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One-dimensional magnetized Tonks–Girardeau gas properties in an external magnetic field

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Abstract
With Girardeau's Fermi–Bose mapping, we have constructed the eigenstates of the Tonks–Girardeau (TG) gas in an external magnetic field. When the number of bosons N is commensurate with the number of potential cycles M, the probability of this TG gas in the ground state is bigger than the TG gas raised by Girardeau in 1960. Through the comparison of properties between this TG gas and Fermi gas, we find that the following issues are always the same: their average value of particle coordinates and potential energies, system total momenta, single-particle densities and pair distribution functions. But the reduced single-particle density matrices and their momentum distributions between them are different.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The problem of a one-dimensional (1D) hard-core gas was first studied classically by Tonks [1]. Girardeau [2, 3] continued the research in quantum by putting forward the Fermi–Bose mapping to solve the energy spectrum and the corresponding wavefunctions of a one-dimensional Tonks–Girardeau (TG) gas. After that, Lieb and Liniger [4] considered N Bose particles interacting via a repulsive δ-function potential with a coupling constant γ. In fact, the TG gas can be considered as the Lieb–Liniger gas when $\gamma \to \infty$.

Over the past decades, the study on the TG gas has undergone a rapid development in theory and experiment [5–17]. In particular, Lenard [5] indicated that the off-diagonal parts of the one-body density matrix and the momentum distribution show significant differences in both TG gas and Fermi gas. Lapeyre *et al* [8] studied the momentum distribution of a harmonically trapped gas. The most important progress was the realization of the strongly interacting bosons [16] in a one-dimensional optical-lattice trap and the TG gas [17] by trapping ^{87}Rb atoms with a combination of two light traps.

We have known some properties of the one-dimensional TG gas, and we are interested in its properties and features in an external magnetic field. We first reveal some properties of both gases in the same external magnetic field and compare them. With the Fermi–Bose mapping [2, 3], we obtain all the eigenenergies and eigenstates of this TG gas. When the number of bosons N is commensurate with the number of potential cycles M, the TG system in an external magnetic field will be in the ground state with a bigger probability than the TG gas raised by Girardeau in 1960. Many properties of the TG gas and the Fermi gas are always the same even if they are time dependent, such as their average values of particle coordinates and potential energies, system total momenta, single-particle densities and pair distribution functions, but their reduced single-particle matrices and momentum distributions are different.

2. The TG gas in an external magnetic field

In a TG gas, the boson is assumed to have an 'impenetrable' hard core characterized by a radius of a. From Girardeau's work, with the hard core radius $a \to 0$, the interparticle interaction is given by

$$U(x_i, x_j) = \begin{cases} 0, & x_i \neq x_j, \\ \infty, & x_i = x_j. \end{cases} \tag{1}$$

Such an interparticle interaction could be represented by the following subsidiary condition on the wavefunction ψ:

$$\psi(x_1, \ldots, x_N, t) = 0 \qquad \text{if} \quad x_i = x_j, \qquad 1 \leqslant i < j \leqslant N. \tag{2}$$

In order to let the TG gas wavefunction, which must be symmetric with respect to the permutations of any x_i and x_j, satisfy this condition (2), we need the ideas of Fermi–Bose mapping proposed by Girardeau [2, 3]. Using the fact that the antisymmetric Fermi wavefunction, denoted by ψ^F, satisfies condition (2) naturally, a bosonic wavefunction ψ^B of a TG gas can be constructed by

$$\psi^B(x_1, \ldots, x_N, t) = A(x_1, \ldots, x_N)\psi^F(x_1, \ldots, x_N, t) \tag{3}$$

in which

$$A(x_1, \ldots, x_N) \equiv \prod_{i>j}^{N} \operatorname{sgn}(x_i - x_j), \tag{4}$$

and

$$\operatorname{sgn}(x) \equiv \frac{x}{|x|} = \begin{cases} 1, & x > 0, \\ -1, & x < 0. \end{cases}$$

