Unconventional states of matter with cold atoms and dipolar molecules

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We have focused on novel quantum phases and emergent symmetries with ultra-cold atoms that are not easily accessible in usual solid state systems. For bosons pumped into high orbital bands, the concept of unconventional BEC (UBEC) is proposed in analogous to unconventional superconductivity based on symmetry properties. A novel statistical model dubbed the 4-coloring model is proposed to describe the heavy frustration of the UBEC in the diamond lattice, which leads to a 3D critical phase with dipolar correlations. For orbital fermions, an exact theorem is proved for the existence of an itinerant ferromagnetic state. For alkaline-earth fermions, the large SU(2N) symmetry greatly enhances quantum spin fluctuations, which give rises to novel quantum magnetism in the ground state and thermodynamic properties. For the research of synthetic gauge field, we derived the 3D Landau levels with the full 3D rotation symmetry and flat spectra. Their wavefunctions exhibit the elegant quaternionic analyticity, which greatly facilitates the further study of interacting topological states in 3D. We have also identified a novel p-wave Weyl type Cooper pairing instability in magnetic dipolar fermion systems, which is fundamentally different from both He-3 A and B phases.

**14. ABSTRACT**

Orbital physics, quantum magnetism, superfluidity, topological states of matter, frustrated magnet
AFOSR YIP (FA9550-11-1-0067), “Unconventional states of matter with cold atoms and dipolar molecules”, was awarded to Congjun Wu (PI, UCSD) (May 15, 2011 – May 14, 2014). The work supported by this award has investigated orbital physics with ultra-cold atoms in high orbital band including both bosons and fermions, novel quantum magnetism with large spin SU(2N) alkaline fermions, novel topological states with synthetic gauge fields, and many-body physics with electric and magnetic dipolar fermions. Our results have greatly deepened our understanding of quantum magnetism, superfluidity, and topological state of matter, and will provide theoretical support for the study of novel states of matter with cold atoms.

Under the support from AFOSR, we have published more than 20 research papers in high profile research journals, including 6 papers in Physical Review Letters, and 1 review paper in Journal of Physics B, AMO, 1 “news-and-views” article in Nature Physics. We have also built up a competitive team in several research directions with strong analytic and numeric capabilities.

Below we present our progress under the support of the AFOSR-YIP award. In Sect. 1, the research progress is presented with a few representative results are explained. The list of publications is given in Sect. 2. In Sect. 3, the education activity and human resource development are reported. In Sect. 4, invited talks at conferences, department seminars, physics colloquium are reported. In Sect. 5, the activity of organizing workshop is reported. In Sect. 1.4, we present the study of many-body physics with both electric and magnetic dipolar interactions. In Sect. 1.5, we present our work in establishing an exact theorem on the itinerant ferromagnetism.

1 Research progress

In this section, we present the research progress in several topics. The research on novel orbital physics with bosons and fermions in high orbital bands is presented in Sect. 1.1. The study of novel quantum magnetism with large spin alkaline earth atoms is presented in Sect. 1.2. In Sect. 1.3, we present our work on the topological states with synthetic gauge fields.

1.1 Novel orbital physics in high bands of optical lattices

Orbital is a degree of freedom independent of charge and spin, which is characterized by two fundamental features: orbital degeneracy and spatial anisotropy. We propose that orbital physics is a natural and promising research direction of cold atom physics. Based on our previous research, we have made further progress in exploring novel orbital physics in optical lattices which does not appear in solid state systems. My group is among the leading groups along this research direction. Our research has already had important impact to the community both experimental and theoretical.
1.1.1 Unconventional BEC with orbital bosons

The ordinary BECs, including most work with cold atoms and $^4$He, obeys the “no-node” theorem, which states that their many-body ground state wavefunctions are positive-definite, thus time-reversal symmetry cannot be spontaneously broken. This is a very general statement applying to almost all the familiar ground states of bosons which implies that time-reversal symmetry cannot be spontaneously broken. It would be exciting to search for novel many-body states of bosons beyond this paradigm.

