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Citation: Chin. Phys. B, 2025, 34 (**3**): 030301. DOI: 10.1088/1674-1056/ada433
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Density distribution of ground state of one-dimensional Bose gas with dipole interaction

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(Received 21 October 2024; revised manuscript received 16 December 2024; accepted manuscript online 31 December 2024)

Using the Bose–Fermi mapping method, we obtain the exact ground state wavefunction of one-dimensional (1D) Bose gas with the zero-range dipolar interaction in the strongly repulsive contact interaction limit. Its ground state density distributions for both repulsive and attractive dipole interactions are exhibited. It is shown that in the case of the finite dipole interaction the density profiles do not change obviously with the increase of dipole interaction and display the typical shell structure of Tonks–Girardeau gases. As the repulsive dipole interaction is greatly strong, the density decreases at the center of the trap and displays a sunken valley. As the attractive dipole interaction increases, the density displays more oscillations and sharp peaks appear in the strong attraction limit, which mainly originate from the atoms occupying the low single particle levels.

Keywords: Bose gas, one-dimensional, dipole interaction

PACS: 03.75.Hh, 05.30.Jp, 67.85.–d

DOI: 10.1088/1674-1056/ada433 **CSTR:** 32038.14.CPB.ada433

1. Introduction

Low-dimensional many-body quantum system has always been the research focus in the condensed matter physics for the interplay of dimensionality effect and strong correlation effect. The rapid progress in the experiment techniques in quantum gas offers an popular platform to investigate the strong correlation in low-dimensional quantum system. With the anisotropic trap and optical lattices cold atoms can be frozen to the ground state in the tranversal direction and remain move freely in the longitudinal direction,[1–4] and the system becomes an effective one-dimensional (1D) quantum gas. In this situation the atomic interaction is reduced to the effective 1D one dependent on the three-dimensional (3D) anisotropic potential. One of the intriguing properties of cold atoms is the tunability of the atomic interaction with the Feschbach resonance and confined induced resonance technique.[5,6] The manipulation of the confinement geometry and atomic interaction are important techniques in the field of quantum gas,[7–9] and their effects are drawn much attention by both experimentalists and theorists. The paradigmatic model for the 1D Bose gas with contact interaction is the Lieb–Liniger model.[10,11] Its exact solution offers us the most solid theoretical description for the 1D interacting Bose quantum gases although it was solved initially as a mathematics model. It is shown that in the strongly interacting regime the ground state density distribution of 1D Bose gas, i.e., the Tonks–Girardeau (TG) gas, exhibits the same shell structure as that of spin-polarized fermions.[12] In this limit the ground state wavefunction and therefore all properties can also be given with Bose–Fermi mapping method.[13,14]

Besides the short-range contact interaction the magnetic atoms such as ^{52}Cr,[15,16] ^{164}Dy,[17] and ^{168}Er[18] draw considerable interests for the long-range interparticle dipolar interactions. Furthermore the dipole interaction exists in heteronuclear molecules,[19–22] Rydberg atoms,[23–25] and it is more interesting that in trapped ion systems the tunable-range interactions can be realized.[26] The dipolar interaction induces very rich phenomenology for its long-range nature and anisotropy.[27] The competition between kinetic energy, contact interaction, and polar interaction leads to the produce of new matter states such as the supersolids[28–31] and the quantum droplet.[32–35] In different phases the quantum gas displays unique properties. For example, unlike the quantum gas phase the quantum droplet shows the flat-topped density distribution.[36–39] Although the 1D Bose gas with δ-interaction can be exactly solved analytically, to solve the many-body Schrödinger equation with long-range dipole interaction is a task far to reach so far. The analytical solution can be obtained only in some specific limit. In Ref. [40], Jakub *et al.* derived the analytical solitonic solution to the 1D Bose gas of infinitely strong contact interactions with zero-range dipolar interaction by solving the Lieb–Liniger–Gross–Pitaevskii equation beyond the mean-field theory. For the strong correlation in 1D quantum gas, the theory based on mean-field cannot describe the system accurately and we have to turn to more exact theory beyond mean-field and perturbation theory. Since the eigen-equation of zero-range dipolar gases without contact interaction can be solved, we can con-

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struct the exact ground wavefunction in the infinite repulsion limit with Bose–Fermi mapping method. It is more accurate than that beyond mean-field theory and can describe the strong correlation effect in a better way.

