Quantum phases of a one-dimensional dipolar Fermi gas

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We quantitatively obtain the quantum ground-state phases of a Fermi system with on-site and dipole-dipole interactions in one-dimensional lattice chain within density matrix renormalization group. We show, at a given spin polarization, the existence of six phases in the phase diagram and find that phases are highly dependent on the spin degree of freedom. These phases can be constructed using available experimental techniques.

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Introduction — Cold dipolar atom gases have attracted a lot of attention due to the novel anisotropic and long-range character of dipole-dipole interactions [1]. For high enough densities, the atomic de Broglie wavelength becomes larger than the typical inter-particle distance and thus quantum statistics governs the many-body dynamics of cold atom systems. Moreover, for strong fermion-fermion interactions, when the average interaction energy becomes larger than the corresponding kinetic energy, one can expect drastic changes of the properties of the system. Strong correlations are at the center of activity of various scientific disciplines such as optical, condensed matter physics, chemistry and quantum science ranging from high-temperature superconductivity [2], superfluidity (SF) [3], metal-insulator transition [4], Fulde-Ferrel-Larkin-Ovchinkov (FFLO) [5], orbital ordering and other certain structural phase transitions [6].

One of the current challenges of condensed matter physics is to understand the distinctive exotic paired states and quantum phases that are realized when particles have different on-site and long-range interactions. It has been predicted that in Bose lattice systems, the presence of finite interactions gives rise to novel quantum phases in two-dimensional [7] and one-dimensional (1D) [8] systems. A quantum phase diagram of a fermionic dipolar gas in a planar array of one-dimensional tubes has been studied [9] and the elementary excitations and the Luttinger components for various correlation functions were found. Unconventional SF in a two coupled fermionic chains has been proposed [10] in which an admixture of spin singlet and triplet SF pairings were occurred with purely repulsive interactions. The recent experimental investigations [11, 12] in creating degenerate cold polar molecules/atoms, rely on the dipole-dipole interaction and using the many internal degree of freedom in molecules to engineer effective spin-spin interactions offers promising orientations for exploring novel and strong correlated many-body physics. In this Letter, we employ the density matrix renormalization group (DMRG) [13], which is one of the sophisticated methods for investigating 1D many-body system, to study the phase diagram of 1D dipolar Fermi systems.

Numerical simulations based on DMRG have been used to investigate quantum phases of 1D Bose lattice [14] and no accurate phase diagram has been reported for 1D dipolar Fermi system so far. We find that paired states near the vanishing on-site energy of a quarter filling state (one fermion per two sites, $n = 1/2$) are significantly different from those paired states of a half filling state (one fermion per site, $n = 1$). The resulting phase diagram shows the existence of six phases, illustrated in Fig. 1 for the unpolarized case, have rich exotic phases of 1D dipolar Fermi gas. We explain below the whole states by computing at their ordered parameters and Luttinger exponents and showing that phase diagrams are different from those results obtained by the extended Hubbard model using constant interaction potentials. We also examine the phase diagrams at finite spin polarization and find that phases are sensitive to the spin degree of freedom.

Theory and Numerical results — The fermionic molecules/atoms interact with other fermionic molecules/atoms with an on-site Coulomb repulsion when two atoms occupy the same orbital. The Hamiltonian of such interacting ultracold atoms on a lattice is given by the Hubbard model [15] which serves as one of the most prominent models for a solid. The extended Hubbard model describing the low-energy physics of interacting dipolar spin-1/2 fermionic in a 1D lattice is given by

$$
H = -t \sum_{i,\sigma} (c_{i+1,\sigma}^\dagger c_{i,\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i,r>0} V_i \frac{n_{i\sigma} n_{i+r\sigma}}{r^3}
$$

