behavior is evident in Figs. 6(b), 6(e), and 6(h). These similarities suggest that confinement-induced thermal energy builds up through the quantum migration process. In essence, quantum migration disrupts the homogeneity of local energy within the system as temperature rises, leading to the observed accumulation of thermal confinement energy.

IV. DISCUSSION

A. Negativity of the apparent local heat capacity versus positivity of the corrected one

The apparent local heat capacity at constant size is defined as the temperature derivative of the local energy under fixed domain sizes L ,

$$c_0 = \left(\frac{\partial u}{\partial T} \right)_L = n \left[\frac{\partial(u/n)}{\partial T} \right]_L + \left(\frac{u}{n} \right) \left(\frac{\partial n}{\partial T} \right)_L, \quad (18)$$

which, in dimensionless form per particle, becomes

$$\hat{c}_0 = \frac{1}{nk_B} \left(\frac{\partial u}{\partial T} \right)_L = \left[\frac{\partial(\tilde{T}\hat{u})}{\partial \tilde{T}} \right]_L - \hat{u}\hat{\gamma}_L. \quad (19)$$

The first term on the right-hand side of (19) represents the temperature derivative of the local energy per particle. Since the energy per particle increases monotonically with temperature, this contribution is strictly positive.

The second term involves the product of the energy per particle and the local thermal expansion coefficient (the negative sign of the temperature derivative of density). In confined systems, particles with longer de Broglie wavelengths preferentially accumulate in the central region, where the quantum probability density is maximized. As the temperature increases, particles are excited into higher-energy states with shorter wavelengths. These shorter wavelengths allow

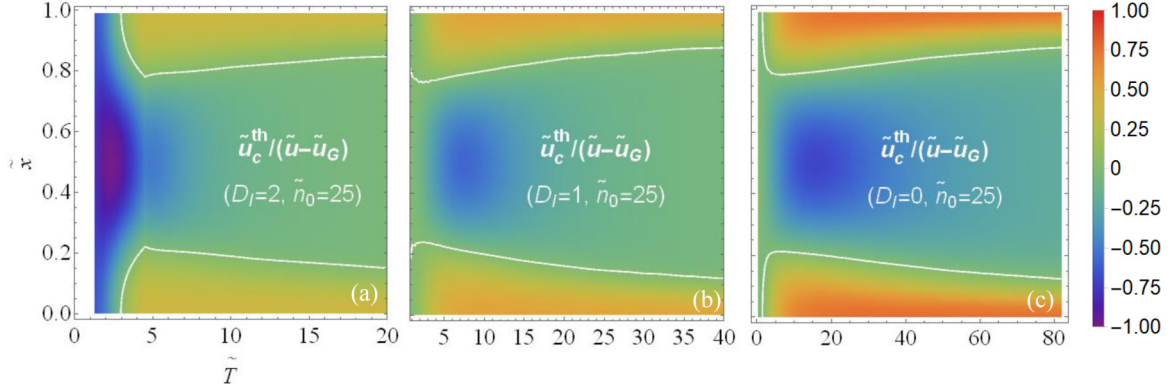


FIG. 10. For $\tilde{n} = 25$, position and temperature dependencies of the percentage of the thermal part of confinement energy defined by Eq. (16) for the different confinement domains shown in Fig. 1. The white curves indicate the zero-crossing points.

particles to access regions closer to the boundaries, thereby reducing the central density and increasing the boundary density. Consequently, the temperature derivative of the local density is negative in the central region and positive near the boundaries.

