Quantum Phases of Quadrupolar Fermi Gases in Optical Lattices
S. G. Bhongale, L. Mathey, Erhai Zhao, S. F. Yelin, and Mikhail Lemeshko
Phys. Rev. Lett. 110, 155301 — Published 8 April 2013
DOI: 10.1103/PhysRevLett.110.155301
Quantum phases of quadrupolar Fermi gases in optical lattices

S. G. Bhongale,1 Ludwig Mathey,2 Erhai Zhao,1 Susanne F. Yelin,3,4,5 and Mikhail Lemeshko4,5,*

1School of Physics, Astronomy, and Computational Sciences, George Mason University, Fairfax, VA 22030
2Zentrum für Optische Quantentechnologien and Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany
3Department of Physics, University of Connecticut, Storrs, Connecticut 06269
4ITAMP, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138
5Department of Physics, Harvard University, 17 Oxford Street, Cambridge, MA 02138

(Dated: February 8, 2013)

We introduce a new platform for quantum simulation of many-body systems based on nonspherical atoms or molecules with zero dipole moment but possessing a significant value of electric quadrupole moment. We consider a quadrupolar Fermi gas trapped in a 2D square optical lattice, and show that the peculiar symmetry and broad tunability of the quadrupole-quadrupole interaction results in a rich phase diagram encompassing unconventional BCS and charge density wave phases, and opens up a perspective to create topological superfluid. Quadrupolar species, such as metastable alkaline-earth atoms and homonuclear molecules, are stable against chemical reactions and collapse and are readily available in experiment at high densities.

Quantum gases of ultracold atoms have provided a fresh perspective on strongly-correlated many-body states, by establishing a highly tunable environment in which both open questions of solid state physics and novel, previously unobserved, many-body states can be studied [1]. An important landmark was reached by cooling and trapping dipolar atoms and molecules, bosonic and fermionic [2–7], near or into quantum degeneracy, which extended the range of features available to quantum simulation in ultracold atom systems beyond contact interactions. Numerous exotic states such as supersolids, quantum liquid crystals and bond-order solids have been predicted, extended Hubbard models with 3-body interactions, and highly tunable lattice spin models for quantum magnetism have been proposed [8–13]. The crucial feature of the interactions in dipolar gases is their anisotropic and long-range character tunable with static and radiative fields [13–15], which is key to the intriguing many-body effects that have been predicted.

In this Letter we propose to study quadrupolar quantum gases. This constitutes a new class of systems in ultracold physics, which can be used as a platform for quantum simulation. Quadrupole interactions are most visible in an optical lattice at half-filling. We find that several unconventional phases emerge, such as bond order solids and p-wave pairing, and discover the intriguing possibility of creating topological ground states of $p_+ + ip_0$ symmetry. While dipolar quantum gases were also shown to host novel many-body phases, quadrupolar particles are available in experiment at higher densities and are stable against chemical reactions [16] and collapse [17].

In order to determine the quadrupole-quadrupole interaction energy, we consider the potential of a classical quadrupole with moment $q = \int \rho(\vec{r}) r^2 (3 \cos^2 \theta - 1) d\vec{r}$ located at $\vec{r}_0 = 0$ aligned in $\hat{k}$-direction. Here $\rho(\vec{r})$ is the electron charge density and $\cos \theta \equiv \hat{k} \cdot \hat{r}$ [46]. In this work we focus on systems possessing cylindrical symmetry, for which only one component $q$ of the quadrupole moment tensor $q_{ij}$ is nonzero. The electric field potential generated by the quadrupole is given by $\phi(\vec{r}) = \frac{q}{4\pi} (3 \cos^2 \theta - 1)$. If a second quadrupole with the same alignment $\hat{k}$ is placed at location $\vec{r}$, the resulting interaction energy is

$$E_{int} = \frac{1}{2} \int \int \frac{\rho(\vec{r}_1) \rho(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|^3} d\vec{r}_1 d\vec{r}_2$$

FIG. 1: Recipe for realization of quadrupolar particles: (a) with alkaline-earth atoms in long-living $^3P_2$ levels; and (b) with homonuclear molecules in rotational states with $J > 0$. (c) Angular “shape” of quadrupolar particles exemplified by $|2, M\rangle$ states.

PACS numbers: 67.85.-d, 75.30.Fv, 71.10.Fd
The quadrupole moment is a tensorial quantity that arises in the description of electric and magnetic interactions. It is defined as the multipole moment of a given system, and it is given by the formula:

\[ q_{\alpha\beta} = \frac{1}{8\pi} \frac{\partial^2 V}{\partial r^2} \]

where \( V \) is the potential energy of the system, \( r \) is the distance from the center of the system, and \( \alpha, \beta \) are indices that label the components of the tensor.

The quadrupole moment is a second-rank tensor, and it has six independent components in three-dimensional space. It can be expressed in terms of the dipole moment and a constant, which is usually taken to be zero for simplicity.

The quadrupole operator couples the states with \( \Delta J = 2 \) and \( \Delta M = 1 \) to states with \( \Delta J = 0 \) and \( \Delta M = 0 \), and it is given by the formula:

\[ \sum_{\alpha=2}^{3} \langle \alpha \rangle \frac{q_{\alpha\beta}}{r^5} \]

where \( q_{\alpha\beta} \) are the components of the quadrupole moment tensor.

The quadrupole moment is a useful tool for studying the properties of particles, such as the electric field of atoms and molecules. It is also used in the study of many-body systems, such as quantum gases and condensed matter systems.
quantitatively accounted for. As another intriguing example, in the vicinity of \((40^\circ, 5^\circ)\), \(V_z\) is strongly attractive while \(V_y\) is strongly repulsive. As we show below, the ground state in this region is neither a BCS state nor conventional charge density wave (CDW). These two examples show that the actual ground state may be of an unexpected nature. Exposing the true ground state thus demands a theory that is (i) unbiased with respect to the initial ansatz, and (ii) includes fluctuations.

