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14. ABSTRACT
We develop and apply computational methods to investigate correlation effects in atomic and molecular systems, and in optical lattice systems. Problems from both classes are studied synergistically. We quantified effects of many-body correlations in trapped atomic Bose gases; developed auxiliary-field quantum Monte Carlo method for Bosons

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Report Title

Computational Studies of Strongly Interacting Ultracold Atoms -- Final Report

ABSTRACT

We develop and apply computational methods to investigate correlation effects in atomic and molecular systems, and in optical lattice systems. Problems from both classes are studied synergistically. We quantified effects of many-body correlations in trapped atomic Bose gases; developed auxiliary-field quantum Monte Carlo method for Bosons and fermions whose computational cost scales as N^3-N^4 with system size; benchmarked the method in molecular systems using Gaussian basis functions; demonstrated that its accuracy is comparable to the preeminent quantum chemistry coupled-cluster method CCSD(T) for systems near equilibrium geometry, and better than the latter when bonds are stretched or broken; developed methods to correct for finite-size errors to drastically improve the efficiency of many-body simulations by reaching larger and more realistic system sizes; formulated an approach to eliminate spin contamination in auxiliary-field calculations; examined spin-density waves states in simple models of metallic systems; showed the existence of incommensurate spin-density waves in two-dimensional optical lattices with positive scattering lengths.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Wirawan Purwanto, Shiwei Zhang,
"Correlation effects in the ground state of trapped atomic Bose gases,"
Phys. Rev. A 72, 053610 (2005)

W. A. Al-Saidi, Shiwei Zhang, Henry Krakauer, "Auxiliary-field quantum Monte Carlo calculations of molecular systems with a Gaussian basis,"
J. Chem. Phys. 124, 224101 (2006)

W. A. Al-Saidi, Henry Krakauer, Shiwei Zhang,
"Auxiliary-field quantum Monte Carlo study of first- and second-row post-d elements," J. Chem. Phys. 125, 154110 (2006)

W. A. Al-Saidi, Henry Krakauer, Shiwei Zhang, "A study of H+H$_2$ and several H-bonded molecules by phaseless auxiliary-field quantum Monte Carlo with planewave and Gaussian basis sets,"
Journal of Chemical
Physics, 126, 194 105 (2007).

Malliga Suewattana, Wirawan Purwanto, Shiwei Zhang, Henry Krakauer, Eric J. Walter, "Phaseless auxiliary-field quantum Monte Carlo calculations with planewaves and pseudopotentials--applications to atoms and molecules," Phys. Rev. B 75, 245123 (2007)

W. A. Al-Saidi, Shiwei Zhang, Henry Krakauer
"Bond breaking with auxiliary-field quantum Monte Carlo,"
Journal of Chemical Physics 127, 144101 (2007).

Hendra Kwee, Shiwei Zhang, Henry Krakauer
"Finite-size correction in many-body electronic structure calculations,"
Phys. Rev. Lett. 100, 126404 (2008)

Shiwei Zhang and D. M. Ceperley
"The Hartree-Fock ground state of the three-dimensional electron gas,"
Phys. Rev. Lett. 100, 236404 (2008)

Wirawan Purwanto, W. A. Al-Saidi, Henry Krakauer, Shiwei Zhang
"Eliminating spin contamination in auxiliary-field quantum Monte Carlo: realistic potential energy curve of F2," J. Chem. Phys. 128, 114309 (2008)

Chia-Chen Chang and Shiwei Zhang, "Spatially inhomogeneous phase in the two-dimensional repulsive Hubbard model," Phys. Rev. B 78, 165101 (2008)

Kenneth P. Esler, Jeongnim Kim, David M. Ceperley, Wirawan Purwanto, Eric J. Walter, Henry Krakauer, Shiwei Zhang, Paul R. C. Kent, Richard G. Hennig, Cyrus Umrigar, Michal Bajdich, Jindrich Kolorenc, Lubos Mitas, and Ashok Srinivasan, "Quantum Monte Carlo algorithms for electronic structure at the petascale; the endstation project," J. of Phys.: Conf. Ser. 125 012057: 1-15 (2008).

