Ground state of low-dimensional dipolar gases: Linear and zigzag chains

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We study the ground-state phase diagram of ultracold dipolar gases in highly anisotropic traps. Starting from a one-dimensional geometry, by ramping down the transverse confinement along one direction, the gas reaches various planar distributions of dipoles. At large linear densities, when the dipolar gas exhibits a crystal-like phase, critical values of the transverse frequency exist below which the configuration exhibits transverse patterns. These critical values are found by means of a classical theory, and are in full agreement with classical Monte Carlo simulations. The study of the quantum system is performed numerically with Monte Carlo techniques and shows that the quantum fluctuations smoothen the transition and make it completely disappear in a gas phase. These predictions could be experimentally tested and would allow one to reveal the effect of zero-point motion on self-organized mesoscopic structures of matter waves, such as the transverse pattern of the zigzag chain.

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I. INTRODUCTION

Ultracold atoms and molecules are an attractive playground for studying fundamental properties of matter. Theoretical and experimental investigations pursue a fundamental understanding of the quantum dynamics of matter at ultralow temperatures and explore applications for quantum technologies, such as quantum metrology and information processing [1,2]. One relevant issue in this context is the realization and control of strongly correlated systems with cold atoms. In this respect, ultracold dipolar gases play an important role, as the nature of the dipolar interaction allows one to observe the interplay between quantum degeneracy and long-range forces. For this reason they are also interesting candidates for studying statistical theories of quantum long-range interacting systems [3]. Dipolar gases of ultracold atoms have been experimentally realized with chromium atoms [4,5]. In these experiments the strength of the s-wave scattering interaction is conveniently controlled by tuning the Feshbach resonance and can be made vanishing, thus leading to the realization of purely dipolar systems. Stability against collapse is warranted by polarizing the gas in a two-dimensional geometry, such that the dipolar interactions are purely repulsive [6,7].

Different phases of dipolar gases of atoms or polar molecules have been theoretically predicted as a function of density and dimensionality. In two dimensions, in the presence of periodic potentials the effect of long-range forces gives rise to the appearance of quantum phases [8]. In a bulk system, recent theoretical work predicted the creation of selforganized structures in two dimensions: the ground state may exhibit the typical features of a crystal or of a quantum fluid depending on the density [6,7]. In a one-dimensional geometry, Luttinger liquid models describe the long-range properties of dipolar gases at ultralow temperatures [9]. In this case, by tuning the density, the phase of the gas undergoes a crossover from a Tonks-Girardeau gas to a crystal-like phase [10]. The effect of transverse quantum correlations in twodimensional and one-dimensional systems, arising from the long-range dipolar force, have been analyzed in stacks of pancake traps [11] and in planar arrays of one-dimensional tubes [12]. Quasiordered systems of polar molecules in one and two dimensions have been recently considered for quantum information processing [13,14].

One-dimensional systems can be experimentally realized with highly anisotropic traps [15,16]. Classically, trapped ultracold dipolar systems may exhibit long-range order in one dimension at vanishing temperatures, such that the equilibrium configuration is solely determined by the interplay between the classical repulsive potential and the external confinement. In the quantum regime the effect of zero-point motion is expected to modify substantially the crystalline properties. This situation must be compared with trapped ultracold ions, interacting via Coulomb repulsion, where structural phase transitions in self-organized structures have been extensively studied [16,17]. Here, the effects of quantum degeneracy [18] are negligible in typical experimental setups [19], and the structures at experimentally accessible low temperatures are essentially determined by the classical potential.

In this paper we study theoretically the competition of long-range interactions and quantum fluctuations in the transverse stability of a one-dimensional ultracold dipolar gas in a highly anisotropic trap. We determine the properties of the quantum ground state using quantum Monte Carlo methods. In particular, we analyze transverse correlations in the parameter regime in which the gas is in the quasiordered phase, and where the one-dimensional structure is unstable with respect to increasing the atomic density and/or to reducing the transverse potential. We see that transverse patterns are formed, giving rise to mesoscopic quantum structures, where the transverse density distribution exhibits first two peaks, and then, by further opening the trap, multiple peaks. Differing from ionic Coulomb crystals, here quantum fluctuations smoothen the transition from the single- to the double-peaked distribution. Nevertheless, we observe a relatively sharp transition to the various transverse structures for parameter regimes, which can be identified by means of a classical theory.