We have proposed the concept of “unconventional BEC” in analogy of unconventional superconductivity based on symmetry analysis. The condensate wavefunctions of unconventional BEC belong to non-trivial representations of the lattice point group. The unconventional BECs have been realized in A. Hemmerich’s group as proposed before in high orbital bands of optical lattices. The resultant many-body wavefunctions are complex-valued and thus break time-reversal symmetry spontaneously. Exotic phenomena in these states include BECs at nonzero momenta, and the ordering of orbital angular momentum moments.

Under the support from the AFOSR-YIP program, my group has deepened the theoretical study of the UBEC. In particular, we focused on the quantum phase transition from a real-valued BEC to the complex-valued BEC. We have used both the weak-coupling approach (PRA 84, 033635(2011)) and the non-perturbative method of quantum Monte-Carlo simulations (PRB 87, 224505(2013)). We have also proposed a phase-sensitive detection scheme to identify the unconventional $p_x \pm ip_y$ symmetry of the condensate wavefunctions (PRA 86, 051601(2012)) by using the impulsive Raman operation combining with time-of-flight imaging. This scheme provides smoking gun evidence for unconventional unconventional BEC with nontrivial condensation symmetries.

We have further proposed a novel concept of “frustrated BECs”. Frustration is a concept usually applied in antiferromagnetic systems in non-bipartite lattices, but not in superfluid systems. We have found that the UBEC in the $p$-orbital bands can exhibit frustrations (PRB 86, 060517(2012)) even in the cubic lattice. Furthermore, the $p$-band diamond lattice is heavily frustrated, for which we proposed a novel four-coloring model (PRL 112, 020601 (2014)). The superfluid phases of the condensate wave functions on the diamond-lattice bonds are mapped to four distinct colors at low temperatures. The fact that a macroscopic number of states satisfy the constraints that four differently colored bonds meet at the same site leads to an extensive degeneracy in the superfluid ground state. We demonstrate that the phase of the superfluid wave function as well as the orbital angular momentum correlations exhibit a power-law decay in the degenerate manifold that is described by an emergent magneto-static theory with three independent flux fields. Our results thus provide a novel example of critical superfluid phase with algebraic order in three dimensions.

1.1.2 Novel physics of orbital fermions

We have also found that fermions in the $p$-orbital bands exhibit exotic properties, such as an exactly solvable model of orbital ice and the realization of FFLO phase.

We demonstrate the existence of orbital Coulomb phase as the exact ground state of $p$-orbital exchange Hamiltonian on the diamond lattice (Phys. Rev. E 84, 061127 (2011)). The Coulomb phase is an emergent state characterized by algebraic dipolar correlations and a gauge structure resulting from local constraints (ice rules) of the underlying lattice models. For most ice models on the pyrochlore lattice, these local constraints are a direct consequence of minimizing the energy of
each individual tetrahedron. On the contrary, the orbital ice rules are emergent phenomena resulting from the quantum orbital dynamics.

We present the study of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) pairing states in the $p$-orbital bands in both two and three-dimensional optical lattices (Phys. Rev. A 83, 063621 (2011)). Due to the quasi one-dimensional band structure which arises from the unidirectional hopping of the orthogonal $p$-orbitals, the pairing phase space is not affected by spin imbalance. Furthermore, interactions build up high dimensional phase coherence which stabilizes the FFLO states in 2D and 3D optical lattices in a large parameter regime in phase diagram. Their entropies are comparable to those of the normal states at finite temperatures.

1.2 Large spin physics with cold atoms studied by QMC simulations

We have pointed out that the large spin cold atomic systems are fundamentally different from the large spin solid state systems (Nat.Phys. 8, 784784 (2012)). In the solid state context, large spin is not considered interesting because large spin means classical, i.e., quantum fluctuations are suppressed by the $1/s$-effect. Although on each lattice site several electrons combine to a large spin through Hund’s rule, the intersite coupling is dominated by the exchange of a single pair of electrons, which suppresses quantum fluctuations as $s$ goes larger. In contrast, such restriction does not occur in cold atom large spin systems because each atom, which carries large spin, moves as an entire object. Even the exchange of a single pair of cold atoms can completely flip the spin configuration. This dramatically enhances quantum spin fluctuations.