Chia-Chen Chang and Shiwei Zhang, "Spin and charge order in doped Hubbard model: long- wavelength collective modes,"
Phys. Rev. Lett. 104, 116402 (2010)

Number of Papers published in peer-reviewed journals: 12.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

Shiwei Zhang, Huihai Zhao, and Tao Xiang "The sign problem in quantum Monte Carlo," invited plenary paper in 10,000 Major Scientic Challenges (published in Chinese by Science Press, ISBN: 9787030242679, 2009).

Number of Papers published in non peer-reviewed journals: 1.00

(c) Presentations

Shiwei Zhang, ``Electronic structure calculations by auxiliary-field quantum Monte Carlo,'' invited talk at the psik-2005 (European electronic structure network) conference, Schwabisch Gmund, Germany, Sep.~17-21, 2005.

* Shiwei Zhang, ``Quantum Monte Carlo method using Gaussian basis sets (part I) {and} a method for computing forces in diffusion Monte Carlo (part II),'' workshop on Ab-Initio Simulation methods beyond Density Functional Theory, CECAM, Lyon, France, Sep.~23-25, 2005.

* Shiwei Zhang, ``Recent developments in electronic structure calculations by auxiliary-field quantum Monte Carlo,'' invited talk at New Developments in Quantum Monte Carlo Techniques workshop in Tempe, AZ May 14-18, 2006.

* Wissam Al-Saidi, ``Auxiliary-field quantum Monte Carlo with localized basis sets,'' 18th Annual Workshop on Recent Developments in Electronic Structure Methods, Columbus, Ohio, USA 22-25 June, 2006.

* Shiwei Zhang, ``An auxiliary-field approach for electronic structure computations,'' invited talk at {\em the international workshop on ``Density functional theory meets strong correlation,''\/} Montauk, NY, Sept.~5-8, 2006.

* Shiwei Zhang, ``Recent advances in auxiliary-field methods --- simulations in lattice models and real materials,'' invited talk at the March Meeting of the American Physical Society, Denver, CO, Mar.~5-9, 2007.

* Shiwei Zhang, "Auxiliary-field methods", two lectures at the summer school on Computational Materials Science --- Quantum Monte Carlo from Minerals and Materials to Molecules, University of Illinois at Urbana-Champaign, Jul 9-19, 2007

* Shiwei Zhang, "Finite-size correction in many-body electronic structure calculations", invited talk at Advances in continuum quantum Monte Carlo methods, CECAM, Aug. 27-31, 2007.

* Shiwei Zhang, ``Recent progress in many-body electronic structure calculations with auxiliary-fields,'' invited talk at the {\em International Workshop on Computational Physics and Materials Science: Progress in Computational Electronic Structure Theory\/}, Bonn, Germany, Jan.~10-12, 2008.

* Shiwei Zhang, ``Auxiliary-field quantum Monte Carlo methods: from lattice models to real materials,'' lectures at International {\em Advanced School on Quantum Monte Carlo Methods in Physics and Chemistry\/}, ICTP, Trieste, Italy, Jan.~21-Feb.~2, 2008.

* Shiwei Zhang "A stochastic independent-electron approach for correlated system,"invited talk at the 20th Annual Workshop on Recent Developments in Electronic Structure Methods, Urbana, Illinois, Jun.~18-20, 2008.

* Shiwei Zhang, "Bridging quantum Monte Carlo and density functional calculations," invited talk at the International Symposium on the Multi-scale Modeling and Simulation of Materials, Shanghai, China, Jul.~7-11, 2008.

* "Finite-size corrections and recent developments on auxiliary-eld

methods," invited talk at Quantum Monte Carlo in the Apuan Alps conference, Vallico Sotto, Italy, July 25-August 1, 2009.

* "Phaseless auxiliary-eld quantum Monte Carlo method for correlated systems," invited talk at the 238th American Chemical Society (ACS) National Meeting, Washington, DC, August 16-20, 2009.