As the wavefunction of the ground state of the Bose system is non-negative [19], mapping (3) for the stationary ground state of a system reduces to a simplified form [2]

$$\psi^B(x_1, \ldots, x_N) = |\psi^F(x_1, \ldots, x_N)|. \tag{5}$$

To illustrate our general ideas, we now study the case that magnetized bosons in an external magnetic field $B(x) = -B\cos(2\omega x)$. For simplicity, we take $B(x)$ as independent of t. Therefore,

$$\hat{H} = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + V(x_i) \right]. \tag{6}$$

in which

$$V(x) = \begin{cases} \mu B\cos(2\omega x), & 0 \leqslant x_i \leqslant \dfrac{L}{\omega}, \\ 0, & \text{else}. \end{cases} \tag{7}$$

We suppose $L = M\pi$, where M is an integer and μ is the magnetic moment of the atom. For the sake of simplicity, we assume that both N and M are odd. (As a result of the introduction of $A(x_1, \ldots, x_N)$, ψ^B is periodic if N is odd and antiperiodic if N is even [2, 12].) From Bloch theory, the corresponding energy spectrum of the system in periodic potentials has an energy band structure. We use the notation n as the band index and k as the Bloch wavevector in the first Brillouin zone. For convenience, we use $\alpha = \{n, k\}$ to denote both the band index and the Bloch wavevector. Without considering the interparticle interaction, every particle in $x \in [0, L/\omega]$ is governed by

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \mu B\cos(2\omega x)\right]\varphi_\alpha(x) = E_\alpha\varphi_\alpha(x). \tag{8}$$

Substitute $z = \omega x$, $q = \frac{m\mu B}{\hbar^2\omega^2}$ and $\lambda = \frac{2mE}{\hbar^2\omega^2}$ into equation (8); then this equation becomes

$$\frac{\mathrm{d}^2\varphi(z)}{\mathrm{d}z^2} + [\lambda - 2q\cos(2z)]\varphi(z) = 0, \qquad z \in [0, L]. \tag{9}$$

It is called Mathieu's differential equation, which can be solved with Shirts's [18] method. Using Bloch's theorem, we first set

$$\varphi(z) = \exp(\mathrm{i}\nu z)u(z), \tag{10}$$

$$\varphi(z) = \varphi(z + \pi), \tag{11}$$

$$u(z) = u(z + L), \tag{12}$$

$$\nu = \frac{2l}{M}, \qquad \left(l \in 0, \pm 1, \ldots, \pm\frac{M-1}{2}\right). \tag{13}$$

Since $u(z)$ is periodic with period π, it can be expanded in the Fourier series:

$$\varphi(z) = \exp(\mathrm{i}\nu z)\sum_n c_n \exp(\mathrm{i}2nz). \tag{14}$$

Then substituting (14) into (9), we obtain an infinite symmetric tridiagonal matrix equation, that is, eigenequation.

$$\begin{pmatrix} \ddots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & (\nu-4)^2 & q & 0 & 0 & 0 & \cdots \\ \cdots & q & (\nu-2)^2 & q & 0 & 0 & \cdots \\ \cdots & 0 & q & \nu^2 & q & 0 & \cdots \\ \cdots & 0 & 0 & q & (\nu+2)^2 & q & \cdots \\ \cdots & 0 & 0 & 0 & q & (\nu+4)^2 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ c_{-2} \\ c_{-1} \\ c_0 \\ c_1 \\ c_2 \\ \vdots \end{pmatrix} = \lambda \begin{pmatrix} \vdots \\ c_{-2} \\ c_{-1} \\ c_0 \\ c_1 \\ c_2 \\ \vdots \end{pmatrix}. \tag{15}$$

By truncating the matrix in each direction (centered at the smallest diagonal element ν^2) at sufficiently large dimensions, approximations to the desired eigenvalues can be obtained to any desired precision. We could obtain the eigenvalues and eigenfunctions easily using Mathematica or Matlab. In practice, the eigenvalue and eigenfunction converge quickly as