We numerically study the quantum magnetism of ultracold alkali and alkaline-earth fermion systems including both the ground state magnetism and finite temperature thermodynamic properties. We nonperturbatively investigate the ground state magnetic properties of the 2D half-filled SU(2$N$) Hubbard model in the square lattice by using the projector determinant quantum Monte Carlo simulations combined with the method of local pinning fields (PRL 112, 156403 (2014); PRB 88, 125108 (2013)). Long-range Neel orders are found for both the SU(4) and SU(6) cases at small and intermediate values of $U$. In both cases, the long-range Neel moments exhibit non-monotonic behavior with respect to $U$, which first grow and then drop as $U$ increases. This result is fundamentally different from the SU(2) case in which the Neel moments increase monotonically and saturate. In the SU(6) case, a transition to the columnar dimer phase is found in the strong interaction regime.

We have also performed a systematical quantum Monte-Carlo simulations on the thermodynamic properties (PRL 110, 220401(2013)). The large number of hyperfine-spin components enhances spin fluctuations, which facilitates the Pomeranchuk cooling to temperatures comparable to the superexchange energy scale in the case of SU(6). This result is particularly useful for the current on-going experiments.

1.3 Novel topological states with synthetic gauge fields

My group is among the pioneers in this direction. Our first paper studying spin-orbit coupled BEC was posted in arxiv in 2008 before the experiments. After that my group has done a series of work focusing on the topological aspect of states with synthetic gauge fields. We have written a review article published as J. Phys. B (AMO), 46, 134001 (2013).
1.3.1 Topological textures with spin-orbit coupled BECs

The spin-orbit coupling with bosons gives rise to novel properties that are absent in usual bosonic systems. The linear dependence of the spinorbit coupling leads to complex-valued condensate wavefunctions beyond this theorem. We have systematically studied this class of unconventional BECs focusing on their topological properties. Both the 2D Rashba and 3D $\vec{\sigma} \cdot \vec{p}$-type Weyl spinorbit couplings give rise to Landau-level-like quantization of single-particle levels in the harmonic trap. Interacting condensates develop the half-quantum vortex structure spontaneously breaking the time-reversal symmetry and exhibit topological spin textures of the skyrmion type. In particular, the 3D Weyl coupling generates topological defects in the quaternionic phase space as an SU(2) generalization of the usual U(1) vortices (arXiv:1205.2162). In the Mott-insulating states in optical lattices, quantum magnetism is characterized by the Dzyaloshinskii-Moriya-type exchange interactions (Phys. Rev. A 85, 061605(R) (2012)).

1.3.2 Topological states of matter with high dimensional Landau levels

The 2D quantum Hall states are among the earliest studied topological electronic states, which are based on Landau level quantization. However, the recent research focus of the 3D topological insulators is focusing on the Bloch wave band structures. Compared to Bloch-wave band structures, Landau levels are simple, explicit with elegant analytical properties. Furthermore, their spectra are flat and thus interaction effects are non-perturbative. These features may facilitate the future study of high dimensional fractional topological states of interacting electrons in 3D.

However, the usual Landau level are based on 2D geometry, and thus cannot easily be extended to 3D. My group generalized Landau levels to 3D with the full spherical rotation symmetry for both relativistic (Phys. Rev. B 85, 085132 (2012)) and non-relativistic fermions (Phys. Rev. Lett. 110, 216802 (2013); Phys. Rev. B 85, 125122 (2012)). In particular, we found that the lowest Landau level wavefunctions in the 3D systems possess an elegant properties: they are quaternionic analyticity. We know that the complex analyticity of the 2D Landau level wavefunctions play an important role in the study of the interacting fractional QHE state. We anticipate that the quaternionic analytic will also greatly facilitate the study of fractional topological states in 3D.