This work is organized as follows. In Sec. II we introduce the theoretical model for a two-dimensional gas of dipolar bosons in the presence of tight transverse confinement and identify the relevant length scales. In Sec. III we discuss the phase diagram of the system, which we obtain using full quantum numerical simulations; we identify the parameter regime where the linear-zigzag chain transition could be observed. In Sec. IV the conclusions are drawn.

II. THEORETICAL MODEL

We consider a system of ultracold bosons (atoms or polar molecules) of mass m possessing large dipole moments, which are confined in the x-y plane, while their dipolar moments are aligned perpendicularly to the plane by an external field. In this limit the interaction is the repulsive dipolar potential

$$V(\rho) = \frac{C_{dd}}{4 \pi |\boldsymbol{\rho}|^3},$$

where ρ is the polar coordinate on the plane and C_{dd} denotes the dipolar interaction strength. Here, s-wave scattering is neglected, assuming that it vanishes due to a properly tuned Feshbach resonance (see, for instance, Ref. [5]). The gas is assumed to be homogeneous along the x direction, where it is characterized by the linear density n, and it is confined along the y direction by a harmonic potential of frequency ν_t . This external potential sets the characteristic length

$$a_{ho} = \sqrt{\frac{\hbar}{m\nu_t}},$$

determining the transverse size of the single-particle wave packet, and which we choose as unit length. Denoting by $\mathbf{\varrho}_j = \mathbf{\rho}_j/a_{ho} = (\widetilde{x}_j, \widetilde{y}_j)$ the rescaled coordinates, the corresponding dimensionless Hamiltonian $\widetilde{H} = H/\hbar \nu_t$ reads

$$\widetilde{H} = \frac{1}{2} \sum_{j} \left(-\frac{\partial^{2}}{\partial \widetilde{x}_{j}^{2}} - \frac{\partial^{2}}{\partial \widetilde{y}_{j}^{2}} + \widetilde{y}_{j}^{2} + \sum_{i \neq j} \frac{\widetilde{r}_{0}}{|\boldsymbol{\varrho}_{i} - \boldsymbol{\varrho}_{j}|^{3}} \right), \tag{1}$$

where the parameter $\tilde{r}_0 = r_0/a_{ho}$ is the characteristic length of quantum coherence in dipolar gases,

$$r_0 = \frac{mC_{dd}}{4\pi\hbar^2},$$

in units of a_{ho} .

The effective one-dimensional Hamiltonian is recovered from Eq. (1) when the chemical potential μ is much smaller than the level spacing of the transverse oscillator, $\mu \ll \hbar \nu_t$. In the quasiordered phase, for $nr_0 \gg 1$, this corresponds to the inequality $E_{\rm cr}^{({\rm 1D})}/N \ll \hbar \nu_t$, where $E_{\rm cr}^{({\rm 1D})} = N(nr_0)^3 \zeta(3)\hbar^2/(mr_0^2)$ is the potential energy of a classical crystal [10], and which leads to the relation $n \ll r_0^{-1/3}$. In the quantum gas regime, for $nr_0 \ll 1$, the gas is essentially described by a Tonks-Girardeau gas [20] and the condition to be fulfilled is $E_{\rm TG}^{({\rm 1D})}/N = \pi^2 \hbar^2 n^2/(6m) \ll \hbar \nu_t$, which is equivalent to the requirement $na_{ho} \ll 1$. The expression for $E_{\rm TG}^{({\rm 1D})}/N$ does not depend on the strength of the dipolar interaction, as the interparticle distance is large and the potential interaction can be neglected.

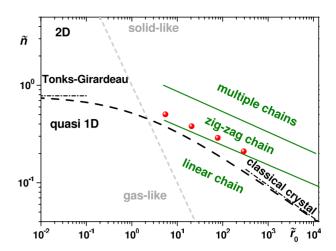


FIG. 1. (Color online) Phase diagram as a function of the parameters \tilde{r}_0 and \tilde{n} . The dashed black line corresponds to the curve $E^{1D}/N=\hbar\nu_t$ and identifies the two regimes, where the dynamics is essentially one or two dimensional. The Tonks-Girardeau and the classical crystal limits are explicitly indicated in the plot (dashed-dotted lines). The short-dashed gray line, at $\tilde{n}\tilde{r}_0=1$, localizes the crossover between gas- and solidlike phases. The green solid lines separate different phases (linear, zigzag, multiple chain) in the classical system. The red circles are the results of quantum Monte Carlo calculations and correspond to the appearance of a double-peak structure in the radial density profile (see the text and Fig. 4). The size of the symbols denotes the error bars.

