

Ground state of hard-core bosons in one-dimensional periodic potentials

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With Girardeau's Fermi-Bose mapping, we find the exact ground states of hard-core bosons residing in a one-dimensional periodic potential. The analysis of these ground states shows that when the number of bosons N is commensurate with the number of wells M in the periodic potential, the boson system is a Mott insulator whose energy gap, however, is given by the single-particle band gap of the periodic potential; when N is not commensurate with M , the system is a metal (not a superfluid). In fact, we argue that there may be no superfluid phase for any one-dimensional boson system in terms of Landau's criterion of superfluidity. The Kronig-Penney potential is used to illustrate our results.

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I. INTRODUCTION

A Tonks-Girardeau (TG) gas is a one-dimensional strongly correlated system consisting of bosons with hard-core interaction. This model of a one-dimensional gas was first studied by Tonks [1], who treated it as a classical gas. Later studies were nevertheless focused mostly on its properties as a quantum boson gas [2,3]. As the milestone development in this model, Girardeau [4,5] found that this boson gas can be mapped into a spinless fermion system and obtained all of its eigenstates.

This idealized TG gas had only been a curiosity of theorists until the realization of Bose-Einstein condensation with dilute atomic gases [6–10]. It was soon noticed that the TG gas could be realized experimentally from a Bose-Einstein condensate trapped in tightly confined waveguides [11]. This work renewed interest in the TG gas and led to a series of further theoretical studies [12–20]. In particular, Lapeyre *et al.* studied the momentum distribution of a harmonically trapped TG gas [15] and Forrester *et al.* [17] obtained highly accurate results on the TG gas's long-range off-diagonal behavior [21,22]. Finally, in 2004, the TG gas was first realized from a Bose-Einstein condensate trapped in two perpendicular optical lattices [23,24]. An overview of studies in this interesting subject can be found in a recent review by Yukalov and Girardeau [25].

In this paper we study the TG gas in a periodic potential. We focus on the case that the hard-core interaction between bosons is a repulsive infinite-contact interaction. By applying Girardeau's Fermi-Bose mapping [4,5], this boson gas can be mapped into a spinless free Fermi system. As a result, we can obtain all the eigenstates and eigenenergies of this TG gas. We are particularly interested in its ground properties. Our analysis of the ground states shows that such a TG gas has two quantum phases, Mott insulator and metal. When the number of bosons N in the gas is commensurate with the number of wells M in the periodic potential, the boson system is a Mott insulator; however, its energy gap is given by the single-particle band gap of the periodic potential. When N is not commensurate with M , the system is a metal. We emphasize that this boson metal is not a superfluid as it cannot support any superflow with finite critical velocity. In fact, in this sense there may be no superfluid phase for any one-

dimensional boson systems including soft-core bosons.

The Kronig-Penney potential is used to illustrate our results. Various properties of the ground state are computed, such as the pair distribution function, single-particle density matrix, and momentum distribution. Before we proceed with full discussion, we note that the hard-core bosons in a lattice have been actively studied under the single-band approximation with the Jordan-Wigner transformation [26–29]. It is also studied as a limiting case in Ref. [30].

II. TG GAS IN PERIODIC POTENTIAL

Normally, the boson in a TG gas has an “impenetrable” hard core characterized by a radius of a . In this study, we focus on the case that the hard core is a point with no radius, that is, the interparticle interaction is given by

$$U(x) = \begin{cases} \infty, & x = 0, \\ 0, & x \neq 0. \end{cases} \quad (1)$$

Such an interaction is equivalent to a constraint on the wave function $\psi(x_1, \dots, x_N)$,

$$\psi = 0 \quad \text{if} \quad x_i = x_j, \quad 1 \leq i < j \leq N. \quad (2)$$

This means that this TG gas can be viewed as a group of “free” bosons governed by the following Hamiltonian:

$$\hat{H} = \sum_{j=1}^N \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + V(x_j) \right\}, \quad (3)$$

while its wave function is subject to the constraint in Eq. (2). Based on the observation that the constraint in Eq. (2) is automatically satisfied by any wave function of a Fermi system due to its antisymmetry, Girardeau [4,5] found a natural mapping that allows one to construct wave functions for a TG gas from wave functions of a free Fermi system. The mapping is

$$\psi^B(x_1, x_2, \dots, x_N) = A \psi^F(x_1, x_2, \dots, x_N) \quad (4)$$

where ψ^B is the Bose wave function and ψ^F the Fermi wave function. A is called the unit antisymmetry function and is defined as

$$A(x_1, x_2, \dots, x_N) = \prod_{i>j} \text{sgn}(x_i - x_j), \quad (5)$$

where sgn is the sign function. This Fermi-Bose mapping is one to one and, therefore, the energy spectrum of a TG gas of infinite contact potential is the same as that of a free spinless Fermi system [4,5].