* "Petascale condensed matter physics and quantum chemistry," invited talk at the American- Chinese Cyberinfrastructure and E-Science workShop (ACCESS) 2009 , Beijing, China, Septem- ber 7-10, 2009.

* "Phaseless auxiliary- eld quantum Monte Carlo method for correlated systems," invited talk at the The 12th Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN12), Beijing, China, Oct. 26-28, 2009.

Number of Presentations: 16.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Kenneth P. Esler, Jeongnim Kim, David M. Ceperley, Wirawan Purwanto, Eric J. Walter, Henry Krakauer, Shiwei Zhang, Paul R. C. Kent, Richard G. Hennig, Cyrus Umrigar, Michal Bajdich, Jindrich Kolorenc, Lubos Mitas, and Ashok Srinivasan, "Quantum Monte Carlo algorithms for electronic structure at the petascale; the endstation project," J. of Phys.: Conf. Ser. 125 012057: 1-15 (2008).

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts): 1

(d) Manuscripts

Number of Manuscripts: 0.00

Patents Submitted

Patents Awarded

Graduate Students

NAME	PERCENT_SUPPORTED
Hendra Kwee	0.15
FTE Equivalent:	**0.15**
Total Number:	**1**

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Chia-Chen Chang	1.00
FTE Equivalent:	**1.00**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Shiwei Zhang	0.08	No
FTE Equivalent:	**0.08**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:.....	0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:.....	0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):	0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:	0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Hendra Kwee
Total Number: 1

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Appendix to Final Report: Statement of the problem studied, and summary of the most important results

Our project aimed to develop and apply computational methods to investigate correlation effects in atomic and molecular systems, and in ultracold atomic gases. Below the most important results are summarized. The twelve (12) journal publications listed earlier describe the findings in detail; the work was also presented in about 25 invited talks at international meetings [including at annual meetings of the American Physical Society (APS) and the American Chemical Society (ACS)], workshops, and conferences, and also as seminars/colloquia at academic instutitions around the world.

A Correlation effects in the ground state of trapped atomic Bose gases.

We studied the effects of many-body correlations in trapped ultracold atomic Bose gases [1]. We calculate the ground state of the gas using a our ground-state auxiliary-field quantum Monte Carlo (QMC) method [2]. We examine the properties of the gas, such as the energetics, condensate fraction, real-space density, and momentum distribution, as a function of the number of particles and the scattering length. We find that the mean-field Gross-Pitaevskii (GP) approach gives qualitatively incorrect result of the kinetic energy as a function of the scattering length. We present detailed QMC data for the various quantities, and discuss the behavior of GP, modified GP, and the Bogoliubov method under a local density approximation.

B Phaseless auxiliary-field method – quantum chemistry applications and benchmark.

Accuracy, or predictive power, is a key requirement of a successful paradigm for strongly correlated systems. The GTO formulation and chemistry applications have been crucial in establishing the phaseless AFQMC method as a general approach that can now be applied to correlated systems. To benchmark the method, we have to date applied it to close to 100 systems, including first- and second-row molecules [3, 4], transition metal oxide molecules [5], simple solids [6, 7], post-d elements [8], and van der Waals systems [9]. Figure 1 illustrates the results on molecules using both planewave and GTOs. In these calculations we have operated largely in an automated mode, inputting only the DFT or HF solutions. The method demonstrated excellent accuracy, consistently able to correct errors in the mean-field trial wave function. In molecules, we find that the accuracy of the phaseless AFQMC is comparable to the coupled-cluster method CCSD(T), the gold standard in chemistry [10, 11], near equilibrium geometry. [The computational cost of CCSD(T) scales as N^7 with system size, while QMC is N^3-N^4.]