For later convenience, we introduce the rescaled density

$$\tilde{n} = na_{ho}$$

such that when $\widetilde{nr_0} \gg 1$ the system is in the quasiordered phase, while for $\widetilde{n} \ll 1$ it is a Tonks-Girardeau gas.

III. PHASE DIAGRAM

Using the criteria in Sec. II, we can identify different phases of the ground state of the dipolar system in a phase diagram with axes \tilde{r}_0 and \tilde{n} , and which is reported in Fig. 1. Here, the black dashed line corresponds to the curve $E^{(1\mathrm{D})}/N=\hbar \nu_{t}$, where the energy per particle of the onedimensional dipolar gas, given in [10], is equal to the level spacing of the transverse confinement $\hbar \nu_t$. This line separates the two regimes, where the dynamics is essentially one or two dimensional. The short-dashed line corresponds to the curve $\widetilde{n}\widetilde{r}_0 = 1$, which separates the gas from the quasiordered phase. These lines are to be intended as indicators, the transition of the gas from one phase to another (from onedimensional to two-dimensional; from gas to quasiordered phases) being a crossover. The behavior deep below the black dashed line of this phase diagram has been studied in Ref. [9], where it was shown that the dipolar system is essentially a Luttinger liquid with Luttinger parameter K < 1. Although there is only one phase as the thermodynamic functions are continuous, nevertheless signatures of quasiorder, due to the dipolar interactions, can be identified in the energy and in the structure form factor [10].

A. Classical theory at T=0

We now focus on the quasiordered regime, where $\widetilde{nr_0} > 1$, and first study the dipolar structure by discarding the kinetic term in the Hamiltonian (1). We stress that this approach gives only a qualitative description, as long-range order cannot exist in one dimension at finite temperatures in a dipolar gas, nor at T=0 in a quantum dipolar gas. The predictions of this classical model are expected to be valid in the asymptotic limit $\widetilde{nr_0} \rightarrow \infty$ of a quantum system. Keeping this in mind, we assume that the dipoles are located along the x axis with interparticle distance a=1/n, such that their dimensionless equilibrium positions are $\widetilde{x_j} = j/\widetilde{n}$ and $y_j = 0$. The stability of this configuration requires the linear density being smaller than a critical value, $\widetilde{n} < \widetilde{n_c}$, where

$$\widetilde{n}_c = \mathcal{E}(\widetilde{r}_0)^{-1/5}$$
,

and hence depends on the trap frequency ν_t , while $\mathcal{E} = \{8/[93\zeta(5)]\}^{1/5} = 0.6078...$ is a constant. For $\tilde{n} > \tilde{n}_c$ the equilibrium positions are distributed in different planar structures, depending on the value of \tilde{n} . The first structure encountered is a zigzag configuration, where now $\tilde{y}_j = (-1)^j b/2$ with b fulfilling the equation

$$\sum_{k=0}^{\infty} \mathcal{F}_k b^{2k} = \frac{1}{12(\tilde{n}\tilde{r}_0)\tilde{n}^4},$$

$$\mathcal{F}_k = \frac{\Gamma(-3/2)\zeta(5+2k)(1-2^{-5-2k})}{\Gamma(1+k)\Gamma(-3/2-k)}\tilde{n}^{2k}.$$
 (2)

These equations are found by evaluating the stable equilibrium points of the potential in Eq. (1) [17]. The expression for the displacement from the axis of the chain close to the critical value \tilde{n}_c reduces to the expression

$$b \simeq \frac{\mathcal{B}}{\tilde{n}_c} \sqrt{1 - \left(\frac{\tilde{n}_c}{\tilde{n}}\right)^5}, \quad \mathcal{B} = \sqrt{\frac{8}{5}} \frac{31\zeta(5)}{127\zeta(7)}, \tag{3}$$

which provides the critical exponent of the parameter b for the classical phase transition. At larger values of n the system exhibits abrupt transitions to more complex structures. Similar behaviors are also observed in one-dimensional Wigner crystals [16,21]. Figure 2 displays the transverse width of the chain $\sqrt{\langle y^2 \rangle}$ as a function of \tilde{n} obtained with a classical Monte Carlo simulation, while the solid line is the solution of Eq. (2). The critical value at which the classical second-order phase transition occurs is indicated by an arrow. The critical parameters for the linear phase transition in a classical system are shown in Fig. 1 as straight solid lines.