Issue (ii) can be adequately addressed within the renormalization group (RG) analysis at weak couplings, where the low energy physics near the Fermi surface is extracted by successively integrating out the high energy degrees of freedom [34]. In order to satisfy criterion (i), we employ the exact (or “functional”) renormalization group (FRG) which keeps track of all the interaction vertices, including both the particle-particle and particle-hole channels, and treats all instabilities on equal footing [35–38].

The FRG phase diagram, Fig. 3 (a), features several different kinds of BCS and CDW phases with symmetry indicated by the the polar plots of Fig. 3 (b). CDW\(_s\) is a CDW phase with a checkerboard modulation of on-site densities, occurring in regions where the repulsive interaction between nearest neighbors dominates, see Fig. 2. This happens for all values of \(\phi_F\) when \(\theta_F \lesssim 25^\circ\), and also for \(\phi_F \lesssim 22^\circ\) at large \(\theta_F \gtrsim 60^\circ\). In addition, two novel types, CDW\(_{ps}\) and CDW\(_{ps'}\), are present. They correspond to a checkerboard modulation of the effective hopping between nearest neighbors along the \(x\) and \(y\) direction respectively, i.e., \((c_i^\dagger c_j)\) with \(r_i - r_j = \hat{x}\) or \(\hat{y}\), with the average taken over the many-body ground state.

We refer to these phases as to bond order solids (BOS). In comparison, the \(s\)-wave CDW order corresponds to modulations of \((c_i^\dagger c_j)\). Furthermore, we find a small region of CDW\(_{s+d}\) that involves a mixture of extended \(s\) and \(d\)-waves. Together they give rise to a checkerboard modulation of effective hopping between the next-nearest neighbor sites. The CDW\(_{ps}\), CDW\(_{ps'}\), and CDW\(_{s+d}\) can be thought of as a 2D generalization of the bond-order-wave phase occurring in the extended Hubbard model in one dimension [36–38]. While BOS is expected for dipolar fermions in 2D [12], it occupies a significantly larger region of the parameter space for quadrupolar interactions (e.g., it is stabilized as soon as \(\theta_F\) approaches \(25^\circ\)). Moreover, the angular dependence of quadrupolar interactions is substantially more complex, resulting in competition between BOS phases of different symmetry, resulting in frustration. Thus, fermions with dominant quadrupolar interactions provide an interesting setup for studying many-body physics with competing phases. For example, in the vicinity of \((90^\circ, 45^\circ)\) both \(V_z\) and \(V_y\) are attractive, while \(V_{\hat{z}+\hat{x}}\) is repulsive (see Fig. 2). On general grounds, one would expect a BCS type ground state resulting from condensation of Cooper pairs due to the attractive \(V_z\) and \(V_y\) couplings. However, the repulsive \(V_{\hat{z}+\hat{x}}\) interaction, if significant, may lead to the insur-
sis shows that the BCS phase can be stable even though the next-nearest neighbor interaction is weakly repulsive. We find that the symmetry of the BCS order parameter is $p_x$ or $p_y$, depending on whether $V_3$ or $V_5$ is more attractive. Along the line of $\theta_F \sim 65^\circ$, these two BCS phases are degenerate. This raises the possibility of realizing $p_x + ip_y$ topological superfluid order. By analogy with the proposal of Ref. [39], using an AC field to periodically modulate the direction of $(\theta_F, \phi_F)$, one can lift the degeneracy and engineer the chiral $p_x + ip_y$ state.

In conclusion, we have shown that ultracold Fermi gases with quadrupole-quadrupole interactions can be used to study unconventional BCS, CDW, and topological phases, and gain insight into the physics of competing ground states. While we have focused on the specific case of a square lattice at half-filling, the functional RG methods of this work can be applied to study other fillings and lattice geometries. Temperatures achieved for degenerate Fermi gases of alkaline-earth atoms in experiment are $T = 0.26 T_F$ and $T = 0.37 T_F$ respectively [29, 30]. The optimal $T_c$ for the CDW and BCS phases predicted here is estimated to be on the order of $0.03 T_F$, for intermediate couplings, $V \sim t$. Thus these many-body phases seem to be within experimental reach in the near future.

Since quadrupolar interactions occur in numerous subfields of physics, from molecular photofragmentation [40] and structure of $f$-electron compounds [41] to nuclear reactions [42] and gravitation of black holes [43], the proposed quantum simulation platform can in principle be applied beyond the many-body physics of fermionic gases. Finally, we note that ground-state atoms can be provided with significant quadrupole moments by means of Rydberg dressing, i.e. admixing a highly-excited electronic state possessing a large quadrupole moment with far-detuned laser light [44, 45].

We are grateful to Charles Clark, Robin Coté, Hendrik Weimer, and Shan-Wen Tsai for discussions. S.B. and E.Z. are supported by NSF (PHY-1205504) and NIST (60NANB12D244). L.M. acknowledges support from the Landesexzellenzinitiative Hamburg, which is financed by the Science and Research Foundation Hamburg and supported by the Joachim Herz Stiftung, and from the Deutsche Forschungsgemeinschaft under SFB 925. M.L. acknowledges support from NSF through a grant for the Institute for Theoretical Atomic, Molecular, and Optical Physics at Harvard University and Smithsonian Astrophysical Observatory. S. F. Y. acknowledges financial support from the National Science Foundation and Air Force Office of Scientific Research.
[45] Details on the FRG approach are provided in the supplemental online material.