In systems strongly confined in at least one spatial direction, the energy per particle can grow arbitrarily large depending on the confinement strength. As a result, the second terms in (19) may become significantly negative in the central region, leading to a negative apparent local heat capacity. However, when local net particle migration occurs, the heat capacity cannot be defined solely as the temperature derivative of the local energy. Instead, corrections due to migration must be included. Incorporating the quantum migration correction yields

$$c = c_0 - \left(\frac{U - \Phi}{N} \right) \left(\frac{\partial n}{\partial T} \right)_L. \quad (20)$$

Substituting Eq. (18) into Eq. (20) gives

$$c = n \left(\frac{\partial(u/n)}{\partial T} \right)_L + \left(\frac{u}{n} - \frac{U}{N} \right) \left(\frac{\partial n}{\partial T} \right)_L + \left(\frac{\Phi}{N} \right) \left(\frac{\partial n}{\partial T} \right)_L. \quad (21)$$

In dimensionless form per particle,

$$\hat{c} = \frac{c}{nk_B} = \left[\frac{\partial(\tilde{T}\tilde{u})}{\partial \tilde{T}} \right]_L + (\hat{U} - \hat{u})\hat{\gamma}_L - \hat{\Phi}\hat{\gamma}_L, \quad (22)$$

which, using the last equality in Eq. (13), may be rewritten as

$$\hat{c} = \left[\frac{\partial(\tilde{T}\tilde{u})}{\partial \tilde{T}} \right]_L + (\hat{U} - \hat{u})\hat{\sigma}_l(\hat{U}_\sigma - \hat{u}_\sigma) - \hat{\Phi}\hat{\sigma}_l(\hat{U}_\sigma - \hat{u}_\sigma). \quad (23)$$

The first term on the right-hand side of Eq. (23) is always positive as mentioned before. The second term reflects the extra heat required due to internal energy variations, $\hat{U} \neq \hat{u}$, that arise during particle migration, $\hat{\gamma}_L \neq 0$. This contribution is always positive because when $\hat{U} \geq \hat{u}$ also $\hat{U}_\sigma \geq \hat{u}_\sigma$, which means $\hat{\gamma}_L \geq 0$ in the central region, while $\hat{U} \leq \hat{u}$ also $\hat{U}_\sigma \leq \hat{u}_\sigma$, meaning $\hat{\gamma}_L \leq 0$ near the boundaries. This

follows from the de Broglie wavelength dependence: high-energy particles, with shorter wavelengths, are more likely to approach the boundaries, while low-energy particles, with longer wavelengths, are preferentially located near the center. Consequently, the energy per particle at the domain center is always lower than the global average, and vice versa near the edges.

The last term represents the flow-work contribution to local heat exchange. Note that in the thermodynamic limit (macroscopic systems), $-\Phi$ reduces to the pressure, whereas in finite systems it deviates from pressure, as discussed after Eq. (9). According to the definition of $\hat{\Phi}$ in Eq. (15b), it is always negative, and thus the sign of this last term is determined by $\hat{\gamma}_L = \hat{\sigma}_l(\hat{U}_\sigma - \hat{u}_\sigma)$ as $\hat{\sigma}_l$ is a positive-definite quantity. A positive value of the third term indicates that more heat is required to drive particles outward from the local volume due to local expansion ($\hat{\gamma}_L > 0$). Specifically, $-\hat{\Phi}\hat{\gamma}_L$ reaches its largest positive values in the central region, where $\hat{\gamma}_L$ attains its maximum for any finite domain, while $\hat{\Phi}$ remains constant as a global quantity. The Positivity of the third term thereby ensures the positivity of the total local heat capacity at the central region—even when the apparent local heat capacity is negative. This conclusion is not restricted to rectangular domains but applies to arbitrary confinement geometries.

Near the boundaries, however, where $\hat{U}_\sigma < \hat{u}_\sigma$, the third term becomes negative, implying that less heat is needed to raise the temperature since local compression work partially offsets the thermal requirement. Nevertheless, we have shown numerically that this negative contribution near the boundaries is never large enough to change the sign of the sum of these three terms and $\hat{c} \geq 0$ holds for the considered rectangular domains. On the other hand, a rigorous analytical proof of $\hat{c} \geq 0$ for arbitrary confinement domains, including near the boundaries, remains an open challenge.