Thermal and quantum fluctuations modify this behavior, thereby affecting the form of transverse correlations as a function of the linear density or of the transverse frequency ν_t . Their effect is analyzed below by means of numerical techniques.

B. Numerical methods

We resort to Monte Carlo techniques to study numerically the properties of the dipolar many-body system. The classi-

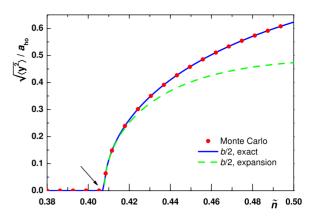


FIG. 2. (Color online) Radial width $\sqrt{\langle y^2 \rangle}/a_{ho}$ as a function of \tilde{n} for the classical dipolar gas at T=0 and $\tilde{n}\tilde{r}_0=3$ close to linear-zigzag transition. The solid line corresponds to the solution of Eq. (2), which describes the transition from a linear chain to a zigzag configuration, the symbols to the results of a classical Monte Carlo simulation, the dashed line is an expansion close to transition point, Eq. (3), and the arrow shows the transition point.

cal (CLS) system at finite temperatures is studied by means of a classical Monte Carlo calculation, where we sample the Boltzmann distribution $p_{CLS} = \exp\{-E/k_BT\}$ by using the Metropolis algorithm. The quantum ground-state properties are determined by means of variational and diffusion Monte Carlo methods [22]. The trial wave function is chosen in a Bijl-Jastrow form

$$\psi_T(\boldsymbol{\rho}_1, \dots, \boldsymbol{\rho}_N) = \prod_{i=1}^N f_1(\boldsymbol{\rho}_i) \prod_{i=k}^N f_2(|\boldsymbol{\rho}_i - \boldsymbol{\rho}_k|), \qquad (4)$$

where the one-body term is $f_1(\rho) = \exp\{-\alpha y^2/a_{ho}^2\}$. If the system is in the quasi-one-dimensional regime, where the transverse oscillator is in the ground state, the variational parameter is the same as for the ground state of the harmonic oscillator, $\alpha = 1/2$. Outside the quasi-one-dimensional regime, the system spreads in the radial direction and accordingly the value of α is reduced. The two-body term is chosen as in Ref. [6],

$$f_{2}(\boldsymbol{\rho}) = \begin{cases} C_{1}K_{0}(2\sqrt{r_{0}/|\boldsymbol{\rho}|}), & 0 < |\boldsymbol{\rho}| < R_{par} \\ C_{2} \exp\left\{-\frac{C_{3}}{|\boldsymbol{\rho}|} - \frac{C_{3}}{L_{x} - |\boldsymbol{\rho}|}\right\}, & R_{par} \leq |\boldsymbol{\rho}| < L_{x}/2 \\ 1, & L_{x}/2 \leq |\boldsymbol{\rho}|, \end{cases}$$

$$(5)$$

where $K_0(|\boldsymbol{\rho}|)$ is the modified Bessel function of the second kind, and coefficients C_1, C_2, C_3 are fixed by the conditions of the continuity of the wave function and its first derivative. The parameter R_{par} is free; it varies in the interval $0 < R_{par} < L_x/2$ and is optimized by a variational procedure. When the distance between two particles is small, the influence of other particles can be neglected and $f_2(\rho)$ is well approximated by the solution of the two-body scattering problem [see the short distance behavior of Eq. (5)]. In this way the divergent behavior of the interaction potential does not cause any numerical instability. At large distances the two-body

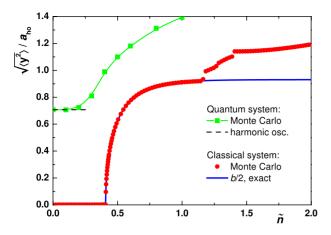


FIG. 3. (Color online) Radial width $\sqrt{\langle y^2 \rangle}/a_{ho}$ as a function of \widetilde{n} for $\widetilde{n}\widetilde{r}_0=3$ in the classical and quantum dipolar gases at T=0. Circles correspond to the results of a classical Monte Carlo simulation; the blue solid line corresponds to the solution of Eq. (2). For $\widetilde{n} < 1.2$ (i.e., for linear and zigzag configurations) both results coincide. A sudden transition to another, broader, planar structure is observed at larger values of $\widetilde{n} > 1.2$. Squares (the connecting line is drawn as a guide to the eye) correspond to the results of quantum Monte Carlo calculations; the dashed line corresponds to the radial width of the transverse harmonic oscillator, $\sqrt{\langle y^2 \rangle} = a_{ho}/\sqrt{2}$.

term is written in a symmetric way. This ensures that $f'(L_x/2)=0$ and periodic boundary conditions are properly satisfied.