where $c_{i\sigma}^\dagger$ stands for the creation operator with spin $\sigma$ at site $i$ and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the density operator. $t$ represents the transfer energy between the nearest-neighbor sites and $V_i = V$ is the strength of dipole-dipole interaction and it can change from a positive value to negative one depending on the direction of the interacting dipolar. This interaction, in general, has two important features; namely anisotropic and long-ranged, i.e. it decays...
FIG. 1. (Color online) DMRG phase diagrams of the fermion atoms with dipolar interactions in the unpolarized 1D lattice chain. At the half filling, (top panel) a quantum TSF phase occurs mainly for all $|U/t| < 2$ and $|V/t| < 0.5$ whereas SSF phase takes place for $|V/t| < 0.5$ and $U < -1.4t$. The BOW is located in a narrow strip between the SDW and CDW phases. The PS phase occurs for the region where $V/t < -0.75$ and the boundary disperses as a function of $U$. For the attractive dipolar interaction values, an inhomogeneous cluster type phase occurs. For the case at the quarter filling (bottom panel) rich quantum phases including CDF for $0.2 < V/t < 3$ and $-3.3t < U < 0$, a large region of the SSF phase for $U < 0$ and $V > 0$, SDF phase, SDW, and a large area of PS occur. In addition, TSF phase is located around small negative $V$ and $U > 0$ next to the SDF phase.

Like $1/r^3$ at large distances. Therefore, it is natural to expect intriguing properties in dipolar gas systems [16]. We accurately investigate the ground-states and phase diagrams of the system described by Eq. (1) at half and quarter fillings in terms of the positive and negative values of $U$ and $V$. The variation of $V$ corresponds to the change of the polarization direction with respect to the lattice orientation. Meanwhile, polar molecules are easily manipulated by external electric fields and thus their dipole moments can be tuned. The DMRG with open-end boundary conditions is employed to obtain the ground-state and low-lying excited-states energies and expectation values of order parameters in the thermodynamic limit, $L \to \infty$. Therefore, the finite-size scaling analysis based on the $L$ dependence of quantities are needed and we thus perform the finite-size scaling for all quantities.

To determine the phase diagrams shown in Fig. 1, several physical expectation values are calculated. We first obtain the charge and spin gaps as follows

$$\Delta_c = [E(N_{\uparrow} + 1, N_{\downarrow} + 1, S_z) + E(N_{\uparrow} - 1, N_{\downarrow} - 1, S_z) - 2E(N_{\uparrow}, N_{\downarrow}, S_z)]/2$$

$$\Delta_s = [E(N_{\uparrow} + 1, N_{\downarrow} - 1, S_z) + E(N_{\uparrow} + 1, N_{\downarrow} - 1, S_z)]$$

where $E(N_{\uparrow}, N_{\downarrow}, S_z)$ is the ground-state energy for a given number of atoms with spin-up (spin-down) $N_{\uparrow}$, $(N_{\downarrow})$ and total spin in the $z$ direction, $S_z$. The competition between the on-site and dipolar energies gives rise to the stable phase. At half filling, near bond order wave (BOW) phase [17] and charge density wave (CDW), which are insulating phases, the spin gap is suppressed and moreover the system is a Mott insulator phase with $2k_F$ spin density wave (SDW) for $V \leq U/2$. Therefore, we introduce local order parameters for these two gapful phases as $O_{CDW} = \sum_j (\hbar)^2 n_j$ and $O_{BOW} = \sum_j (\hbar)^2 (\bar{c}_{j\sigma}^c c_{j+1,\sigma} + h.c.)$. For the finite value of $<O_{CDW}> < O_{BOW}>$, a long-range order of the CDW(BOW) state appears. Notice that both charge and spin gaps are zero in a region near the $U = V = 0$. In this region, system is a gapless Luttinger liquid [18]. In the BOW phase with insulating gap nature of the Mott type, both charge and spin gaps are finite. The occurrence of the BOW phase for $2.5 \leq U/t \leq 6$ can be understood as the result of increasing frustration in the spin degree of freedom.

As $V$ increases, the charge fluctuations enhance and thus a transition from SDW to BOW occurs. The boundary is determined where the spin gap begins to develop. In order to specify the SDW-BOW critical point precisely, we examine the charge-charge and spin-spin correlation functions

$$S_{\pm}(\mathbf{q}) = \frac{1}{L} \sum_j \sum_{j'} e^{i\mathbf{q}(j-j')} \langle (n_{\uparrow,j} \pm n_{\downarrow,j})(n_{\uparrow,j'} \pm n_{\downarrow,j'}) \rangle$$

$$- \langle (n_{\uparrow,j} \pm n_{\downarrow,j}) \rangle \langle (n_{\uparrow,j'} \pm n_{\downarrow,j'}) \rangle$$

