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Ground-state properties of a one-dimensional system of dipoles

A. S. Arkhipov[+], *G. E. Astrakharchik*[+*], *A. V. Belikov*[+], *Yu. E. Lozovik*[+1)]

[+]*Institute of Spectroscopy, 142190 Troitsk, Moscow reg., Russia*

[*]*Dipartimento di Fisica, Università di Trento, and BEC-INFM, I-38050 Povo, Italy*

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A one-dimensional (1D) Bose system with dipole-dipole repulsion is studied at zero temperature by means of a Quantum Monte Carlo method. It is shown that in the limit of small linear density the *bosonic* system of dipole moments acquires many properties of a system of non-interacting *fermions*. At larger linear densities a Variational Monte Carlo calculation suggests a crossover from a liquid-like to a solid-like state. The system is superfluid on the liquid-like side of the crossover and is normal deep on the solid-like side. Energy and structural functions are presented for a wide range of densities. Possible realizations of the model are 1D Bose atom systems with permanent dipoles or dipoles induced by static field or resonance radiation, or indirect excitons in coupled quantum wires, etc. We propose parameters of a possible experiment and discuss manifestations of the zero-temperature quantum crossover.

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Up until now Bose–Einstein condensation has been realized in many different atom and molecule species with short-range interactions. At low temperatures such an interaction can be described by a s-wave scattering length and is commonly approximated by a contact pseudopotential. In contrast, some recent work has focused on the realization of dipole condensates [1 – 5]. In these systems, the dipole-dipole interaction extends to much larger distances and significant differences in the properties (such as the phase diagram and correlation functions) are expected. Another appealing aspect of a system of dipole moments is the relative ease of tuning the effective strength of interactions [6] which makes the system highly controllable. Dipole particles are also considered to be a promising candidate for the implementation of quantum-computing schemes [7 – 9].

On the theoretical side dipole condensates have been mainly studied on a semiclassical (Gross–Pitaevskii) [10] or Bogoliubov [11] level. A model Bose–Hubbard Hamiltonian has been used to describe a dipole gas in optical lattices and a rich phase diagram was found [12, 5]. So far there have been no full quantum microscopic computations of the properties of a homogeneous system.

Recently the Monte Carlo method was used to study helium and molecular hydrogen in nanotubes [13]. Such a geometry, which is effectively one dimensional, leads to completely different properties compared to a three-dimensional sample.

We consider N repulsive dipole moments of mass M located on a line. The Hamiltonian of such a system is given by

$$\hat{H} = -\frac{\hbar^2}{2M}\sum_{i=1}^{N}\frac{\partial^2}{\partial z_i^2} + \frac{C_{dd}}{4\pi}\sum_{i<j}\frac{1}{|z_i - z_j|^3}. \qquad (1)$$

We keep in mind two different possible realizations.

1) Cold bosonic atoms, with induced or static dipole momenta, in a transverse trap so tight that excitations of the levels of the transverse confinement are not possible and the system is dynamically one-dimensional (1D). The dipoles themselves can be either induced or permanent. In the case of dipoles induced by an electric field E the coupling has the form $C_{dd} = E^2\alpha^2$, where α is the static polarizability. For permanent magnetic dipoles aligned by an external magnetic field one has $C_{dd} = m^2$, where m is the magnetic dipole moment. The interaction between the atoms, apart from the dipole forces, contains a short-range scattering part which is conveniently described by the s-wave scattering length a. Usually this contribution is large compared to the dipole force, but recent progress in applying Feshbach resonance techniques to tune a, and even to make it zero, opens exciting prospects of obtaining a system with purely dipole-dipole interactions. The strength of the effective coupling C_{dd} can be tuned by changing the electric field in the case of induced dipoles, and the special technique of fast rotation of the electric or magnetic field can be applied to permanent dipoles[6].

2) Spatially indirect excitons in two coupled quantum wires. A quantum wire is a semiconductor nanos-

[1)]e-mail: lozovik@isan.troitsk.ru

tructure where an electron or a hole is allowed to move only in one direction and excitations of the transverse quantization levels are negligible. In two parallel quantum wires, one containing only holes, and the other only electrons, holes and electrons couple forming indirect excitons. If such a system is dilute enough, it constitutes a 1D set of dipoles. In this case $C_{dd} = e^2D^2/\varepsilon$, where e is an electron's charge, ε is the dielectric constant of the semiconductor, and D is the distance between the centers of the quantum wires. This system is 1D counterpart of 2D indirect exciton system in coupled quantum wells, which was extensively studied both theoretically [14–17, 5] and experimentally [18]. The properties of 1D and 2D systems differ essentially (see below Tonks-Girardeau regime, etc.), thus an experimental study of the 1D system is of a great importance.