The results of classical simulations are obtained using an annealing procedure. This means that the classical simulation is started at a large temperature, $k_BT/\hbar\nu_t\approx 1$, and then the temperature is gradually reduced to very small values, where the classical system is frozen. By starting the simulation at a high temperature one is able to explore more effectively the phase space and this helps to avoid the system finding a local minimum instead of a global one. We repeat the annealing procedure several times for each set of parameters \tilde{n} and \tilde{r}_0 , thus choosing the lowest energy.

C. Numerical results

In the quantum system we study the transition from a linear to a planar configuration by considering the radial spreading $\langle y^2 \rangle$ as a function of density and trap frequency. In particular, when the chain is in the ground state of the transverse harmonic oscillator, then $\langle y^2 \rangle = a_{ho}^2/2$, while it becomes larger as the transverse potential is excited. In Fig. 3 the radial spreading for the quantum-mechanical case is shown as a function of \tilde{n} and compared with the classical result at T=0. Quantum fluctuations clearly smoothen the transition, and in particular, introduce a basic uncertainty related to the oscillator length a_{ho} . Similarly, the transition is smoothened in the classical system at finite temperatures. It is interesting to notice that the second value, at which one observes another discontinuity of the classical radial spreading, is a transition to multiple chains and it is expected to be of first order [21]. The quantum-mechanical behavior at this point will be the object of future studies. The results of the quantum MC simulations correspond to the circles in Fig. 1 and have been

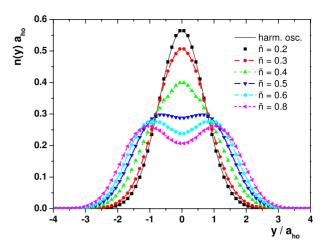


FIG. 4. (Color online) Radial density profile n(y) for fixed $\widetilde{nr_0}$ = 3 and at \widetilde{n} =0.2,0.4,0.5,0.6,0.8 (decreasing the height at y=0). This choice of the parameters corresponds to effectively changing the frequency of the harmonic confinement. The radial confinement is normalized to unity, $\int_{-\infty}^{\infty} n(y) dy$ =1. The solid line corresponds to the single-particle wave packet of the transverse harmonic oscillator and is plotted for comparison. For these parameters, the value at which the classical phase transition occurs is $\widetilde{n}_c \approx 0.408$.

determined by the critical value of the parameters for which two maxima are formed in the radial density profile. We note that the position of the transition in a quantum system is close to the predictions of a classical theory with the agreement being even better as \tilde{r}_0 is increased. Oppositely, for small values of \tilde{r}_0 the two-peak structure, characteristic for a zigzag chain, disappears due to an increased role of quantum fluctuations and the crystal gets completely melted.

Figure 4 displays the radial density profile at fixed nr_0 for various values of \tilde{n} , which are distributed across the value \tilde{n}_c =0.408... at which the classical phase transition linearzigzag occurs for the chosen value of nr_0 . For $\tilde{n} < \tilde{n}_c$ the radial density profile is a single-peaked curve, a Gaussian of width a_{ho} , centered at y=0. This is the situation we expect for the quantum linear chain. For $\tilde{n} > \tilde{n}_c$, the density distribution becomes double peaked, the peaks being symmetrical about y=0. The density in the center is, however, significantly different from zero: this effect originates from zeropoint quantum fluctuations, which prevent the particles from being localized at the minima of the potential energy, which for $\tilde{n} > \tilde{n}_c$ is a double-well potential. At larger values of nr_0 , nevertheless, one recovers the expected zigzag configuration for values of \tilde{n} closer to \tilde{n}_c : in this regime the size of zigzag spreading is comparable to the oscillator length. The size of the region, where quantum fluctuations are relevant, shrinks as the interaction strength, here represented by the parameter \tilde{r}_0 , is increased. These planar structures are of mesoscopic nature as the number of chains is small. Here, the radial density profile cannot be described by the local density approximation, which, instead, is generally applicable in a macroscopic system. Figure 5 displays characteristic examples of the pair-correlation function, showing that for sufficiently large values of the interaction a zigzag distribution of dipoles is observed.