Recently, we have a new progress along this direction. We have generalized the Landau levels to 3D in the SU(2) Landau type gauge (Phys. Rev. Lett. 111, 186803 (2013)). As known in 2D, Landau levels in the Landau gauge are spatially separated 1D chiral plane waves. We found their high dimensional counterparts: the 2D helical Dirac modes with opposite helicities and 3D Weyl modes with opposite chiralities are spatially separated along the third and fourth dimensions, respectively. We further studied the quantized charge pumping in 4D Landau levels. Just like the 2D quantum Hall effect can be viewed as chiral anomaly on two spatially separated 1D edges, the 4D counterpart is the spatially separated chiral anomaly on the 3D boundaries.

1.4 Many-body physics with dipolar interactions

We have investigated the many-body physics with both electric and magnetic dipolar interactions. Actually, fermion systems with these two different dipolar interactions are quite different from each other.
1.4.1 Spin-orbit coupled magnetic dipolar systems

Although the energy scale of the magnetic dipolar interaction is much weaker than that of the electric one, it is conceptually more interesting if magnetic dipoles are not aligned by external fields. Magnetic dipole moments are proportional to the hyperfine spin up to a Lande factor, thus, they are quantum-mechanical operators rather than the non-quantized classic vectors as electric dipole moments are. Furthermore, there is no need to use external fields to induce magnetic dipole moments. In fact, the unpolarized magnetic dipolar systems are isotropic. The dipolar interaction does not conserve spin nor orbit angular momentum but is invariant under simultaneous spin-orbit (SO) rotation. This is essentially a spin-orbit coupled interaction. Different from the usual spin-orbit coupling of electrons in solids, this coupling appears at the interaction level but not at the kinetic-energy level.

We investigate Fermi liquid states of the ultra-cold magnetic dipolar Fermi gases in the simplest two-component case including both thermodynamic instabilities and collective excitations (Phys. Rev. B 85, 205126 (2012)). The Landau interaction matrix is calculated and is diagonalized in terms of the spin-orbit coupled partial-wave channels of the total angular momentum $J$. The leading thermodynamic instabilities lie in the channels of ferromagnetism hybridized with the ferronematic order with $J = 1^+$ and the spin-current mode with $J = 1^-$, where $+\text{ and } -$ represent even and odd parities, respectively. An exotic propagating collective mode is identified as spin-orbit coupled Fermi surface oscillations in which spin distribution on the Fermi surface exhibits a topologically nontrivial hedgehog configuration.

We have also found that the magnetic dipolar interaction also gives rise to a robust mechanism for a novel pairing symmetry: orbital $p$-wave ($L = 1$) spin triplet ($S = 1$) pairing with total angular momentum of the Cooper pair $J = 1$ (Scientific Report 2, 392 (2012)). This pairing is markedly different from both the $^3$He-B phase in which $J = 0$ and the $^3$He-A phase in which $J$ is not conserved. It is also different from the $p$-wave pairing in the single-component electric dipolar systems in which the spin degree of freedom is frozen.

1.4.2 Interaction effects in Majorana flat bands

We have also been working on the topological aspect of the pairing states with electric dipolar fermions, focusing on the interaction effects in the surface flat band of Majorana zero modes. We found an important result that interactions always open up the gap in these surface Majorana flat bands by spontaneously breaking time-reversal symmetry (New J. Phys. 15 085002 (2013)). This project is closely related to the current experiment effort of searching Majorana fermions in semiconducting wires.

We first considered an array of these wires with the $p_z$-pairing connected by the inter-chain tunneling. Each wire is in the topological pairing state with a Majorana zero mode on the boundary. These zero modes do not couple at the single particle level as a result of time-reversal symmetry, and thus form a flat band. However, the band flatness is unstable toward the spontaneous generation of vortex loops near the boundary, which lowers the energy by opening the gap.

We have also considered the more experimental relevant systems of spin-orbit coupled wires (Phys. Rev. B 89, 174510 (2014)). The bulk exhibits topologically distinct gapped phases and an intervening gapless phase. Even though the bulk pairing structure is topological, the interaction between Majorana zero modes and superfluid phases leads to spontaneous time-reversal symme-
try breaking. Consequently, edge supercurrent loops emerge and edge Majorana fermions are in
general gapped out except when the number of chains is odd, in which case one Majorana fermion
survives.