Nevertheless, since quantum migration is unavoidable in nanoconfined systems, and since the laws of thermodynamics are valid at the nanoscale, one may conjecture that the quantum-corrected local heat capacity in Eq. (9c) [or equivalently Eq. (23)] is a positive-definite quantity in any confinement domain for noninteracting systems, as required by thermodynamic stability.

B. Effects of boundary conditions

For particles confined in a rectangular box with Dirichlet boundary conditions (DBC), the ground state has finite energy with a probability density peaked at the center and vanishing at the boundaries. Under Neumann boundary conditions (NBC), however, the ground-state energy vanishes and the corresponding probability density becomes uniform. Excited states then exhibit maximum probability density at the boundaries, opposite to the DBC case. This inversion of boundary versus central probability density also reverses the density distribution: the central density is minimized ($\tilde{n} < 1$) while the boundary density is maximized ($\tilde{n} = 2$). With increasing temperature, density increases in the central region while it decreases near the boundaries, although the boundary density itself remains pinned at its maximum ($\tilde{n} = 2$). Consequently, the sign of $\hat{\gamma}_L$ reserves $\hat{\gamma}_L < 0$ at the central region and $\hat{\gamma}_L \gg 0$ near the edges. Thus, particles migrate inward rather than outward, the opposite trend compared to the DBC case.

The same reversal behavior appears for profile, which now exhibits a maximum at the center and a local minimum close to the edges before turning upward again. Reversing the profile of $\hat{\gamma}_L$ inverts the behavior of $\tilde{c}$ and $\tilde{c}_{\text{cnd}}$ while $\tilde{c}_{\text{qmh}}$ maintains its form but with reduced amplitude relative to DBC. As a result, the giant local heat-capacity enhancement appears at the boundaries instead of the center. Furthermore, because the ground-state energy is zero, its contributions to local and global state functions vanish for the case of NBC. Therefore, the negative values of the apparent heat capacity $\tilde{c}_0$ due to migrated confinement energy disappear, while $\tilde{c}_0$ still fails to predict correct values as it neglects the corrections of quantum migration. For the global heat capacity, the peak appears at a lower temperature and with a reduced maximum for the NBC case, reflecting the fact that the ground-state energy is zero. It is important to note that, for proper comparison, the dimensionless temperature in the NBC case should be defined relative to the energy of the first excited state rather than the (vanishing) ground-state energy.

In the case of soft-wall boundary conditions, confinement weakens for high-energy states that penetrate the finite barrier, reducing central density enhancement and flattening near-boundary profiles. The degree of suppression depends directly on barrier height, with softer walls producing smaller quantum-migration effects.

For nonrectangular geometries, the key parameter is the effective confinement length along the surface normal. As long as boundary curvature exceeds the thermal de Broglie wavelength λ_{th} , results remain essentially unchanged; significant shape effects appear only when local domain sizes fall below λ_{th} , allowing boundary layers to overlap.

Finally, for periodic boundary conditions (PBC), the situation is qualitatively different. The wave functions satisfying periodicity across the domain lead to discrete momentum eigenstates but with uniform probability density. In this case, translational symmetry is preserved, no central-boundary asymmetry arises, and quantum migration effects are expected to disappear. Local thermodynamic quantities remain homogeneous, while global properties are modified from those of the bulk system due to finite-size momentum quantization. Thus, PBC represent a special limit that removes

boundary-induced effects while retaining discreteness in the spectrum due to finite system size.

C. Effects of interactions

In the presence of interparticle interactions, both global and local heat capacities are influenced by the additional potential energy. Moreover, interactions modify the quantum probability density distribution, since the positions of the nodes shift. These shifts induce new patterns in the density profile, which in turn affect quantum migration processes and related quantities.

Attractive interactions typically enhance the central density and increase the strength of $\hat{\gamma}_L$. This occurs because the symmetric attractions among particles in the central region tend to cancel out, whereas asymmetry near the boundaries leads to a net attraction toward the center. Repulsive interactions produce the opposite effect. The detailed effects of interactions, however, depend on multiple factors: particle statistics, interaction strength, interparticle spacing (density), system dimensionality, boundary conditions, temperature, and the strength of confinement. Together, these factors form a rich spectrum of problems for future investigation. Particle-wall interactions add another layer of complexity, requiring further analyses.