In this paper, we study the case where the external potential $V(x)$ is periodic, $V(x)=V(x+d)$, with d being the period. Due to the Fermi-Bose mapping (4), we consider first a system of N free spinless fermions residing in this periodic potential. According to the basic knowledge of solid state physics [31], when the number of fermions N in the gas is commensurate with the number of wells M in the periodic potential, the fermions can fill up exactly N/M Bloch bands and thus the Fermi system is an insulator with its energy gap determined by the periodic potential. When N is not commensurate with M , the fermions can fill up the bands only partially and the Fermi system is a metal.

Because of the Fermi-Bose mapping (4), the TG gas has the same energy spectrum as this free Fermi system. This allows us to conclude immediately that when N is commensurate with M , the TG gas is an insulator. However, we emphasize that this insulator is a Mott insulator unlike its mapping target, the free Fermi system, where the insulator is a band insulator. This leads to a quite peculiar situation: the energy gap of a Mott insulator is completely dictated by the periodic potential and is given by the single-particle band gap. For the other situation where N is not commensurate with M , the TG gas is a metal.

We emphasize that this Bose metal is a real metal, not a superfluid according to Landau's criterion of superfluidity [32]. Landau's criterion is that the system is a superfluid if it has phonons as its only low-energy excitations. Plotted in Fig. 1 is the excitation spectrum of a TG gas in a periodic potential for the noncommensurate case, which is marked by the shading. It is clear from this figure that there are two kinds of low-energy excitations, one at $k=0$ and the other at $k=2k_{\text{max}}$. The low-energy excitation at $k=0$ may barely be called a phonon since the phonon relation $\epsilon=ck$ exists only at the limit $k \rightarrow 0$ and the excitation spectrum immediately spreads out at $k \neq 0$. The most destructive results are the low-energy excitations at $2k_{\text{max}}$, which are not phonons. The presence of these low excitations causes vanishing of the minimum slope of $\epsilon(k)/k$, which gives the critical velocity of possible superfluidity. Therefore, we can conclude that this TG gas cannot support a superflow with finite critical velocity and it is not a superfluid.

What is more interesting is that the TG gas is not an isolated case. According to Ref. [33], a boson gas with finite repulsive δ -function interaction has a very similar excitation spectrum as our TG gas. This means that such a gas is not superfluid, either. This prompts us to speculate that any one-dimensional boson system is not a superfluid. We are aware that there are different definitions of superfluidity [34]. In particular, according to Leggett [35], our TG gas (in his version it is a spinless fermion) is a superfluid since it has the so-called nonclassical rotational inertia. Because of this, we

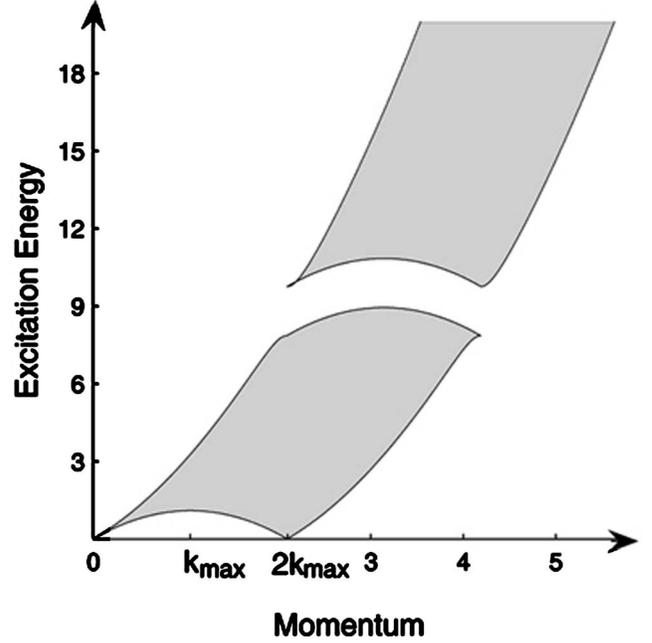


FIG. 1. Excitation spectrum of a TG gas in a periodic potential for the noncommensurate case. The shading shows all the possible excitations. k_{max} is the largest possible value of k , similar to the Fermi wave vector in the fermion case.

state again that we are talking about superfluid in the sense of Landau's criterion.