1.5 Exact theorems on itinerant ferromagnetism

Although ferromagnetism (FM) was discovered more than 2000 years ago, it remains one of the
major challenges of contemporary condensed matter physics. Ferromagnetism is not only a strong-
correlation phenomenon; it is also a highly non-perturbative phenomenon. Exact theorems are,
therefore, indispensable for understanding the precise mechanism of ferromagnetism. Historically,
the Lieb-Mattis theorem proved that one-dimensional systems of itinerant electrons can never be
ferromagnetic no matter how strong the interactions are. Previously known examples of ferro-
magnetism in two and three dimensional systems usually fall into one of the two paradigms: the
“Nagaoka ferromagnetism” as a result of coherent hopping of a single hole in lattices under infi-
nite repulsion, or, the “flat-band ferromagnetism” arising from Wannier-like localized states on line
graphs, where zero penalty from kinetic energy greatly assists the development of ferromagnetism.

We have proved a set of new theorems of the ground state itinerant ferromagnetism as published
(PRL 112, 21720 (2014). It applies for all generic fillings in a general class of multi-orbital Hubbard
models in two and three dimensions. The theorems established here provide a concrete playground
of itinerant ferromagnetism pertinent to experimental systems and may provide useful guidance for
the current experimental efforts to search for itinerant ferromagnetism in both condensed matter
and ultra-cold atom systems.

The new mechanism here differs from the “Nagaoka ferromagnetism” in that it is valid for
any generic electron filling, and also differs from the “flat-band ferromagnetism” where kinetic
energy is suppressed. In this paper, the orbital degree of freedom, i.e. the shape of electron cloud
which plays a key role in solids, gives rise to quasi-one dimensional kinetic bands as well as to
on-site inter-orbital Hunds rule coupling. We prove that, in the strong coupling limit, the Hund’s
rule coupling at each site drives the ground states to fully saturated itinerant ferromagnetic states
for any generic filling. The ground states are unique apart from the trivial spin degeneracy, and
the wave functions are nodeless in a properly defined basis. Our theorems apply to a large class
of two- and three- dimensional strongly correlated multi-orbital lattice systems with quasi-one-
dimensional band structures, including the $d_{xz}$ and $d_{yz}$-orbital bands in transition-metal-oxide layers
or interfaces, and the $p$-orbital bands in optical lattices with ultra-cold fermions. We believe that
this paper will have important impact in condensed matter and cold atom physics as well as in
mathematical physics.

2 Publication list under AFOSR-YIP support

1. Gu-Feng Zhang, Yi Li, Congjun Wu, “The honeycomb lattice with multi-orbital structure:
topological and quantum anomalous Hall insulators with large gaps”, Phys. Rev. B 90,
075114 (2014).

2. Da Wang, Zhou-Shen Huang, Congjun Wu, “The fate and remnant of Majorana zero modes


3 Education and Human resource development

Under the AFOSR-YIP support, the PI has build up a competitive research group for the study of novel states with ultra-cold atoms. This project provides excellent theoretical training to students and postdoctoral researchers on various theoretical and numerical skills. These include band structure calculations, self-consistent mean-field theory, field theoretical methods, symmetry and topological analysis, and quantum Monte-Carlo simulations. My group members also receive training on analyzing deep physics behind the experimental phenomena.

3.1 Mentoring graduate students

1. There are two graduate students received their Ph. D. degree during the period of this AFOSR-YIP support: Hsiang-hsuan Hung (Sept. 2011), and Yi Li (Jun. 2013). Part of their support was from this award.

2. My former student Yi Li, a woman student, worked on the proposed research of this award as her thesis topic. She is very successful in academic record, and was among the top candidates in the postdoc job market of condensed matter physics in 2013 in the US. She is current a postdoctoral researcher at Princeton Center of Theoretical Sciences. I believe that she will be very successful in her academic career.

3. In Sept 2013, I recruited three graduate researchers for the projects supported by AFOSR.

4. I hold regular group meetings, which are open to both my group members and other students in the department. I educate them the general background on the research frontier of condensed matter and cold atom physics, and organize them to form study groups for classic papers. This activities have reached a satisfactory effect.