Nevertheless, the main conclusions of this study remain valid when the interparticle interaction energy per particle is smaller than the confinement energy, in the regime of weak interactions or strong confinement. Noticeable deviations may arise in the opposite limit (weak confinement or strong interactions). In summary, while interactions enrich the phenomenology, they do not alter the central conclusions of this work provided that either the ground-state energy or the thermal energy exceeds the characteristic interaction energy.

D. Model validity in the nondegenerate limit

In nanoscale systems, the discreteness of energy levels becomes significant, particle densities can be high, and the total number of particles may be relatively small. In such cases, calculations over discrete levels require replacing continuum-based integrals with exact summations or with accurate approximations such as the Poisson summation, and the Euler-Maclaurin or Abel-Plana formulas.

At high particle densities, quantum statistics (Bose-Einstein or Fermi-Dirac) become necessary when the average interparticle distance is comparable to or smaller than λ_{th} . In systems with only a small number of particles, strong fluctuations may occur, sometimes even exceeding the ensemble averages. In general, however, fluctuations scale as $\sim 1/\sqrt{N}$, and are negligible even in nanoscale systems provided that $N \gg 1$.

For nanoscale systems, the condition $N \gg 1$ can be satisfied either by maintaining sufficiently high particle density or by ensuring that at least one of the system sizes is much larger than λ_{th} . Thus, even in confined systems, Maxwell-Boltzmann (MB) statistics remain valid if λ_{th} is much shorter than the average interparticle spacing in at least one spatial direction. This condition ensures that the average ground-state occupation remains much less than one—the key prerequisite

for MB statistics. For the domains shown in Figs. 1(a)–1(c), the condition for MB statistics is $\lambda_{\text{th}} \ll \sqrt{L_I^{D_I} L_S/N}$, which is fulfilled even at low temperatures, as long as L_I (for $D_I \neq 0$) or L_S (for $D_I = 0$) is sufficiently large to guarantee $N \gg 1$.

V. CONCLUSION

Building upon the understanding of TIQM in finite Maxwell-Boltzmann gases, this study extends the framework to Bose gases to understand and analyze the influence of quantum degeneracy, particularly on local heat capacity. Our analysis reveals that TIQM is enhanced by quantum degeneracy in a Bose gas, leading to a giant local heat capacity. Furthermore, the existence of a maximum global heat capacity in a finite 2D Bose gas is explained by the contribution of quantum migration, and TIQM emerges as a key mechanism for excess global heat capacity in finite 3D systems. The thermal confinement energy, responsible for many unusual features of confined systems, is also explained by the TIQM process for a Bose gas.

For further extension, the effect of TIQM on the local heat capacity of a finite Fermi gas can be considered. In such systems, Friedel oscillations induced by confinement are expected to drive oscillations in TIQM contributions. Therefore, oscillations in both density and TIQM (related with the thermal expansion coefficient of density, $\tilde{\gamma}_L$) may interfere with each other and can induce some unusual behavior especially in local heat capacity. TIQM may also provide a mechanism for oscillations observed in the global heat capacity of finite Fermi gases. The influence of TIQM on local heat capacity in interacting Bose and Fermi gases constitutes another natural and important extension for future studies.

The predicted giant local heat capacity in a finite Bose gas offers a promising route for the experimental observation and verification of TIQM. Recently developed optical box traps [54,58] can create the confinement geometry of a “particle in a box,” enabling the trapping of Bose gases within these potentials. These traps can confine up to 3500 atoms. Furthermore, the integration of single-atom detection in these new traps allows for direct measurements of quantum atom statistics.