We now construct explicitly the exact eigenfunctions of this TG gas. The single-particle eigenstate $\varphi_{n,k}(x)$ is a Bloch state that satisfies the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \varphi_{n,k}(x) = E_{n,k} \varphi_{n,k}(x). \quad (6)$$

The notation n is for the band index and k is the Bloch wave vector in the first Brillouin zone. For convenience, we use $\alpha=\{n,k\}$ to denote both the band index and the Bloch wave vector. Then according to Eq. (4) the Bose eigenfunction is given by the Slater determinant

$$\psi^B(x_1, x_2, \dots, x_N) = \frac{A}{\sqrt{N!}} \begin{vmatrix} \varphi_{\alpha_1}(x_1) & \varphi_{\alpha_2}(x_1) & \cdots & \varphi_{\alpha_N}(x_1) \\ \varphi_{\alpha_1}(x_2) & \varphi_{\alpha_2}(x_2) & \cdots & \varphi_{\alpha_N}(x_2) \\ \vdots & \vdots & \vdots & \vdots \\ \varphi_{\alpha_1}(x_N) & \varphi_{\alpha_2}(x_N) & \cdots & \varphi_{\alpha_N}(x_N) \end{vmatrix}. \quad (7)$$

As one can check, this symmetric wave function satisfies both the Schrödinger equation with the Hamiltonian (3) and the constraint (2). The corresponding eigenenergy is

$$E = \sum_{j=1}^N E_{\alpha_j}. \quad (8)$$

For the ground state, the N eigenfunctions in the Slater determinant are for the N lowest eigenstates. For convenience, we shall assume that both N and M are odd in the following discussion.

III. TG GAS IN THE KRONIG-PENNEY POTENTIAL

We now use the Kronig-Penney (KP) potential to illustrate our general results of the TG gas in the last section. The Kronig-Penney potential is given by

$$V(x) = \gamma \sum_j \delta(x - jd) \quad (9)$$

where γ is the strength of the δ potential. We follow the standard procedure in solid state physics [31] by placing the

$$\varphi_\alpha(x) = \begin{cases} f(x) = A_\alpha e^{ip_\alpha x} + B_\alpha e^{-ip_\alpha x}, & x \in [0, 1) \\ e^{iks} f(x-s), & x \in [s, s+1) \quad (s = 1, 2, \dots, M-1) \end{cases} \quad (11)$$

with the coefficients determined by

$$k = \frac{2\pi l}{M} \quad \left(l \in 0, \pm 1, \dots, \pm \frac{M-1}{2} \right),$$

$$\cos p_\alpha + \frac{V}{2p_\alpha} \sin p_\alpha = \cos k,$$

$$A_\alpha = \frac{\sqrt{2} e^{-ip_\alpha d/2} p_\alpha \sin[(p_\alpha + k)/2]}{\sqrt{[(2p_\alpha^2 + V) \sin p_\alpha - p_\alpha V \cos p_\alpha] M \sin p_\alpha}},$$

$$B_\alpha = \frac{\sqrt{2} e^{ip_\alpha d/2} p_\alpha \sin[(p_\alpha - k)/2]}{\sqrt{[(2p_\alpha^2 + V) \sin p_\alpha - p_\alpha V \cos p_\alpha] M \sin p_\alpha}}. \quad (12)$$

The corresponding eigenenergy is $E_\alpha = p_\alpha^2$.

As we have demonstrated in the last section, when a TG gas of exactly M bosons is placed in the KP potential, the system is a Mott insulator. The energy gap between the first and the second Bloch bands is plotted in Fig. 2. This figure shows that this gap initially increases with the lattice strength V and eventually saturates at the energy difference between the first excited state and the ground state in a square well potential.