Thermal fluctuations in the classical systems give rise to a qualitatively similar behavior. The curves here obtained for

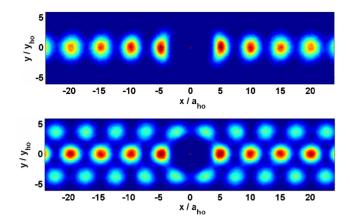


FIG. 5. (Color online) Two-dimensional contour plot of a pair distribution function $\langle n(\mathbf{0})n(x,y)\rangle$ in a quantum system for a fixed value of one-dimensional density $\widetilde{n}\widetilde{r}_0$ =40. Bright colors correspond to high values of the pair distribution function. Upper plot, \widetilde{r}_0 =100 (linear chain); lower plot, \widetilde{r}_0 =200 (zigzag chain).

the quantum system are qualitatively reproduced by using a classical system at the effective temperature $T_{\rm eff} = \hbar \nu_t / 2 \kappa_B$.

D. Discussion

The phase diagram in Fig. 1 can be experimentally explored by changing the density \tilde{n} , thereby moving vertically, and by varying the transverse frequency ν_t , thereby moving parallel to the straight short-dashed line. Typical parameters of 1D experiments [15], with $a_{ho} \approx 35$ nm and 60–400 atoms per tube of length 15–50 μ m, are $\tilde{r}_0 \approx 0.07$, $\tilde{n} \approx 0.04-0.3$. While ⁵²Cr has the largest value of r_0 =2.4 nm among all atom species with which condensation has been reached [5], the use of polar molecules such as CO, ND₃, HCN, and CsCl with r_0 =5 nm-340 μ m would permit one to cover regions of the phase diagram up to the classical region ($\tilde{n}\tilde{r}_0 \gg 1$).

The formation of the zigzag structure can be experimentally revealed in the structure form factor. The latter, in fact, exhibits an additional peak at the y component of the wave vector $k_y=2\pi/b$, where b is the distance between the two chains forming the zigzag structure.

An important question is whether the system under consideration is superfluid or not. The problem of superfluidity is very delicate when treating (quasi-) one-dimensional systems. While different definitions of the superfluidity coincide in homogeneous two- and three-dimensional systems, they lead to contradictive conclusions when applied to a one-dimensional system. Indeed, the excitation spectrum of one-dimensional Luttinger liquids touches zero for a nonzero value of momentum, $k=2\pi n$. Thus, such systems are always normal from the point of view of the Landau criterion. Alternatively, one can use the winding number technique [24] to calculate the superfluid fraction. Applied to the exactly known ground-state wave function (for example, the Calogero-Sutherland system) it predicts a completely super-

fluid system. In the mean-field limit a system with short-range interactions is well described by the Gross-Pitaevskii equation. It is natural to think that in this regime, where the description of a pure condensate applies, the system is superfluid.

A possible way out, proposed in Ref. [25], is based on the calculation of the energy dissipation caused by dragging a small probe through the system. The conclusion is that there is always some dissipation, which ranges from negligibly small (in the Gross-Pitaevskii limit) to the same as in a normal system (in the Tonks-Girardeau limit). There is a continuous crossover from a (quasi)superfluid to a normal system. In our case, the limit of small density $\tilde{n} \rightarrow 0$ corresponds to the Tonks-Girardeau regime, where the system is normal. Indeed, in this regime the wave function of the system can be mapped onto a wave function of an ideal normal Fermi gas. At larger values of \tilde{n} the dipolar system corresponds to a Luttinger liquid with even stronger interactions than in the Tonks-Girardeau regime. As a result our system remains normal for all densities.

IV. CONCLUSIONS

To conclude, we have studied the ground state of a dipolar gas of bosons at T=0 in low dimensions starting from quasione-dimensional geometry and opening the radial trap, so that a two-dimensional structure develops. We do an analytical study of the system in the classical limit close to the transition to the zigzag configuration by applying Landau theory and compare these predictions with numerical simulations using classical Monte Carlo methods. We determine the phase diagram numerically using quantum Monte Carlo methods, and study in detail the effect of quantum fluctuations on the linear-zigzag transition. The transition from a one-dimensional to a planar configuration occurs with the creation of a mesoscopic structure in the transverse direction, which exhibits the main features of the transition from a single to a double and then a multiple chain distribution of dipoles, while quasiorder is observed also in the transverse pair correlation function at large densities. Such patterns are characterized by nonlocal correlations, which arise from zero-point fluctuations, and which may be important resources for the realization of quantum simulators [1,23]. Moreover, the control of atomic patterns has potential applications for nanostructuring processes [26].

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