As an energy-filtering particle transport process, TIQM is generally expected to influence not only local heat capacity but also other local properties, including, e.g., the local distribution of magnetic and superconducting orders in materials. Therefore, this study further underscores the crucial role of TIQM in understanding the temperature-dependent local quantities of quantum confined systems.

DATA AVAILABILITY

The data that support the findings of this article are openly available [62], embargo periods may apply.

APPENDIX A: GENERALIZED DERIVATION OF GLOBAL HEAT CAPACITY OF A BOSE GAS CONFINED IN THE DOMAINS ILLUSTRATED IN Fig. 1

Based on the dimensionless energy per particle, $\tilde{\epsilon}_i = \epsilon_i/k_B T = (\alpha_i k_i)^2$, and the defined confinement parameter relations $\alpha_S^2 = 1/\tilde{T}$, $\alpha_I = \alpha_S/r_I$, and $\alpha_G = \alpha_S r_G$, the following

equation can be written to find the chemical potential Λ :

$$N = \sum_{k_S=1}^{\infty} \int_0^{\infty} \frac{dk_{I1} \dots dk_{ID_I}}{\exp \left[-\Lambda + \frac{k_S^2}{\tilde{T}} + \frac{(2-D_I)r_G^2}{\tilde{T}} + \frac{(k_{I1}^2 + \dots + k_{ID_I}^2)}{r_I^2 \tilde{T}} \right] - 1}. \quad (\text{A1})$$

Notice that integral and ground-state approaches are used to calculate the contributions of summations over k_{Ii} and k_{Gi} , respectively. The total dimension $D = 3$ and there is only one α_S , while the numbers of α_I and α_G are D_I and $2 - D_I$. By considering the change of variable $u_i = k_{Ii}/(r_I \sqrt{\tilde{T}})$ and transforming the cartesian coordinates to spherical ones for $dk_{I1} \dots dk_{ID_I}$, as $dk_{I1} \dots dk_{ID_I} = [2\pi^{D_I/2} s^{D_I-1} ds]/(2^{D_I} \Gamma(D_I/2))$, Eq. (A1) is rewritten as

$$N = \left(\frac{r_I \sqrt{\tilde{T}}}{2} \right)^{D_I} \frac{2\pi^{D_I/2}}{\Gamma(D_I/2)} \sum_{k_S=1}^{\infty} \int_0^{\infty} \frac{s^{D_I-1} ds}{\exp \left[-\Lambda + \frac{k_S^2}{\tilde{T}} + \frac{(2-D_I)r_G^2}{\tilde{T}} + s^2 \right] - 1}. \quad (\text{A2})$$

Calculating the integral in Eq. (A2), calling the equality $N = (\sqrt{\pi} r_I/2)^{D_I} \tilde{n}_0$ and using the modified dimensionless chemical potential $\Lambda_C = \Lambda - (2 - D_I)r_G^2/\tilde{T}$, the following normalization equation is obtained for chemical potential, which is the one given in Eq. (1):

$$\tilde{n}_0 = \tilde{T}^{D_I/2} \sum_{k_S=1}^{\infty} \text{Li}_{D_I/2} \left(\exp \left[\Lambda_C - \frac{k_S^2}{\tilde{T}} \right] \right). \quad (\text{A3})$$

Using the same variables, the total energy is expressed as

$$U = k_B T \sum_{k_S=1}^{\infty} \int_0^{\infty} \frac{\left[\frac{k_S^2}{\tilde{T}} + \frac{(2-D_I)r_G^2}{\tilde{T}} + \frac{(k_{I1}^2 + \dots + k_{ID_I}^2)}{r_I^2 \tilde{T}} \right] dk_{I1} \dots dk_{ID_I}}{\exp \left[-\Lambda + \frac{k_S^2}{\tilde{T}} + \frac{(2-D_I)r_G^2}{\tilde{T}} + \frac{(k_{I1}^2 + \dots + k_{ID_I}^2)}{r_I^2 \tilde{T}} \right] - 1}. \quad (\text{A4})$$

