The low-energy excitation spectrum of one-dimensional dipolar quantum gases

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We determine the excitation spectrum of a bosonic dipolar quantum gas in a one-dimensional geometry, from the dynamical density-density correlation functions simulated by means of Reptation Quantum Monte Carlo techniques. The excitation energy is always vanishing at the first vector of the reciprocal lattice in the whole crossover from the liquid-like at low density to the quasi-ordered state at high density, demonstrating the absence of a roton minimum. Gaps at higher reciprocal lattice vectors are seen to progressively close with increasing density, while the quantum state evolves into a quasi-periodic structure. The simulational data together with the uncertainty-principle inequality also provide a rigorous proof of the absence of long-range order in such a super-strongly correlated system. Our conclusions confirm that the dipolar gas is in a Luttinger-liquid state, significantly affected by the dynamical correlations. The connection with ongoing experiments is also discussed.

Introduction.- Ultracold quantum gases with dipolar interactions are currently being produced in laboratory, where atomic $^{52}$Cr atoms have been Bose-condensed [1, 2], following earlier theoretical predictions [3, 4]. Experiments have been suggested [5, 6] aimed to produce molecular gases with large dipolar strengths, and a few laboratories worldwide are working along these lines. In fact, dipolar quantum gases are emerging as competitive realizations of quantum devices [6] and as a laboratory for investigating strongly correlated regimes [7, 8] and novel quantum phases [9, 10], in which quantum fluctuations dominate. When applied to specific systems, the inequality may allow to rule out the existence of long-range order, as in the case of, e.g., 1D antiferromagnets and crystals [22]. Both questions above would have a definite answer if the system were in a Luttinger-liquid state, for which there is no long-range order nor roton minimum.

In this Brief Report, we find that this is indeed the case, after computing by RQMC the low-energy excitation spectrum up to eight reciprocal lattice vectors $G_m/n = 2\pi m$ in the whole crossover. The evolution of quasi-long-range order from the TG to the DDW state emerges as a progressive closing of the gaps in the excitation spectrum with increasing the order $m$. By the same token, we demonstrate the absence of a roton minimum at $2\pi$ in the whole crossover and that dynamical effects play a significant role in building the Luttinger state. Our results, analyzed by means of the uncertainty-principle inequality [22], also confirm that the 1D dipolar gas is in a Luttinger-liquid state.
The model and the RQMC method. We model the 1D dipolar Bose gas by considering $N$ atoms with mass $M$ and permanent dipoles moments arranged along and orthogonal to a line, yielding purely repulsive interactions. The Hamiltonian is

$$H = -\frac{1}{r_s^2} \sum_i \frac{\partial^2}{\partial x_i^2} + \frac{1}{r_s^3} \sum_{i<j} \frac{1}{|x_i - x_j|^3},$$

in effective Rydberg units $Ry^* = \hbar^2/(2Mr_s^2)$. The effective Bohr radius $r_0 \equiv MC_{dd}/(2\pi\hbar^2)$ is expressed in terms of the interaction strength $C_{dd} = \mu_0/2$ for magnetic and $C_{dd} = d^2/\epsilon_0$ for electric dipoles [31]. The dimensionless parameter $r_s = 1/(nr_0)$ determines the interacting regime in terms of $r_0$ and of the linear density $n$. Since the potential-to-kinetic energy ratio scales as $1/r_s = nr_0$, large densities yield to strong correlations, at variance with Coulomb systems.

We determine the ground-state properties and the excitation spectrum by resorting to the Reptation Quantum Monte Carlo technique [20]. This is in essence a path-integral method at zero temperature, where the ground-state distribution is directly sampled in the internal part of the path. Thus, the computation of the structure of the fluid and of the imaginary-time correlation functions for suitable long projection times is conceptually straightforward and practically easy, since possible biases arising from mixed averages are ruled out by definition. In particular, from an analysis of the imaginary-time density-density correlation function we determine the low-energy excitation spectrum while the parameter $nr_0$ spans the whole crossover from the TG to the DDW state.

We use a trial wave-function that is a product of two-body Jastrow factors $\psi_{\text{trial}} = \prod_{i<j} e^{u(|z_i - z_j|)}$. As we are interested in long-range behavior, we actually take the Luttinger-liquid expression

$$\psi_{\text{trial}}(R) \propto \prod_{i<j} \sin(\frac{\pi}{K} (x_i - x_j))^{1/K},$$

which in the low-density limit implies $K = 1$ [2] and recovers the wave-function of spinless non-interacting fermions. Different choices of the wave functions, such as the product of gaussians centered on the lattice sites $R_m = nn^{-1}$, result into different time-step extrapolations, but eventually lead to negligible differences in the computation of the static and dynamic structure factors.