The Hamiltonian (1) can be written in dimensionless form by expressing all distances $\tilde{z} = z/r_0$ in units of $r_0 = MC_{dd}/2\pi\hbar^2$ and energies in units of $\mathcal{E}_0 = \hbar^2/Mr_0^2$. All properties of such a system are defined by the dimensionless parameter nr_0 with $n = N/L$ being the linear density and L the size of the system.

Our aim is to determine the ground state energy in wide range of densities and to check the evidence of a possible quantum crossover. In order to define the structural properties we calculate the pair distribution function (PDF). In terms of the many-body ground state wave function of the system Ψ_0 PDF is written as

$$g_2(|z_1-z_2|) = \frac{N(N-1)}{n^2}\frac{\int|\Psi_0(z_1,..,z_N)|^2dz_3..dz_N}{\int|\Psi_0(z_1,..,z_N)|^2dz_1..dz_N}. \tag{2}$$

The static structure factor is directly related to the pair distribution function

$$S(k) = 1 + n\int e^{ikz}[g_2(z)-1]\,dz. \tag{3}$$

The technique of Bragg scattering provides access to the static structure factor in experiments on bosonic atoms. For the system of indirect excitons measurements of spatial structure of photoluminescence can give information about possible crystallization, etc.

We apply Diffusion Monte Carlo (DMC) method, which is one of the most efficient theoretical tools for investigating zero temperature properties of quantum systems [19]. We choose the many-body guiding trial wave function Ψ_T in the Bijl–Jastrow form consisting of one- and two-body terms:

$$\Psi_T(z_1,...,z_N) = \prod_{i=1}^{N} f_1(z_i)\prod_{j<k} f_2(|z_j - z_k|). \tag{4}$$

To describe the liquid-like side of the crossover it is sufficient to have only the term describing pair-correlations. We choose it in the form $f_2(|z|) = \exp\{-[A/(n|z|)]^B\}$, where A and B are variational parameters which we optimize by minimizing variational energy by carrying out Variational Monte Carlo (VMC) calculation. As will be discussed below, in the low density limit the wave function asymptotically approaches the Tonks-Girardeau gas wavefunction $f_2^{TG}(|z|) = |\sin(\pi z/L)|$ [20, 21]. We checked that in this regime there is no large difference between using $f_2^{TG}(|z|)$ and $f_2(|z|)$ even on a variational level. Thus our choice of a two-body term is well suited to describing a liquid even in the strong mean-field regime (see [21]).

We account for the spatial quasi-crystalline order by considering Gaussians with width C for each particle near to a corresponding lattice site $f_1(z_i) = \exp\{-[n(z_i - z_i^c)]^2/2C^2\}$. The sites z_i^c are equally spaced with the distance n^{-1} and the variational parameter C is defined by VMC optimization. For the simulation at high density we keep the same type of two-body term f_2 as on the liquid-like side of the crossover, although the values of optimal parameters may differ.

In Fig.1 we show the comparison of the VMC energy of the liquid-like and solid-like wavefunctions in the

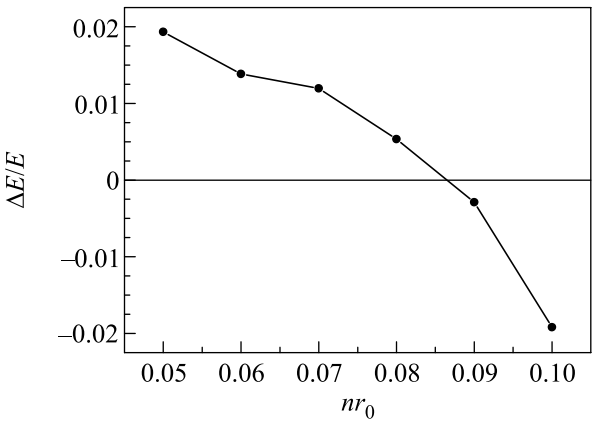

Fig.1. Difference between energy calculated using liquid-like and solid-like wavefunctions $(E_{\text{solid}} - E_{\text{liquid}})/E$ as a function of the dimensionless density

$nr_0 = 0.01 - 0.1$ density range. In this region the optimal parameters are $A = 1.6$, $B = 0.4$, $C = 1.16$. We discover that for densities smaller than $n_c \approx 0.085r_0^{-1}$ the liquid-like wavefunction description is energetically favorable, although at larger densities the ground state of the system is better described by a solid-like *ansatz*. On the contrary to 3D and 2D liquid-solid phase transitions, the energetic difference in 1D system is very small.

This suggests that the transition in a 1D system at zero temperature is of a crossover type.