By following the same change of variables and transformation of integral over cartesian coordinates into a spherical one, Eq. (A4) becomes

$$U = k_B T \left(\frac{\sqrt{\pi} r_I}{2} \right)^{D_I} \tilde{T}^{D_I/2} \left[\sum_{k_S=1}^{\infty} \frac{k_S^2}{\tilde{T}} \text{Li}_{D_I/2} \left[\exp \left(\Lambda_C - \frac{k_S^2}{\tilde{T}} \right) \right] + (2 - D_I) \frac{r_G^2}{\tilde{T}} \sum_{k_S=1}^{\infty} \text{Li}_{D_I/2} \left[\exp \left(\Lambda_C - \frac{k_S^2}{\tilde{T}} \right) \right] + \frac{D_I}{2} \sum_{k_S=1}^{\infty} \text{Li}_{(2+D_I)/2} \left[\exp \left(\Lambda_C - \frac{k_S^2}{\tilde{T}} \right) \right] \right]. \quad (\text{A5})$$

Each term, from the first to last, represents a contribution from confined (S), strongly confined (G), and unconfined (I) directions, respectively. Considering $N = (\sqrt{\pi} r_I/2)^{D_I} \tilde{n}_0$ and Eq. (A3), the dimensionless energy per particle can be expressed

in terms of A functions defined in Eq. (5) by

$$\hat{U} = \frac{U}{Nk_B T} = \frac{{}_1A_0}{{}_0A_0} + \frac{(2 - D_I)r_G^2}{\tilde{T}} + \frac{D_I}{2} \frac{{}_0A_1}{{}_0A_0}. \quad (\text{A6})$$

In terms of $\hat{U}(\tilde{T}, \Lambda_C)$, the dimensionless global heat capacity per particle is expressed as

$$\begin{aligned} \hat{C}_L = \frac{C_L}{Nk_B} &= \left(\frac{\partial \hat{U}}{\partial \tilde{T}} \right)_L = \hat{U} + \tilde{T} \left(\frac{\partial \hat{U}}{\partial \tilde{T}} \right)_{L, \Lambda_C} \\ &+ \tilde{T} \left(\frac{\partial \hat{U}}{\partial \Lambda_C} \right)_{L, \tilde{T}} \left(\frac{\partial \Lambda_C}{\partial \tilde{T}} \right)_L. \end{aligned} \quad (\text{A7})$$

Due to $N = (\sqrt{\pi} r_I / 2)^{D_I} \tilde{n}_0$, the constant number of particles N requires

$$\left(\frac{d\tilde{n}_0}{d\tilde{T}} \right)_L = \left(\frac{\partial \tilde{n}_0}{\partial \tilde{T}} \right)_{L, \Lambda_C} + \left(\frac{\partial \tilde{n}_0}{\partial \Lambda_C} \right)_{L, \tilde{T}} \left(\frac{\partial \Lambda_C}{\partial \tilde{T}} \right)_L = 0, \quad (\text{A8})$$

which gives the following equation in terms of A functions:

$$\left(\frac{\partial \Lambda_C}{\partial \tilde{T}} \right)_L = - \frac{\left(\frac{\partial \tilde{n}_0}{\partial \tilde{T}} \right)_{L, \Lambda_C}}{\left(\frac{\partial \tilde{n}_0}{\partial \Lambda_C} \right)_{L, \tilde{T}}} = - \frac{1}{\tilde{T}} \left[\frac{D_I}{2} \frac{{}_0A_0}{{}_0A_{-1}} + \frac{{}_1A_{-1}}{{}_0A_{-1}} \right]. \quad (\text{A9})$$

For the temperature and chemical potential derivatives of Eq. (A3) in Eq. (A9), the subsequent derivative equalities of A functions are used:

$$\frac{\partial({}_xA_y)}{\partial \tilde{T}} = \frac{1}{\tilde{T}} ({}_{x+1}A_{y-1} - {}_xA_y), \quad (\text{A10})$$

$$\frac{\partial({}_xA_y)}{\partial \Lambda_C} = {}_xA_{y-1}. \quad (\text{A11})$$

The employment of Eqs. (A6), (A9), (A10) and (A11) in Eq. (A7) leads to the global heat capacity given by Eq. (4).