The goal of the present paper is to obtain the ground state wavefunction and therefore the density distribution of 1D TG gases with zero-range dipolar interaction. In Section 2, we firstly give the complete Hamiltonian to describe the 1D Bose gas with contact interaction and dipole–dipole interaction. Then we obtain the ground state wavefunction of TG gases with zero-range dipole–dipole interaction with Bose–Fermi mapping method. In Section 3, we show the ground state density distribution dependent on the strength of 1D effective dipolar interaction. In Section 4, a brief summary is given.

2. Model

The dipole–dipole interaction energy between two dipoles at $\boldsymbol{r}$ and $\boldsymbol{r}'$ which are pointing in the same direction is

$$U_{\rm dd}\left(\boldsymbol{r}-\boldsymbol{r}'\right)=\frac{3a_{\rm dd}\hbar^2}{m}\frac{1-3\cos^2\theta}{\left|\boldsymbol{r}-\boldsymbol{r}'\right|^3}. \tag{1}$$

Here m is the mass of dipoles, $a_{\rm dd}$ is the interacting constant, and θ is the angle between the position vector of two dipoles and the polarization direction. The most appealing topics of dipole interaction is its effect of anisotropy and long-range, and with the change of θ the dipolar interaction can be repulsive or attractive. In the present paper we investigate the 1D quantum gas with dipolar interactions. The quantum gas is confined in transverse tightly with anisotropic potential or strong two-dimensional (2D) optical lattices such that cold atoms are frozen to the ground state of harmonic potential transversely. In this case the quantum gas can be reduced to the effective 1D system and the effective 1D dipolar interaction taken the formula as[41–43]

$$V_{\rm dd}^{\rm 1D}(|x-x'|)=\frac{6\pi a_{\rm dd}\hbar^2}{\sqrt{2}md_\rho}\left[\frac{4}{3}\delta(\sqrt{\omega})+2\sqrt{\omega}-\sqrt{\pi}(1+2\omega)\,{\rm e}^{\omega}(1-{\rm erf}(\sqrt{\omega}))\right] \tag{2}$$

with $\omega=\left[|x-x'|/\sqrt{2}d_\rho\right]^2$, where d_ρ is the radial harmonic oscillator length. In the same way the atomic contact interaction is also reduced as the 1D interaction strength $g_{\rm 1D}=-2\hbar^2/(ma_{\rm 1d})$ and $a_{\rm 1d}$ being the effective 1D scattering length.[44,45]

The 1D quantum gas of N indistinguishable Bose atoms with contact interaction and dipolar interaction can be described by the Hamiltonian

$$\hat{H}=\sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2}+V(x_i)\right]+g_{\rm 1D}\sum_{1\le i<j\le N}\delta(x_i-x_j)+g_{\rm dd}^{\rm 1D}\sum_{1\le i<j\le N}V_{\rm dd}^{\rm 1D}(|x_i-x_j|), \tag{3}$$

where $g_{\rm dd}^{\rm 1D}$ is the effective 1D dipolar interacting constants and $V(x)$ is the external potential. In the present paper, we will focus on the 1D quantum gas in a hard wall potential (with the width being 1) in the strongly repulsive limit $g_{\rm 1D}\to+\infty$. The solution in this limit can be constructed by the solution to the above Hamiltonian without the $g_{\rm 1D}$ term for the fermions with the Fermi–Bose mapping method. That is to say, the exact ground state wavefunction of 1D strongly interacting Bose gases can be calculated based on the wavefunction of fermions $\Psi_{\rm F}(x_1,x_2,\ldots,x_N)$,[13,14]