A. Pair distribution function

The pair distribution function, normalized to $N(N-1)$, is defined as

$$D(x_1, x_2) = N(N-1) \int |\psi_0^B(x_1, \dots, x_N)|^2 dx_3 \cdots dx_N$$

$$= \frac{1}{2} \sum_{\alpha, \alpha'=0}^{N-1} |\varphi_\alpha(x_1) \varphi_{\alpha'}(x_2) - \varphi_\alpha(x_2) \varphi_{\alpha'}(x_1)|^2. \quad (13)$$

It is the joint probability of finding simultaneously one atom at x_1 and another atom at x_2 . When $x_1 = x_2$, the pair distribu-

tion function vanishes by antisymmetry, reflecting physically the impenetrable hard-core interaction between boson particles.

$$\left(-\frac{\partial^2}{\partial x^2} + V \sum_{j=0}^{M-1} \delta(x-j) \right) \varphi_\alpha(x) = E_\alpha \varphi_\alpha(x) \quad (10)$$

where $V = 2m\gamma d/\hbar^2$. The eigenfunction φ_α is given by

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Figure 3 shows gray-scale plots of the pair distribution function $D(x_1, x_2)$ for different numbers of particles of $M=9$. Some qualitative features of the pair distribution function are observed. First, the figure shows that $D(x_1, x_2)$ vanishes at contact, $x_1 = x_2$, reflecting the impenetrability between the particles. Second, the periodicity due to the Kronig-Penney potential is apparent. Third, with the increase of the particle number, the black diagonal stripe becomes thinner. This indicates that the averaged distance between particles decreases.

B. Reduced single-particle density matrix

The reduced single-particle density matrix is given by

$$\rho(x, x') = N \int \psi_0^B(x, x_2, \dots, x_N) \times \psi_0^B(x', x_2, \dots, x_N) dx_2 \cdots dx_N. \quad (14)$$

The existence of the off-diagonal long-range order in this

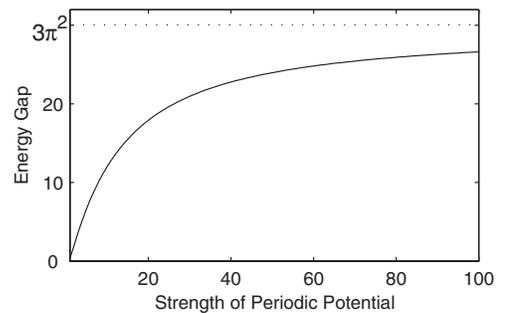


FIG. 2. Width of the energy gap between the first and the second Bloch bands as a function of the strength V of the periodic potential. This is also the energy gap of the Mott insulator when the number of bosons in the TG gas is equal to the number of wells in the periodic potential.

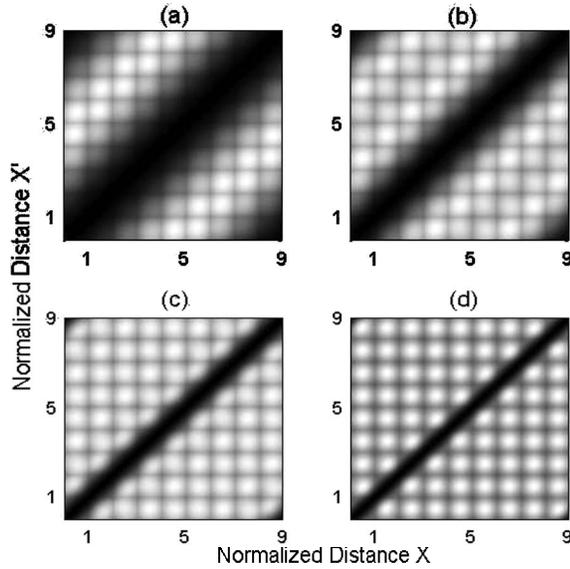


FIG. 3. Gray-scale plots of the pair distribution function $D(x_1, x_2)$. $V=1$. (a) $N=2, M=9$; (b) $N=3, M=9$; (c) $N=6, M=9$; (d) $N=9, M=9$.

matrix indicates the onset of Bose-Einstein condensation [36,37]. Its diagonal term $\rho(x)=\rho(x, x'=x)$ is the single-particle density and is normalized to N ,

$$\int \rho(x, x) dx = N. \quad (15)$$

The multidimensional integral in Eq. (14) is evaluated numerically by Monte Carlo integration. The results are shown in Fig. 4. The relatively darker area of the diagonal in