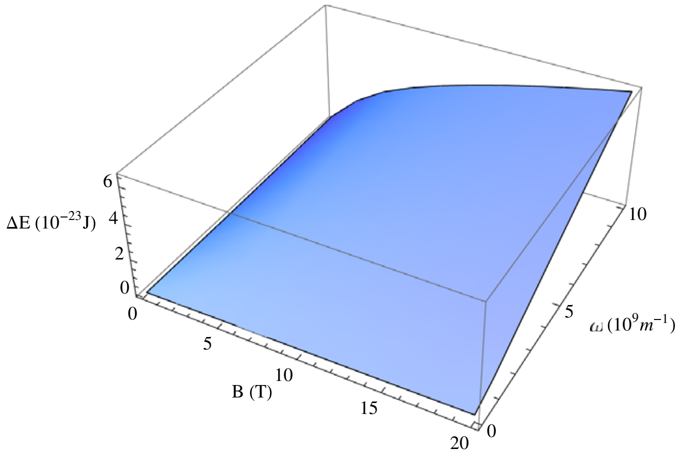

Figure 1. Plots of the energy gap between the first and the second Bloch bands as a function of magnetic induction B and frequency ω. $M = 9$, $m = 1.44 \times 10^{-25}$ kg, $\mu = 9.274 \times 10^{-24}$ JT^{-1}.

the dimension increases when q is not too large. For example, if we choose $\nu = 6/7$ and $q = 1$, the relative difference of the lowest eigenvalue between truncating the matrix at 21-D and 2001-D is only 10^{-38}. For large values of q and high orders, we can use asymptotic expansions instead [20, 21], since the matrix dimension that needs to get accurate eigenvalues and eigenfunctions becomes very large.

With Girardeau's Fermi–Bose mapping (3), the eigenstates of the hard-core Bose system are given by the Slater determinant:

$$\psi^B(x_1, \ldots, x_N) = \frac{A(x_1, \ldots, x_N)}{\sqrt{N!}} \begin{vmatrix} \varphi_{\alpha_1}(x_1) & \varphi_{\alpha_2}(x_1) & \cdots & \varphi_{\alpha_N}(x_1) \\ \varphi_{\alpha_1}(x_2) & \varphi_{\alpha_2}(x_2) & \cdots & \varphi_{\alpha_N}(x_2) \\ \vdots & \vdots & \vdots & \vdots \\ \varphi_{\alpha_1}(x_N) & \varphi_{\alpha_2}(x_N) & \cdots & \varphi_{\alpha_N}(x_N) \end{vmatrix}. \tag{16}$$

The total energy of the system is

$$E = \sum_{i=1}^{N} E_{\alpha_i}. \tag{17}$$

As a result of the Bose–Fermi mapping, the energy spectrums of the Bose and the corresponding Fermi system are identical. When the temperature is 0, the system will be on the ground state—N particles on the N lowest eigenstates, respectively.

Calculations show that the energy gap $\triangle E$ between the first and the second Bloch bands decreases with the decrease of M, and $\triangle E$ is independent of M when M is large. The energy gap as a function of the magnetic field B and the frequency ω are plotted in figure 1. When $B = 0$, raised by Girardeau [2], the energy gap of the TG gas is the smallest (not 0). The energy gap increases as B and ω increase. As the Boltzman distribution law states, $\frac{n_k}{n_{k'}} \propto \exp\left(-\frac{\triangle E}{kT}\right)$, where $\triangle E = E_k - E_{k'}$, n_k and $n_{k'}$ are particle numbers on the corresponding states. So the system has a bigger probability in the ground state with large B and ω than that of the case $B = 0$ when the total number $N = M$. That is to say that one could realize the ground-state TG system more simpler with large q and ω than $q = 0$ when the total number $N = M$.

3. Properties of the TG gas compared with the fermi gas

In this section, we further study the properties of the 1D N magnetized hard-core bosons in the external magnetic field (7), and then compare them with the properties of 1D N magnetized fermions in the 'same' state which hard-core bosons occupy.

3.1. Reduced single-particle density matrix and single-particle density

The reduced single-particle density matrix with normalization $\int \rho(x,x)\,\mathrm{d}x = N$ is given by

$$\rho^B(x,x',t) \equiv N\int \psi^{B*}(x,x_2,\ldots,x_N,t)\psi^B(x',x_2,\ldots,x_N,t)\,\mathrm{d}x_2\ldots\mathrm{d}x_N. \tag{18}$$

For the Fermi gas, the reduced single-particle density matrix can be simplified to

$$\begin{aligned}\rho^F(x,x',t) &= N\int \psi^{F*}(x,x_2,\ldots,x_N,t)\psi^F(x',x_2,\ldots,x_N,t)\,\mathrm{d}x_2\ldots\mathrm{d}x_N\\ &= \sum_{\substack{\alpha=\text{all states}\\ \text{occupied}}} \varphi_\alpha(x,t)^*\varphi_\alpha(x',t).\end{aligned} \tag{19}$$