$$\Psi_{\rm B}(x_1,\ldots,x_N)=A(x_1,\ldots,x_N)\,\Psi_{\rm F}(x_1,\ldots,x_N)$$

with the mapping function

$$A(x_1,\ldots,x_N)=\prod_{1\le i<j\le N}{\rm sign}(x_i-x_j),$$

which change the exchange properties of the wavefunction with the sign function sign(x) being equal to 1, 0, and -1, for $x>0$, $x=0$, and $x<0$, respectively. Because it is a huge challenge to solve the eigen-problem of dipole interacting system, we will include the dipole effect approximately in the mean-field level.[40] Here the Fermi wavefunction $\Psi_{\rm F}(x_1,\ldots,x_N)$ is constructed as the Slater determinant

$$\Psi_{\rm F}(x_1,\ldots,x_N)=\frac{1}{\sqrt{N!}}\det_{l,k=1}^{N}\left[\varphi_{l-1}(x_k)\right],$$

where $\varphi_l(x)$ is the eigen-function of the Schrödinger equation including the dipole term,

$$\hat{H}_{\rm F}\varphi_n(x)=E_n\varphi_n(x) \tag{4}$$

with

$$\hat{H}_{\rm F}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+g_{\rm dd}^{\rm 1D}\int{\rm d}x'\left|\varphi_n(x')\right|^2V_{\rm dd}^{\rm 1D}(|x-x'|).$$

We consider the zero-range dipolar interactions[40] in this limit $V_{\rm dd}^{\rm 1D}(|x-x'|)=g_{\rm dd}^{\rm 1D}\delta(|x-x'|)$. This approximation works well when the aspect ratio is smaller enough but much larger than the mean distance between particles. In this situation the eigen-equation for $\hat{H}_{\rm F}$ can be formualted as the following nonlinear Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+g_{\rm dd}^{\rm 1D}\varphi_n^2(x)\right]\varphi_n(x)=E_n\varphi_n(x). \tag{5}$$

For simplicity, we take the natural unit in the following ($m=\hbar=1$) and the original notations are preserved. The eigen-equation is expressed as

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+g_{\rm dd}^{\rm 1D}\varphi_n^2(x)\right]\varphi_n(x)=E_n\varphi_n(x). \tag{6}$$

The eigen-function to Eq. (6) in the repulsive case ($g_{\rm dd}^{\rm 1D} > 0$) for the hard wall potential is[46]

$$\varphi_n(x) = \sqrt{2k}\,[2n\mathcal{K}(k)]\,/\sqrt{2g_{\rm dd}^{\rm 1D}}\,{\rm sn}\,[2n\mathcal{K}(k)x|k]\,, \tag{7}$$

where the notation ${\rm sn}(x|n)$ is standard Jacobian elliptic function and $\mathcal{K}(k)$ is the complete elliptic integral of the first kind. The corresponding eigenvalue is $E_n = 2\,[n\mathcal{K}(k)]^2\,(1+k)$. k is determined by the normalization condition

$$\frac{[2n\mathcal{K}(k)]^2}{g_{\rm dd}^{\rm 1D}}\left(1-\frac{\mathcal{E}(k)}{\mathcal{K}(k)}\right) = 1 \tag{8}$$

with $\mathcal{E}(k)$ being the complete elliptic integral of the second kind. The eigen-function to Eq. (6) in the attractive case ($g_{\rm dd}^{\rm 1D} < 0$) is[47]

$$\varphi_n(x) = \sqrt{2k}\,[2n\mathcal{K}(k)]\,/\sqrt{2g_{\rm dd}^{\rm 1D}}\,{\rm cn}\,[\mathcal{K}(k)(2nx-1)|k] \tag{9}$$

with the corresponding eigenvalues $E_n = -2\,[n\mathcal{K}(k)]^2\,(2k-1)$ and the normalization condition

$$\frac{(2n)^2\,\mathcal{K}(k)}{g_{\rm dd}^{\rm 1D}}\,[\mathcal{E}(k)-(1-k)\mathcal{K}(k)] = 1. \tag{10}$$