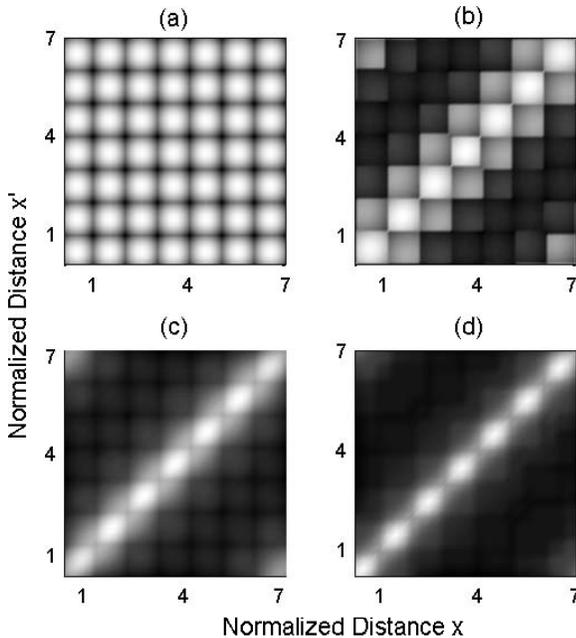


FIG. 4. Gray-scale plots of the reduced density matrix $\rho(x, x')$ of the TG gas. $V=1$. (a) $N=1, M=7$; (b) $N=3, M=7$; (c) $N=5, M=7$; (d) $N=7, M=7$.

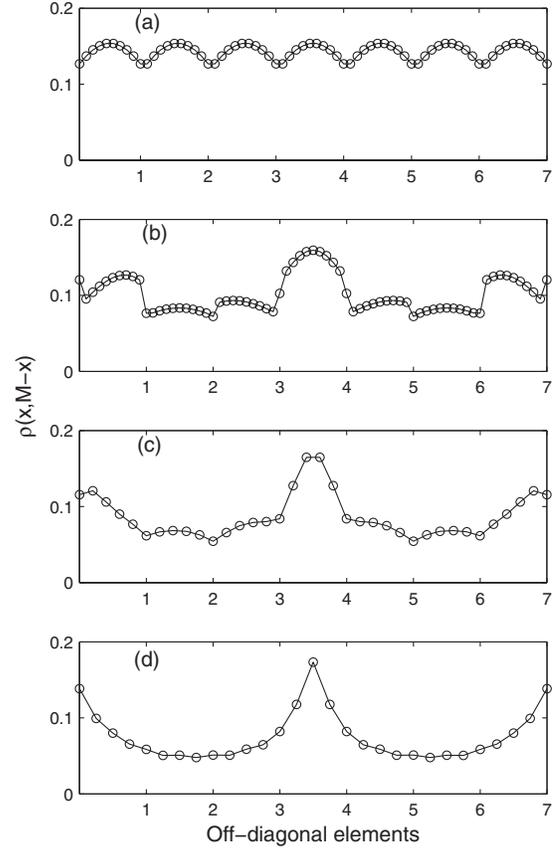


FIG. 5. Off-diagonal elements $\rho(x, M-x)$ of the reduced density matrix. $V=1$. (a) $N=1, M=7$; (b) $N=3, M=7$; (c) $N=5, M=7$; (d) $N=7, M=7$.

the figure is due to δ potentials, which tend to repel the particles. The particles like to stay between δ potentials, i.e., in the brighter diagonal area.

The gray scale in Fig. 4 indicates that the off-diagonal elements decrease as N increases. To see this more clearly, we have plotted the off-diagonal elements $\rho(x, M-x)$ of the reduced density matrix in Fig. 5. It is clear from the figure that, as N increases and the interaction in the system gets stronger, the off-diagonal elements decrease relative to the diagonal. This indicates that the interaction suppresses the off-diagonal terms. It has been proved that there is no real Bose-Einstein condensate in the uniform Tonks-Girardeau gas [17,21,22].