with $\mathbf{q} = 2\pi/L$. Following the Luttinger-liquid (LL) theory [18, 19], the long-wavelength behavior of the $S_{\pm}(\mathbf{q})$ is governed by the LL spin and charge exponents; $K_{\sigma,\pi} = \lim_{q\to0} S_{\pm}(\mathbf{q})/q$. $K_{\sigma}$ LL vanishes in the spin gapped phase, however $K_{\pi} = 1$ everywhere else in the thermodynamic limit. In the weak coupling regime, the metallic phase is a Luttinger liquid and it is still quite hypothetic to assume that this is the case for the model Hamiltonian (1). This assumption [20] is verified by calculating both the identity $2K_{\rho}/(\pi u_\rho) = n^2 \kappa$ where $u_\rho$ is the charge velocity and $\kappa$ is the charge compressibility. In addition, we also test the central charge value.
and evaluate it to be 1 within 2% error considering the dipole-dipole interaction. Moreover, the LL theory has been used for bosonic gases with repulsive power-law interactions. [21] Accordingly, the assumption is applicable in our system in the $\langle V, U \rangle$ space and we thus able to explore metallic phases within LL theory.

Another exciting phase in 1D system is a spin density fluctuation (SDF) where the spin and charge gaps vanish. In order to determine this phase, we compute the LL exponents [22] where the $K_\sigma \geq 4/m^2 \ (n = 2/m$ and $m = 2$ for half filling, for instance) whereas the $K_\rho \leq 4/m^2$. At the quarter filling, SDF having the $K_\rho \leq 1/4$ emerges in a wide region of the parameter space and furthermore a small area of SDW takes place for large $V$ and $U$. Meanwhile, there is a charge density fluctuation (CDF) phase in which the spin gap is finite and both the $K_\sigma$ and $K_\rho$ are smaller than unity. When $U \leq 0$ increases the spin gap opens whereas the charge gap remains zero for certain values of $V$ at the quarter filling. In other words, the ground state of the model is the CDF metal for a weak interacting fermion regime.

Another state is the phase separation (PS) and it occurs when the ground-state is inhomogeneous. PS means the possibility of the system to spontaneously undergo a macroscopic segregation into two phases with different hole concentrations. In the attractive interaction, a pair of the fermion atoms on the same site can not be broken because, it is costly from energy point of view. The unpaired fermion atoms, on the other hand, can move in the region located between pairs, but they can not be on the neighboring sites. In this phase, the charge gap is finite and $K_\rho < 4/m^2$. The simplest way to get a quantitative insight into the instability region is to calculate the compressibility. It turns out [23] that the compressibility of a homogenous Fermi gas becomes negative signalling the instability of the gas leading to a collapse. We calculate the compressibility

$$\kappa = \frac{L}{N^2} \left[ \frac{4}{E_0(N+2) + E_0(N-2) - 2E_0(N)} \right]$$

and thus its divergence illustrates the position of the PS transition. Our accurate calculations show that a wide regime of PS phase takes place at both the quarter and half filling phase with an attractive interaction potential.

**FFLO and SF phases** — The FFLO phase [5] has recently attracted a lot of interest from both experimental and theoretical groups [24] for spin polarized systems. To obtain the FFLO phase, the pairing operator $\Delta_i = \hat{c}_i \hat{c}_i^\dagger$ is no longer useless since a long-range order is forbidden in 1D. The correlation functions of the pairing operator

$$C_{ij} = \langle \Delta_i \Delta_j \rangle$$

for different values of the spin polarization, $\xi = (N_\uparrow - N_\downarrow)/N \ \text{where} \ N = N_\uparrow + N_\downarrow$ can be evaluated and our numerical results for the polarized system, $\xi \neq 0$, show that the pair correlation function decays with a power law $|l - l'|^{-1/K_\sigma}$ at large distances. As $\xi$ values increase, the power law of the correlation function transforms to an oscillation function in the large distances. For $V < 0$, the form of the function differs with respect to the $V > 0$. Moreover the pair correlation function increases by decreasing the $U$ values.