After solving the transcendental equations (8) and (10), we determine the parameter k and therefore obtain the eigen-solutions of the Schrödinger equation. In Fig. 1 we plot the dependence of eigenvalues on the effective 1D dipolar interaction. It is shown that the eigenvalues increase with the increase of the dipolar interaction. In the repulsive case the eigen-levels are always greater than 0, while in the attractive case the eigenvalues are greater than 0 only when the attractive interaction is not so strong. The eigenvalues become negative with the increase of the attractive case for all eigen-levels. The higher levels, the stronger the attraction of the transition from positive value to the negative value.

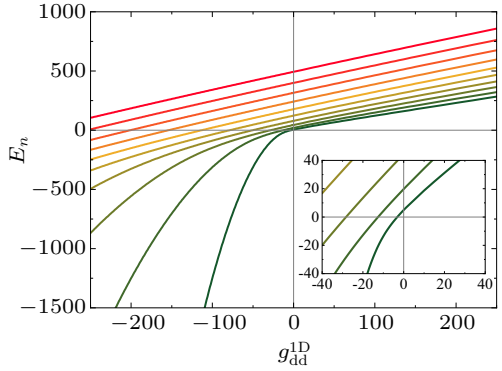


Fig. 1. The eigenvalue E_n dependence on the effective 1D dipolar interaction strength $g_{\rm dd}^{\rm 1D}$.

3. Ground state density distribution

When we have the solution to Eqs. (8) and (10), the eigen-function $\varphi_n(x)$ for different 1D dipolar interactions can be determined. Therefor we can calculate the density distribution $\rho(x) = \sum_{n=1}^{N}\varphi_n^2(x)$ based on the Bose–Fermi mapping method.[13,14] In Fig. 2 we plot the four lowest eigen-functions for different repulsive dipole interactions. It is shown that in the limit of $g_{\rm dd}^{\rm 1D} = 0$ the solution reproduces the results of 1D TG gases $\varphi_n(x) = \sqrt{2}\sin(n\pi x)$. As the 1D dipole interaction increases, the positions of the nodes of eigen-functions do not change but they become more flat in each regions between neighbor nodes. This means that in the limit of strong repulsive dipolar interaction the particles distribute in n separated regions with the homogeneous probability if one particle occupies the n-th eigen-state.

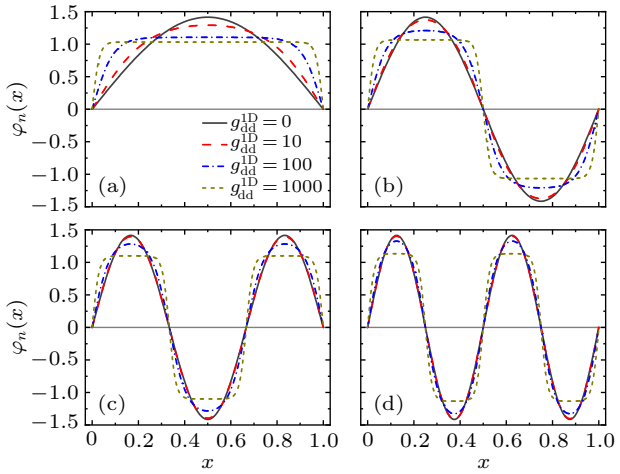


Fig. 2. The four lowest eigen-functions for different repulsive dipole interactions: (a) $n=1$, (b) $n=2$, (c) $n=3$, and (d) $n=4$.