Both the reduced single-particle matrices of hard-core bosons and fermions in the ground state in the external magnetized field (7) are plotted separately in figure 2. The multidimensional integral in equation (18) is evaluated numerically by Monte Carlo integration using Mathematica. Because the relationship between x and z is proportional, for the sake of simplicity, we take z as a variable. From the figure we can see that the off-diagonal elements of the matrices of both two kinds of gases decay quickly as N increases; the bright diagonal stripe of the TG gas is thinner than that of the Fermi gas under the same condition. This reflects the condensate properties of the Bose gas, and the shock of the off-diagonal elements $\rho(z, M\pi - z)$ of the TG gas is smaller than that of the Fermi gas. To see this more clearly, we have plotted the off-diagonal elements $\rho(z, M\pi - z)$ in figure 3. A sudden rise in the border is the result of using periodic boundary conditions.

Using mapping (3), we can prove that the single-particle densities $\rho(x,t)$, normalized to N, of both hard-core bosons and fermions are equal, no matter whether they are on the ground state or not.

$$\begin{aligned}\rho^B(x,t) &= N\int |\psi^B(x,x_2,\ldots,x_N,t)|^2\,\mathrm{d}x_2\ldots\mathrm{d}x_N\\ &= N\int |\psi^F(x,x_2,\ldots,x_N,t)|^2\,\mathrm{d}x_2\ldots\mathrm{d}x_N\\ &= \sum_{\substack{\alpha=\text{all states}\\ \text{occupied}}} |\varphi_\alpha(x,t)|^2\\ &= \rho^F(x,t).\end{aligned} \tag{20}$$

$\rho(x,t)$ is just the element of the reduced single-particle matrix $\rho(x,x',t)$ when $x = x'$. Figure 2 shows that $\rho(x)$ is cyclic, which indicates that the particles tend to stay cyclic when their potential energy is low.

3.2. Pair distribution function

The pair distribution function, which is the probability of finding a second particle as a function of distance from an initial particle, normalized to $N(N-1)$, is defined as

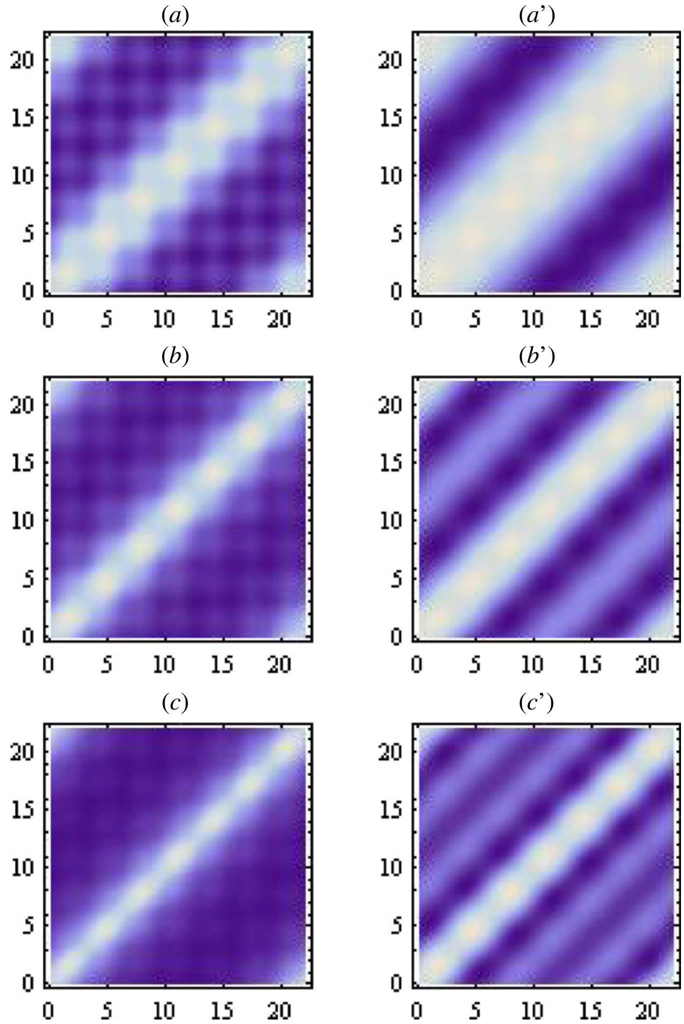

Figure 2. Density plots of $\rho(z, z')$ of the hard-core TG gas (a, b, c) and the Fermi gas (a', b', c'), $M = 7$. The abscissa is z_1, and the ordinate is z_2. (a, a') $N = 3$; (b, b') $N = 5$; (c, c') $N = 7$.