At a very small density one expects that: 1) in the process of two-body collisions particles always get reflected back due to the repulsive interaction which is very intense at short distances, 2) particles stay far apart most of the time, so that the potential energy of the interaction is small compared to the kinetic energy. From above it follows that the system is equivalent to a gas of impenetrable bosons (Tonks–Girardeau gas). It was shown in [20] that the wave function of such a Bose system can be mapped onto the wave function of a system of non-interacting spinless *fermions*. The bosonic system acquires many fermion-like properties (fermionization): the energy is the Fermi energy $E^{TG}/N = \mathcal{E}_0\pi^2(nr_0)^2/6$, and the pair distribution function exhibits Friedel-like oscillations $g_2^{TG}(z) = 1 - \sin^2(\pi nz)/(\pi nz)^2$.

We present the dependence of the energy per particle on the density in Fig.2. At small density $nr_0 \ll 1$ the energy is the same as that of the Tonks-Girardeau gas E^{TG},

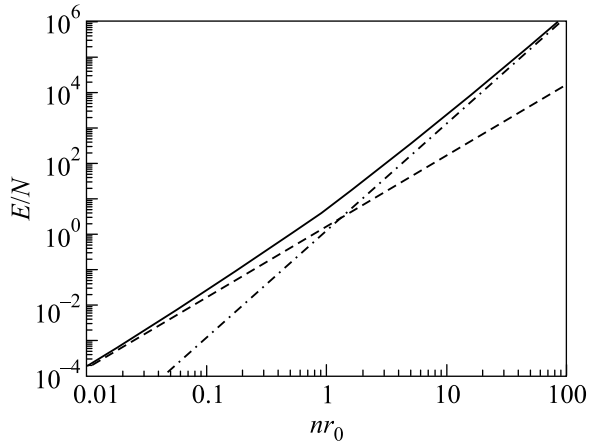

Fig.2. Energy per particle as a function of the dimensionless density (solid line), energy E^{TG} of the Tonks–Girardeau limit (dashed line), potential energy in the strongly interacting limit (dash-dotted line). Everything is measured in units of $\hbar^2/mr_0^2$

which signals fermionization of the system in this regime. At large density the particles are localized at lattice sites with the potential energy $E^{\text{str.int.}}/N = \mathcal{E}_0\zeta(3)(nr_0)^3$ being dominant. In this regime the density dependence of the energy is very strong. Indeed it is cubic, in contrast to the linear dependence on the mean field for the pseudopotential interaction and the quadratic dependence for an exactly solvable model with a $1/z^2$ interaction [22]. This strong dependence comes from the diverging short-range behavior of the dipole-dipole interaction. Although in 3D the dipole-dipole interaction is long-range, this is no longer true in the 1D case (see, for example, [23]) and no special techniques like Ewald summation are required.

We studied the dependence of the energy on the size of the system. The energy has two contributions: one coming from summation over pairs separated by a distance smaller than $L/2$ (this contribution is a direct output of the Monte Carlo calculation) and a tail energy, which is estimated by approximating the density at $L/2$ by the asymptotic bulk value. We find that the energy per particle as a function of the system size quickly saturates to its thermodynamic value and the results obtained for $N = 50, 100, 200$ particles agree within the statistical accuracy present in our calculation. We also find that the "tail energy" contribution is smaller than 0.2% of the total energy. All reported results are obtained using $N = 100$ particles.

The pair distribution function (Eq. (2)) is presented in Fig.3 for a range of densities covering all the regions

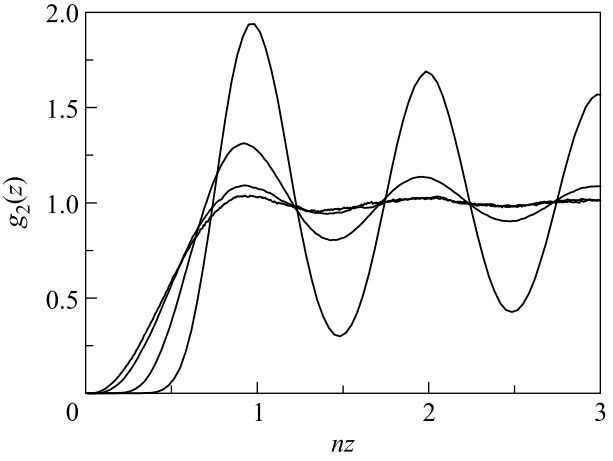

Fig.3. Pair distribution function (2) obtained from a DMC calculation for densities $nr_0 = 10^{-3}, 0.1, 1, 10$ (larger densities have higher peaks)

of interest. In a dilute system we find that amplitude of the oscillation decays rapidly which is characteristic for a liquid. In particular, at the density $nr_0 = 10^{-3}$ it is almost impossible to distinguish the pair distribution function from that of spinless fermions, which is in agreement with the arguments given above. By increasing the density the oscillation becomes more pronounced. Around the critical density $n_c r_0 \approx 0.08$ we enter the solid-like side of the crossover. Further, at larger densities $nr_0 = 1, 10$ we see manifestations of the localization of particles near lattice sites.