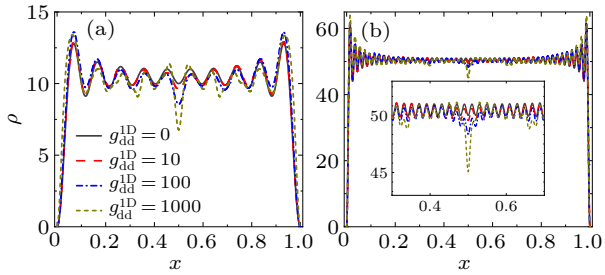


Fig. 3. Density distribution of TG gases with repulsive dipolar interaction: (a) 10 particles, (b) 50 particles.

For the TG gases with strong repulsive contact interaction, the total density is the summation over the lowest N eigen-states. The dependence of density distribution $\rho(x)$ on the repulse dipole interaction is displayed for TG gases with 10 atoms and 50 atoms in Figs. 3(a) and 3(b), respectively. In the case of $g_{\rm dd}^{\rm 1D} = 0$, the quantum gas shows multi-peak shell structure which is the typical density distribution of TG gases. With the increase of the dipole interaction the density does not exhibit obviously different properties until the strong dipole interaction regime. But when the dipole interaction becomes very strong the density displays a sunken valley at the center of the potential trap that means the Bose atoms appear at the potential center with smaller probability in this case. It is interesting to note that the zero-range dipole interaction with

finite strong repusion induces the reduction of the central density profiles although the contact interaction is infinite repulsion. The competition between them only obviously affects the density at the potential center locally. The flattening effect of eigen-functions does not show obviously because the node number of the density profile is equal to the atom number and the density profile oscillates intensively.

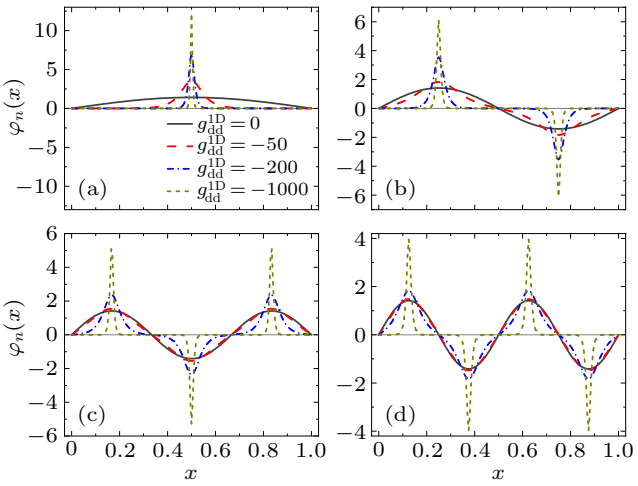


Fig. 4. The four lowest eigen-functions for different attractive dipole interactions: (a) $n=1$, (b) $n=2$, (c) $n=3$, and (d) $n=4$.

The four lowest eigen-functions for attractive dipolar interaction are plotted in Fig. 4. It is shown that with the increase of attraction interaction the eigen-function becomes sharp peaks in separated regions. This means that the attractive interaction prompts atoms to gather in smaller regions. In Fig. 5, we plot the density profiles of TG gases for $N=10$ (Fig. 5(a)) and $N=50$ (Fig. 5(b)). Compared with the typical multi-peak shell structure of TG gases induced by the strong repulsion, the density profiles display more oscillations for the increase of the dipole interaction. As the dipole interaction becomes strong enough, a sharp peak at the center with lower satellite peaks at both sides is shown. Although in the TG limit the atomic repulsion is infinity, it is interesting that the finite attractive dipole interaction induces interesting gathering properties, characterized by the formation of several separated high density locations in equilibrium with a low density background. In order to clarify the origin of these enormously high density regime and satellite peaks, figure 6 shows a comparison between total density distribution ρ and the density of low levels ($\rho_3=\sum_1^3\varphi_n^2$ and $\rho_L=\sum_1^5\varphi_n^2$) and that of high levels ($\rho_H=\sum_6^{50}\varphi_n^2$), for 50 atoms and $g_{dd}^{1D}=-1000$. It is shown that the lowest three levels make major contribution to shape the density distribution, including the central and side peaks, while other higher levels ($\varphi_n(x)$ with $n=6,\ldots,50$) raise the whole density, and induce small fluctuations to the density profiles. The comparison of the total density distribution with the profiles of low levels in Fig. 4 shows that the prominent central density is formed for the atoms occupied the odd levels, in particular the occupations of the lowest level and the third level, while the side peaks neighbor to the central one are mainly form of the occupation of the second lowest level. The atoms in high levels distribute in more different local regimes with equal probability and no more prominent high peaks are displayed. The atoms in the lowest three levels play crucial roles in the appearance of satellite peaks.