$$\begin{aligned} D(x_1, x_2, t) &= N(N-1)\int |\psi^B(x_1, x_2, \ldots, x_N, t)|^2\, \mathrm{d}x_3 \cdots \mathrm{d}x_N \\ &= N(N-1)\int |\psi^F(x_1, x_2, \ldots, x_N, t)|^2\, \mathrm{d}x_3 \cdots \mathrm{d}x_N \\ &= \frac{1}{2}\sum_{\substack{\alpha, \alpha' = \text{all states} \\ \text{occupied}}} |\varphi_\alpha(x_1, t)\varphi_{\alpha'}(x_2, t) - \varphi_\alpha(x_2, t)\varphi_{\alpha'}(x_1, t)|^2. \end{aligned} \tag{21}$$

From the above equation we can see that the pair distribution functions of both hard-core boson gas and Fermi gas are identical. In fact, the averages of particle coordinates and potential energies of both the gases are identical too, as they involve absolute values of the wavefunctions only. We can also say that this feature is determined by the fact that the single-particle densities

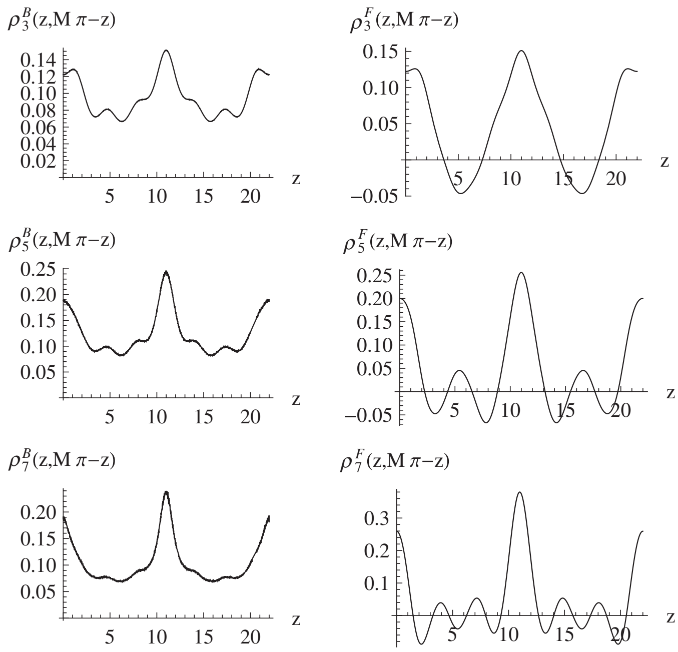

Figure 3. Plots of $\rho(z, M\pi - z)$, $M = 7$. $\rho_n^B(z, M\pi - z)$ stands for $\rho(z, M\pi - z)$ of n hard-core boson particles, and so $\rho_n^F(z, M\pi - z)$.

of both hard-core boson gas and Fermi gas are exactly the same. For the ground state of a system with N particles governed by Hamilton (6), the pair distribution function is

$$D(x_1, x_2) = \frac{1}{2} \sum_{\alpha,\alpha'=0}^{N-1} |\varphi_\alpha(x_1)\varphi_{\alpha'}(x_2) - \varphi_\alpha(x_2)\varphi_{\alpha'}(x_1)|^2. \tag{22}$$

Figure 4 shows the density plots of the pair distribution function of the ground state for a different number of particles. When $x_1 = x_2$, $D(x_1, x_2) = 0$. It is the result of the impenetrable hard-core interparticle interaction. Just like the single-particle density, the pair distribution function reflects the same periodicity and the particles tend to tarry at the low potential energy. As the number of particles increases, the black strip becomes thinner. One of the reason is that the average distance between particles reduces as the number of particles increases while the scope of the potential field is certain. In two distant regions, away from the diagonal in figure 4, $D(z_1, z_2)$ is cyclic. This reflects that the hard-core interaction between particles is local.