C. Momentum distribution

The Bose-Einstein condensation of a Bose system is often characterized by a macroscopic number of bosons occupying the zero-momentum state. It is therefore meaningful to look at the momentum distribution of our TG gas in the ground state. The momentum distribution $\varrho(k)$ is related to the reduced density matrix and given by [15]

$$\varrho(k) = \frac{1}{2\pi N} \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx' \rho(x, x') e^{-ik(x-x')}, \quad (16)$$

which is normalized to 1. As noted by Girardeau [4,5], the Fermi-Bose mapping in Eq. (4) becomes simply $\psi^B = |\psi^F|$ for

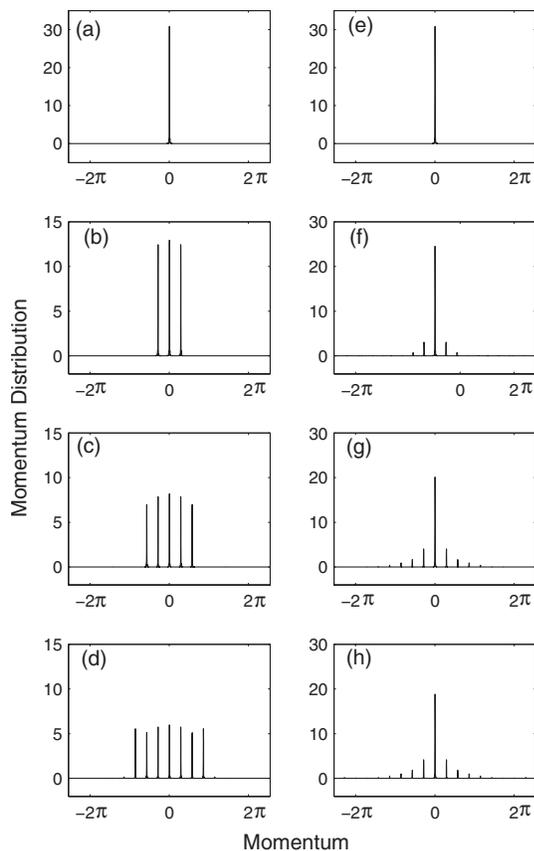


FIG. 6. Normalized momentum distribution function $\rho(k)$. $V=1$. $M=7$. (a)–(d) Free Fermi gas for $N=1, 3, 5, 7$ (from top to bottom); (e)–(h) TG gas for $N=1, 3, 5, 7$ (from top to bottom).

the ground state. This shows that, even though the density distribution $|\psi|^2$ is the same for the TG gas and its mapping counterpart, the free Fermi gas, their momentum distributions are different. It is therefore also interesting to compare the momentum distributions for these two different systems.

In Fig. 6, we have plotted the momentum distributions for both the TG gas and the free Fermi gas in a periodic poten-

tial. The number of wells is $M=7$ and the strength of the periodic potential is $V=1$. The left column (a)–(d) of Fig. 6 is for the Fermi gas and the right column (e)–(h) is for the TG gas. Since higher-order Bragg peaks, e.g., the ones at $\pm 2\pi$, are very small, the plots in Fig. 6 focus on the central Bragg peak, which consists of discrete small peaks due to the finite size of the systems.

We first look at the right column of Fig. 6. For $N=1$, which can be regarded as the free boson case, we see that the Bragg peak is completely located at $k=0$. As the number of bosons increases, the interaction in the system gets stronger. This causes the Bragg peak to spread out as seen in the right column of Fig. 6. When $N=M$, the peak has a width of almost a whole Brillouin zone. It is interesting to compare the TG gas with the free Fermi gas. As shown in the left column of Fig. 6, the Bragg peaks are much “fatter” than for the TG gas (except $N=1$). This demonstrates that even a free Fermi gas has a broader momentum distribution than a the most strongly interacting boson gas.

IV. SUMMARY AND CONCLUSIONS

In summary, we have studied the ground-state properties of a Tonks-Girardeau gas in a periodic potential with Girardeau’s Fermi-Bose mapping. We found that such a TG gas is a metal when the number of particles N is not commensurate with the number of wells M in the periodic potential; it is a Mott insulator when N is commensurate with M . What is more interesting is that the energy gap in the Mott insulator is given by the single-particle band gap of the periodic potential. To illustrate our results, we have employed the Kronig-Penney potential to compute various properties of the ground state, such as the pair distribution function, single-particle density matrix, and momentum distribution.

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