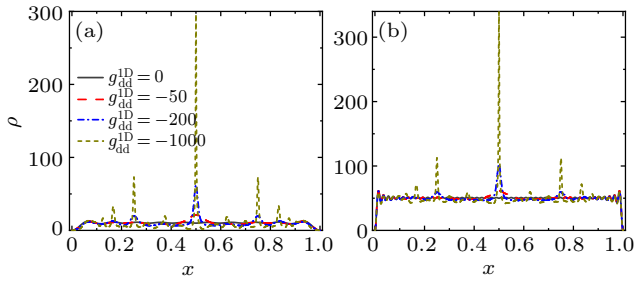


Fig. 5. Density distribution of TG gases with attractive dipolar interactions: (a) 10 particles, (b) 50 particles.

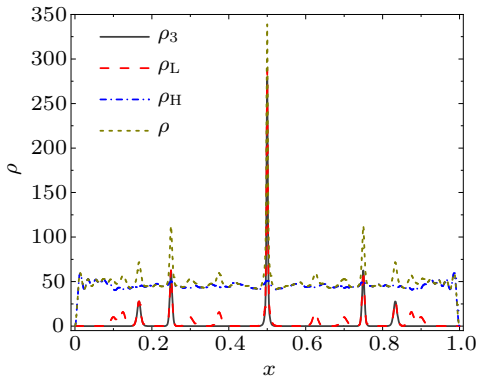


Fig. 6. Low levels contribute more for density distribution. The graph shows ρ, ρ_3, ρ_L, and ρ_H, where $\rho=\rho_L+\rho_H$, given 50 particles and $g_{dd}^{1D}=-1000$.

4. Conclusion

In conclusion we investigated the ground state of TG gases with dipolar interactions. The energy levels and eigenfunctions of single particle Schrödinger equation with zero-range dipolar interaction can be solved analytically. Combing the eigen-functions and the Bose–Fermi mapping method, we constructed the exact ground wavefunction of TG gases with the zero-range dipolar interaction. The effect on the ground state density distributions induced by dipole interaction is exhibited. It is shown that the finite dipole interactions do not affect the density profile obviously and display the similar shell structure to that of Tonks–Girardeau gases. As the repulsive dipole interaction is greatly strong, the density profiles display a sunken valley and atoms populate at the center of the trap with smaller probability. While with the increase of the attractive dipole interaction, the density displays more oscillations compared with that of TG gases. In the strong attraction limit the sharp peaks appear at the potential center and on its sides separately. The strong long-range attraction induces the atoms populate at several separated locations with enormous probability. The comparison of the total density with the density of

low levels and that of high levels indicates that the enormous increase of the density at these locations mainly originate from the occupations of low levels. The present theoretical method is trying to obtain the ground state in a better way than mean-field theory, but the way to dealing with strong dipole interaction is not rigorous and the new method is expected.

Acknowledgement

Project supported by the National Natural Science Foundation of China (Grant No. 11174026).

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