We investigate the oscillatory character of the pair correlation function by studying the Fourier transform of the function. Its Fourier transform is given by

$$G_{\text{pair}}(k) = \frac{1}{2L} \sum_{i,j} C_{ij} e^{ik(i-j)}$$

The peak of the pair momentum distribution (PMD) is the indication of a long-range order pair correlation in the system for the different $\xi$. The PMD can determine the limitation of SF or FFLO phase in the phase diagram. The PMD for different states and different interactions is illustrated in Fig. 2 at the half filling. We obtain a similar structure at the quarter filling. For $U < 0$ and $V > 0$ the PMD has a sharp peak that disappears in a certain value of the dipole-dipole interaction, $V_c$. The value of $V_c$ increases by increasing $U$. For $V < 0$, the PMD is a constant function in the Fourier space. The ground-state, for the unpolarized case, is the SF state characterized by a sharp peak centered at momentum $k = 0$ in the PMD $G_{\text{pair}}(k)$ (Fig. 2(a)). For $\xi \neq 0$, the ground-state
is a 1D FFLO state with $k \neq 0$ (Fig. 2(c)). Then the $k$ value can be understood as an order parameter of the FFLO phase. The momentum of the FFLO state $k_{FFLO}$, at which the $G_{pair}$ shows a strong peak, is $k_{FFLO} = \pi N \xi / L$. We notice that, in Fig. 2(d), the value of $k_{FFLO}$ remains constant for different interaction strengths but it increases when the filling of atoms increases to the half filling value. The PMD function for the quarter filling behaves like the half filling, however its tail as a function of the momentum is different.

The SF or FFLO phase in the fermionic system is the result of the condensation of the pairs of fermions. If the total spin of the pair is zero, the state of the two fermions will be a singlet state (SSF), however the two fermions maybe paired in a triplet state (TSF). Both the SSF and TSF extend to a wide range around $V = 0$ due to the presence of the correlated hopping term (see Fig. 1). For the case of the repulsive interaction, the system undergoes a quantum phase transition from the SF to an insulator state. This can be understood by noting that in the strongly interacting regime, density fluctuations become energetically costly and are therefore suppressed.

Our numerical results of the phase diagram at half filling and for $V > 0$, apart from BOW phase, are in good agreement with those results obtained by a bosonization theory in Ref. [25]. Moreover, results show that there is a discrepancy between quantum phases at half and quarter fillings due to the difference between the on-site and dipolar energies for different fillings. Noticeably, the phase diagrams shown in Fig. 1 are different from those results obtained by the extended Hubbard model [20, 26] due to the impact of the dipole-dipole interaction.

We examine the phase diagram at finite $\xi = 0.5 (N_\uparrow > N_\downarrow)$ and the results are illustrated in Fig. 3. Quantum TSF phase is similar to the case of $\xi = 0$ at half filling, however the SDW expands toward the negative $U$. A small BOW region has taken place for larger $U$ and $V$ values. The CDW is modifies by a mixed state of a combination of the CDW and narrow domains of a ferromagnetic state, since it is energetically favorable. Moreover, at quarter filling, rich quantum phases occur and the CDF expands in the larger $V$ values. These new features are originated from a competition between the on-site and the interaction energies for imbalanced particle densities.

Finally, the system at half filling phase and at fully polarized case is a ferromagnetic Heisenberg chain model, however there is a rich diagram phase at the quarter filling as it is shown in Fig. 4. To determine the phase diagram in this case, we calculate the $K_p$ ($=K_p$), the charge and spin gaps given by Eqs. (2) and (3). The value of $K_p$ is mostly smaller than unity for the range of $V$ values showed in Fig. 4(a). The CDF phase for which the hopping energy is dominated, is obtained by conditions in which $\Delta_c \neq 0$ however $\Delta_s = 0$. PS phase has taken place for the large attractive interaction energy with different hole concentrations. Here we also show the finite size scaling analysis for the $K_p$ at $V = 0$ and the results for every $V$ are extrapolated in $1/L$. The density profile of the different phases are shown in Fig. 4(b). The particle-hole density profile at the large attractive interaction potential is a constant value $n = 0.5$ at $V = 0$ and then emerges to the CDW at the large repulsive interaction potential.

**Conclusions** —We have determined with quite accuracy the ground-state phase diagrams of the fermion atoms with on-site and dipolar interactions in a 1D lattice at half and quarter filling within the extended Hubbard model by utilizing DMRG approach. The competition between the on-site energy, the dipole-dipole interaction and the hopping energy and besides their quantum fluctuations generates different exotic phases in the system. We have elaborated a paring phase in the large area of the repulsive interaction potential at the quarter filling.
We have shown, at a given spin polarization, the existence of six phases in the phase diagram and found that they are sensitive to the spin degree of freedom.

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