A few technical details are in order. We perform simulations for different values of the number $N$ of bosons in a square box with periodic boundary conditions, namely $N = 40, 60, 80, 100$, reaching in selected cases $N = 200$. We check that we are able to take care of finite-size effects by summing the interactions over ten simulation boxes. Finally, the energies are extrapolated to their thermodynamic limit after removing the time-step dependence.

The resulting energy per particle $\epsilon(nr_0)/Ry^*$ as a function of $nr_0$ has been provided in [21, 25], together with an accurate analytical form of it, useful for further applications. We remark here that $\epsilon(nr_0)/Ry^*$ recovers the known limiting behaviors $\epsilon(nr_0)/Ry^* \sim (\pi^2/3)(nr_0)^2$ for $nr_0 \ll 1$ in the TG regime and $\epsilon(nr_0)/Ry^* \sim \zeta(3)(nr_0)^3$ for $nr_0 \gg 1$ in the DDW limit [4]. We set from now on units of $n^{-1}$ for lengths and of $Ry^*$ for energies.

Low energy excitations from dynamical structure factor. We determine the low-energy excitations after computing the imaginary-time correlation function of the density operator [26] $\rho_q = \sum_i \exp(-i\bar{q} \cdot r_i(\tau))$ creating a density fluctuation with wave vector $q$, that is $F(q, \tau) = \langle \rho_q(\tau)\rho_q^*(0) \rangle/N$, where the sum in $\rho_q$ spans over the number of particles $N$ located at position $r_i$ and $\tau$ is the imaginary time. $F(q, \tau)$ is related to the dynamical structure factor by $F(q, \tau) = \int_0^\infty d\omega \exp(-\omega \tau)S(q, \omega)$, yielding the static structure factor for $\tau = 0$, namely $S(q) = F(q, 0) = \int_0^\infty d\omega S(q, \omega)$.

To give a system overview, we first display the $S(q)$ in Fig. 1 as previously determined [2] by RQMC for various densities between the TG and DDW limits. Peaks at $q/n = 2\pi m$ ($m$ integer) progressively disappear with decreasing density as the dipolar gas approaches the spinless fermionic liquid.

We track this smooth evolution by investigating the low-energy excitations as extracted from the dynamical structure factor $S(q, \omega)$. From the expression

$$S(q, \omega) = \sum_n |\langle n|\rho_q|0\rangle|^2 \delta(\omega - \omega_n),$$

we estimate the energy dispersion of the collective excitations by fitting the imaginary-dependence of $F(q, \tau)$ as a sum of exponentials $\sum A_i(q)e^{\omega_i(q)\tau}$ corresponding to multiple modes. Then, the fit yielding the best $\chi^2$ value is chosen.

Fig. 2 displays the resulting RQMC energy dispersion $\omega(q)$, for the case with $N = 40$ at $nr_0 = 1, 10$ and 1000 namely in the low, intermediate and very high density regimes. In spite of the finite size effects, the overall qualitative behavior is already clear. The phonon softens at low $q$-values, while the density decreases. On the
Indeed, the Feynman relation is clearly seen to overestimate an upper bound to $\omega$ of a roton minimum. This is not the case if we use the $S(q/n)$ account for the $\omega$ lower bounds, requires an accurate size effect analysis. Dotted line: periodic replica of the first bump.

Other hand, the gap at $2\pi$ seems to be always closed at all densities. As represented in the inset by the dotted curve, even at $n \tau_0 = 1000$ the RQMC excitation spectrum (solid line) is very different from what could be obtained by replicating the portion from $q = 0$ to $q = 2\pi$ (dotted line), indicating a non periodic structure. The dashed line instead, represents $\omega(q)$ obtained from the Feynman relation $\omega(q) = \epsilon(q)/S(q)$, which provides only an upper bound to $\omega(q)$ in terms of the static structure factor $S(q)$ and of the kinetic energy $\epsilon(q) = \hbar^2 q^2/2m$. Indeed, the Feynman relation is clearly seen to overestimate the RQMC value for $q > 2\pi$, while it seems to account for the $\omega(q)$ between $q = 0$ and $q = 2\pi$. Considering that the Feynman relation is expected to yield better results as $q/n \to 0$, we can also anticipate that at lower densities the range where the Feynman relation is reliable will shrink (see below).