5. I support my graduate students to attend the APS march meeting to present our research results supported by this NSF award.
3.2 Postdoc Mentoring activity

Dr. Zi Cai and Dr. Da Wang were postdoctoral researchers in my group. Both of their participation had greatly accelerated the research progress. The mentoring activity on his research is explained as follows:

1. Dr. Zi Cai was supported from Sept. 2011 to Aug. 2012, and Dr. Da Wang was supported from Sept. 2012 to May 2014 by this AFOSR-YIP award.

2. Under the PI’s guidance, Dr. Zi Cai and Dr. Da Wang made a large contribution to the projects of this award with their expertise on both analytic and numeric skills. Zi Cai worked on unconventional BEC of orbital bosons, and quantum Monte-Carlo simulations. Da Wang worked on the novel quantum magnetism of the SU(2N) fermions by using the quantum Monte-Carlo simulations, and also Majorana fermions. Both of them have grown up as matured researchers in condensed matter physics.

3. The PI provided guidance for both Dr. Zi Cai and Dr. Da Wang’s future career for applying faculty positions. Dr. Da Wang has obtained a faculty position in condensed matter physics in Nanjing University, China, and will join there since Sept 1. 2014. Dr. Zi Cai is working as postdoctoral researcher in Prof. Peter Zoller’s group.

4. Dr. Zi Cai and Dr. Da Wang published many high quality research papers in my group. In particular, both of them published first-authored PRL papers in my group.

5. Teaching and Mentoring Skills: both of them played an important role in training new graduate researchers in my group.

4 Presentations Activities

Physics Colloquium by the PI:

1. Institut fur Laserphysik, University of Hamburg, Germany, Unconventional Bose-Einstein condensation beyond the no-node paradigm, Jan. 31, 2012.

2. Department of Physics, University of Houston, Physics Colloquia, Unconventional metamagnetism and orbital ordering in transition metal oxides, March 27, 2012.

Invited conference talks and condensed matter seminars by the PI:

1. The opening conference of the Tsinghua Sanya International Mathematics Forum, topological insulator workshop, Quaternionic analytic Landau levels, Sanya, China, Dec 18-19, 2013.

2. Department of Physics, Harvard University, Quaternionic analytic SU(2) Landau levels in 3D, Oct. 17, 2013.

3. Hefei National high magnetic-field Lab, China. Interaction effects on topological insulators, 07/24/2013.


8. Department of Physics, The Florida State University, Isotropic Landau Levels of Relativistic and Non-Relativistic Fermions in 3D Flat Space, September 14, 2012.


10. Department of Physics, University of British Columbia, Canada, Isotropic Landau Levels of Relativistic and Non-Relativistic Fermions in 3D Flat Space, March 20, 2012.

11. Department of Physics, University of California, Irvine, Unconventional meta-magnetism and orbital ordering in transition metal oxides, Feb 8, 2012.

Invited talks given by my group members based on projects in this proposal

1. Aspen winter conference on strongly correlated electrons, ”Exact results in orbital-assisted itinerant ferromagnetism”, Yi Li, Feb. 2014.

2. International workshop on Orbital Physics in Cold Atom Systems, Quantum magnetic and charge properties of the SU(2N) Hubbard model: a quantum Monte Carlo study, by Zi Cai, Institute of Physics, Chinese Academy of Sciences, Beijing, Jan.5-6, 2013.

3. Institute for Quantum Information and Matter, California Institute of Technology, Quaternionic analytic Landau levels in 3D and 4D, by Yi Li, Jan. 2013.

4. Department of Physics, University of California - Los Angeles, 3D and 4D Topological Insulators from SU(2) Landau Levels, by Yi Li, Nov. 2012.

5. Department of Physics, Stanford University, 3D and 4D Topological Insulators from SU(2) Landau Levels, by Yi Li, Oct. 2012

5 Organizing workshop

I was one of the organizers of an international workshop on ”Orbital physics of cold atoms” at Institute of Physics, Chinese Academy of Sciences, Beijing in January 2013. Leading experimentalists and theorists in this directions participated this workshop. This workshop were very successful.