3.3. Momentum distribution

The momentum distribution, related to the reduced density matrix, is defined as

$$n(k) = \frac{1}{2\pi} \int \rho(x, x')\, \mathrm{e}^{-\mathrm{i}k(x-x')}\, \mathrm{d}x\, \mathrm{d}x', \tag{23}$$

with the normalization

$$\int n(k)\, \mathrm{d}k = N.$$

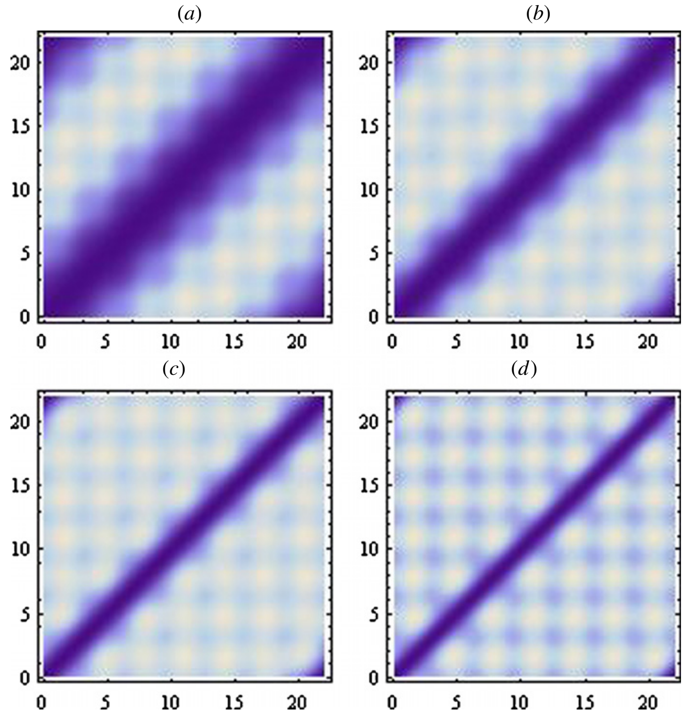

Figure 4. Density plots of the pair distribution function $D(z_1, z_2)$. The abscissa is z_1, and the ordinate is z_2. $M = 7$. (*a*) $N = 2$; (*b*) $N = 3$; (*c*) $N = 5$; (*d*) $N = 7$.

Actually, the momentum distribution is just the Fourier transformation of the reduced density matrix (18). We know that a function and its Fourier series are one-to-one, as the difference of the reduced density matrix $\rho(x, x')$ of the hard-core Bose gas and Fermi gas, the momentum distribution is surely not the same. Lin and Wu [10] have plotted the momentum distributions for both the TG gas and the free Fermi gas in a periodic Kronig–Penney potential, which shows the difference—even a free Fermi gas has a broader momentum distribution than the most strongly interacting boson gas. We would like to add that, although their momentum distribution functions are different, their total momenta are the same. With the equation

$$\left(\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2}\right) \operatorname{sgn}(x_2 - x_1) = 0, \tag{24}$$

we can prove that

$$\sum_{i=1}^{N} \frac{\partial}{\partial x_i} A(x_1, \ldots, x_N) = 0. \tag{25}$$

And then, going ahead, we can obtain

$$\bar{P}(t)^B = \bar{P}(t)^F, \qquad \text{where} \quad P = -\mathrm{i}\hbar \sum_{i=1}^{N} \frac{\partial}{\partial x_i}. \tag{26}$$

4. Summary and conclusions

On solving the eigenfunction of the TG gas in the external magnetic field, we find that the TG system with large B and ω has a higher probability in the ground state than the TG gas raised by Girardeau in 1960 when the number of bosons N is commensurate with the number of potential cycles M. It reveals that we can realize the ground-state TG system more easily. Then we have studied the properties of the magnetized TG and Fermi gases in an external magnetic field. Comparison with each other when they are in the 'same' state reveals that it is impossible to distinguish them just by their average values of particle coordinates and potential energies, system total momenta, single-particle densities and pair distribution functions. But we can distinguish them by their reduced single-particle matrices or their momentum distributions. In order to illustrate our results, we have plotted their reduced single-particle matrices and the momentum distributions when they are in the ground state. Although their momentum distribution functions are different, their total momenta are the same. These results will be helpful for understanding the TG gas.

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