A quantitatively reliable measure of the gap sizes requires an accurate size effect analysis. Fig. 3 displays the $1/N$ scaling of $\omega(q/n = 2\pi)$ for $n \tau_0 = 0.01, 0.1, 1, 10$ and 1000. The fit to the RQMC data (symbols in the figure) yields the linear scaling $\omega_N(q = 2\pi) = c(n \tau_0)/N$ with the constant $c(n \tau_0)$ being an increasing function of $n \tau_0$. Thus, $\omega(q/n = 2\pi) \to 0$ as $1/N \to 0$, the gap is clearly closed at all densities, demonstrating the absence of a roton minimum. This is not the case if we use the Feynman relation, corresponding to a single-mode approximation in Eq. 3. At the intermediate-to-low density $n \tau_0 = 1$ the fit yields a finite gap value (see the inset). Since the Feynman relation is built up from static quantities, we may conclude that dynamical effects, as embodied in the multimode analysis of 3 play a significant role, leading to qualitatively different conclusions. A similar multimode analysis performed at $q = 2m\pi$, $m > 2$ shows the existence of open gaps, which progressively close while the quasi-ordered state is approached.

Absence of long-range order.- Using these results, we can derive a strict upper bound for the order parameter of the solid $\rho \equiv N^{-1}(\sum_m \exp(i \vec{G} \cdot \vec{r}_m))$ with $\vec{G}$ a vector of the reciprocal lattice, and rigorously test the qualitative conclusions from the inset of Fig. 2, namely that no long-range order may exist in our 1D dipolar quantum gas. We closely follow the derivation of Pitaevskii and Stringari 22. By applying the uncertainty-principle inequality $\langle A^\dagger A \rangle \langle B^\dagger B \rangle \leq \langle (A^\dagger B) (A B^\dagger) \rangle^2$ to the operators $A = \hat{\rho}_{\vec{q}+\vec{G}}$ and $B = \hat{\rho}_{\vec{q}}/\partial t$ one has $S(q + G) \int d\omega \omega^2 S(q, \omega) \geq \frac{1}{4\pi^2} \rho_{\vec{q} + \vec{G}}^2(q + G^2)$. From the RQMC data we know that as $q \to 0$, $S(q + \vec{G}) \to |q|^{2K-1}$, while the second moment of $S(q, \omega)$ vanishes as $|q|^{3K-1}$. Thus, the order parameter in the long wavelength limit vanishes as $\rho_{\vec{G}}^2 \leq q_{\text{min}}^{3K-1}$ with $K \geq 0$. Thus no long-ranger order may exist unless $K = 0$, which is however the limit of infinite density.

Dynamical response function and Luttinger-liquid analysis.- These results can be analyzed within the...
Luttinger-liquid theory. We want to calculate the imaginary-time \( \tau \) correlation function \( \tilde{F}(x, \tau) = \langle T_x e^{i\phi(x, \tau)} e^{-i\phi(0, 0)} \rangle \), on a finite size system of length \( L \). It is known [16] from bosonization that \( \tilde{F}(x, \tau) = (\pi \alpha/L)^2 K / \left[ \sin^2 \left( \frac{\pi}{2} \frac{x}{L} \right) + \sin^2 \left( \frac{\pi}{2} \frac{\tau}{L} \right) \right]^K \) valid in the long-time (low-energy) limit \( u \tau \gg \alpha \) where \( \alpha \) is a short-distance cutoff of the order of \( n^{-1} \), \( u \) is the velocity of the excitations and \( K \) the Luttinger exponent. After Fourier transforming \( \tilde{F}(x, \tau) \) in \( q \)-space with \( q = 2\pi j/L \), we get:

\[
F(q, \tau) = \left( \frac{\pi \alpha}{L} \right)^{2K} L 2^{2K+1-j} e^{-\frac{4\pi u}{\pi} (K+j)} \left( 1 + e^{-\frac{2\pi q}{\pi} \alpha} K^j \right) \\
\left[ \Gamma(j+K) \left| \Gamma(K+j+1)^{-1} \right. \right. _2 F_1 \left( K+j, K+j+1; e^{-\frac{2\pi q}{\pi} \alpha} \right) \right]
\]

where \( _2 F_1 \) and \( \Gamma \) are the Hypergeometric and Euler functions.

Using an Ansatz \( e^{-\tau \omega(q)} \) to fit the long-time behavior \( F(q, \tau \to \infty) \sim e^{-\frac{4\pi u}{\pi} (K+j)} \) we get \( \omega(q) = 2\pi u K/L + u 2 \pi j \), where we have used the even parity of the response function. Thus, there should be no roton gap at \( q = 2\pi \) in the infinite size limit. For finite size, an apparent roton gap (vanishing as \( 1/L \) in the infinite size limit). For finite size, an apparent roton gap (vanishing as \( 1/L \) in the infinite size limit). For finite size, an apparent roton gap (vanishing as \( 1/L \) in the infinite size limit).

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[30] By dipolar-density-wave we mean a quasi-ordered state very much analogous to a charge-density-wave.
[31] \( \mu_d \) and \( d \) are the magnetic and electric dipole moments.
and $\mu_0$ and $\epsilon_0$ are the vacuum permittivities.

[32] At fixed density, $1/N$ and $1/L$ scaling are equivalent.