By performing the Fourier transformation (3) we obtain the static structure factor from the pair-distribution function. Knowledge of $S(k)$ is of high importance as

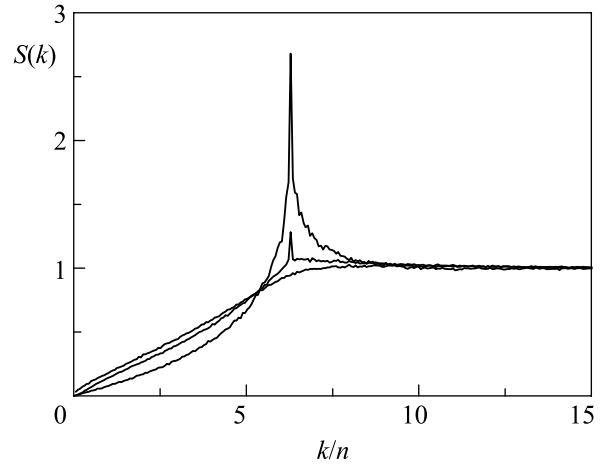

Fig.4. Static structure factor obtained from a DMC calculation for densities $nr_0 = 10^{-3}$, 0.1, 1. A higher first peak corresponds to a higher density

it can be accessed experimentally by using Bragg spectrometry. At small densities the low-momentum region has a linear form which is related to the speed of sound c by the Feynman relation $S(k) = \hbar|k|/2Mc$. In particular, in the Tonks–Girardeau limit the static structure factor takes an extremely simple form: the linear growth matches the asymptotic constant at the wave vector $|k| = 2\pi n$. Increasing the density leads to the formation of a peak structure. Presence of the peak in the $S(k)$ is a consequence of the dipole-dipole interaction, as the peak is absent in a system with only s-wave scattering [24]. In the regime of large density we see several peaks at integer multiples of $2\pi n$.

In order to test superfluidity of the system we use the winding-number technique [25]. The superfluid fraction is given by the ratio of the imaginary time diffusion constants of the center of mass and of a free particle [26]. In contrast to the calculation of the energy, here the symmetry of the trial wavefunction is crucial. We restore symmetry in the trial wavefunction in the solid-like region by performing a summation over all sites $f_1(z_i) = \sum_j \exp\{-[n(z_i - z_j^c)]^2/2C^2\}$. We see negligible differences in the energy (similarly to that found in ^{4}He simulations [27]) which justifies our previous choice of Ψ_T. We find that the system is superfluid on the liquid-like side of the crossover and is normal deep on the solid-like side.

We argue that the critical densities of the quantum crossover can be readily reached in experiments with interacting indirect excitons in two quantum wires. Let us take the GaAs parameters ($\varepsilon = 12.5$, electronic mass $m_e = 0.07m_0$, hole mass $m_h = 0.15m_0$, with m_0 being the free electron's mass) for reference. Then the mass of an exciton is $0.22m_0$. Using quantum wires with a separation between their axes, D, equal to 5 nm, we obtain $r_0 \approx 10^{-6}$ cm and $\mathcal{E}_0 \approx 3$ meV. Then the dimensionless density $nr_0 = 0.08 - 0.09$ corresponds to an achievable linear excitonic density $n \approx 10^5\,\mathrm{cm}^{-1}$. The liquid-like and solid-like regions and the crossover between them should be realized by changing the density of excitons in the quantum wires.

Interactions between chromium atoms can be efficiently tuned as proposed in [6]. Chromium has the advantage of having a large permanent magnetic moment when compared to the other alkali atoms. Research into achieving Bose-condensation in chromium is now a hot topic [1–4]. In permanent dipole chromium atoms the ratio between the strength C_{dd} of the dipole-dipole interaction and s-wave coupling constant is 0.27 for ^{52}Cr. Manipulation of induced electric dipoles is more difficult, although in such a system a ratio of the order of 10^2 can be reached leading to the realization of an almost pure dipole system.

In conclusion we have investigated the ground state properties of a system of dipole moments by means of a quantum Monte Carlo method. We have found the presence of a quantum crossover: at small linear densities nr_0 system stays liquid-like and superfluid, although in a more compressed system the solid-like description is energetically favorable. We have calculated the experimentally accessible pair distribution function and the static structure factor for a wide range of densities. In the dilute limit this Bosonic system becomes similar to a system of spinless fermions (fermionization) and the properties of the system are those of a Tonks–Girardeau gas. On the liquid-like side of the crossover the system is superfluid, although it is normal deep on the solid side.

Finally, we have pointed out that the critical density of the quantum crossover can be achieved in current experiments with interacting excitons in wires and have proposed the parameters of a possible experimental setup.

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