APPENDIX B: DERIVATION OF THE CONDITION FOR EXCESS GLOBAL HEAT CAPACITY FOR $D_I = 0$

When $D_I = 0$, the general global heat-capacity equation, Eq. (4), simplifies to

$$\tilde{C} = \frac{C_L}{Nk_B} = \frac{{}_2A_{-1}}{{}_0A_0} - \frac{{}_1A_{-1}^2}{{}_0A_0 {}_0A_{-1}}. \quad (\text{B1})$$

The exact numerical results in Fig. 3(b) show that the temperature of maximum heat capacity approaches infinity when $\tilde{n}_0 \rightarrow \sqrt{2}$.

In the high-temperature regime ($\tilde{T} \gg 1$), the first two terms of the Poisson summation formula (PSF) (or equivalently, the Euler-Maclaurin formula) provide a very accurate approximation for the summation in the A functions, accounting for the finite-size effects due to confinement. These two terms consist of the integral of the function over the interval $[0, \infty)$ and the subtraction of half of the integrand evaluated at $k_S = 0$. Therefore, the A functions can be approximated using the PSF as ${}_xB_y^{\text{PSF}}$ given by

$$\begin{aligned} {}_xB_y^{\text{PSF}} &= \left(\frac{\sqrt{\tilde{T}}}{2} \right) \Gamma \left(x + \frac{1}{2} \right) \text{Li}_{[(D_I+1)/2]+x+y}[\exp(\Lambda_C)] \\ &- \frac{1}{2} \theta(x) \theta(-x) \text{Li}_{(D_I/2)+y}[\exp(\Lambda_C)], \end{aligned} \quad (\text{B2})$$

where $\theta(x)$ is the right-continuous Heaviside step function, defined as $\theta(x) = 1$ for $x \geq 0$ and $\theta(x) = 0$ for $x < 0$. By considering $z = \exp[\Lambda_C] \rightarrow 0$ in the high-temperature regime, the Polylogarithm functions can also be approximated as $\text{Li}_m(z) \approx z + z^2/2^m + O(z^3)$. Thus, in the high-temperature limit, the simplified form of the ${}_xB_y^{\text{PSF}}$ functions becomes

$$\begin{aligned} {}_xB_y^{\text{PSF}} &\rightarrow \left(\frac{\sqrt{\tilde{T}}}{2} \right) \Gamma \left(x + \frac{1}{2} \right) [z + z^2/2^{[(D_I+1)/2]+x+y}] \\ &- \frac{1}{2} \theta(x) \theta(-x) [z + z^2/2^{[(D_I/2)+y]}]. \end{aligned} \quad (\text{B3})$$

Using Eq. (B3) as an approximation for A functions in Eq. (B1), and applying Taylor expansion for $\tilde{T} \rightarrow \infty$, we obtain the following global heat capacity for $D_I = 0$ at the high-temperature regime:

$$\tilde{C} \approx \frac{1}{2} + \frac{2 - \sqrt{2}\tilde{n}_0}{8\sqrt{\pi}\tilde{T}}. \quad (\text{B4})$$

From Eq. (B4) it is evident that excess heat capacity ($\tilde{C} > 1/2$) is possible only when $\tilde{n}_0 > \sqrt{2}$. Also, its temperature derivative is zero when $\tilde{n}_0 = \sqrt{2}$. Consequently, unlike unbounded (infinite) systems, the global heat capacity of a finite 1D system ($D_I = 0$) exhibits a small maximum, which can be observed only when $\tilde{n}_0 = 1$. Since $N = g_s \tilde{n}_0$ for $D_I = 0$, this implies that, depending on the value of g_s , the system must be a single-particle or few-particle ergodic system to observe this small maximum in such a finite system.

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