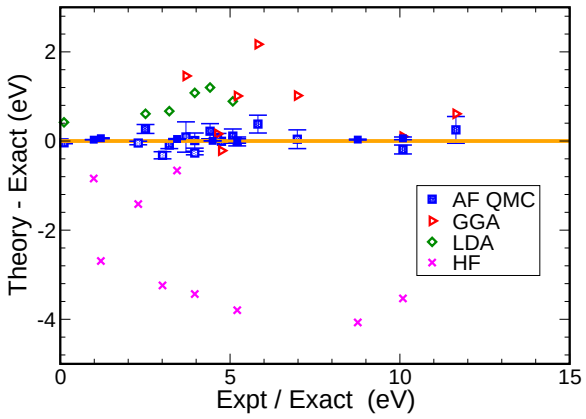

Figure 1: Calculated binding energies [15, 5, 4, 16] of molecules compared with experimental values. The discrepancy between theory and experiment is plotted. The AFQMC is fed a trial wave function to start, which is taken directly from DFT [with either local-density approximation (LDA) or generalized-gradient approximation (GGA) functionals] or Hartree-Fock (HF). The corresponding DFT or HF results are also shown. As can be readily observed, the AFQMC results are in excellent agreement with experiment and significantly improve upon the values from DFT and HF.

C Electron correlation effects from bond stretching and bond breaking.

Bond stretching in molecules and solids mimics different levels of particle correlation and provides a challenging testbed for approximate many-body computational methods. With single Slater determinants from unrestricted Hartree-Fock (UHF) as trial wave function, we find that the phaseless AFQMC method generally gives better overall accuracy and a more uniform behavior than the coupled cluster CCSD(T) method in mapping the potential-energy curve [12, 13, 14]. Calculations were also done in the triple-bond system of N_2, and a chain of 50 H atoms.

D Eliminating spin contamination in the treatment of magnetic properties.

The use of an approximate reference state wave function $|\Psi_T\rangle$ in electronic many-body methods can break the spin symmetry of Born-Oppenheimer spin-independent Hamiltonians. This can result in significant errors. To address the problem, a simple spin-projection method was introduced [13] for AFQMC, which yields spin-contamination-free results, even when a spin-contaminated $|\Psi_T\rangle$ is used. The method was applied to the difficult F_2 molecule, which is unbound within UHF. With a UHF $|\Psi_T\rangle$, spin contamination causes large systematic errors and long equilibration times in AFQMC in the intermediate, bond-breaking region. The spin-projection method eliminated these problems, and delivered an accurate potential energy curve from equilibrium to the dissociation limit using the UHF $|\Psi_T\rangle$. The calculated spectroscopic constants, using large basis sets, were in excellent agreement with experiment.

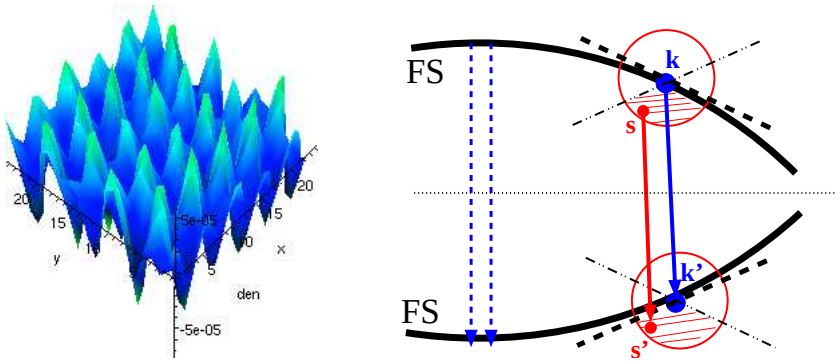

Figure 2: Spin-density wave (SDW) states in the homogeneous electron gas, in Hartree-Fock (HF) theory [19]. The **left** shows the result from our full unrestricted HF calculation. The HF ground state clearly exhibits SDW structure, shown by the spin density for a plane in the supercell. The **right** shows a cartoon depicting our theory explaining the mechanism for the SDW state, which we showed to have characteristic wave vector $q_\sigma < 2k_F$, not $2k_F$ as previously believed [20, 21].

E Finite-size correction in many-body electronic structure calculations

Finite-size effects are a major source of error in many-body electronic structure calculations of extended systems. We have developed a general method to correct for such errors [7]. We showed that many-body finite-size effects can be effectively included in a modified local density approximation calculation. A parameterization for the finite-size exchange-correlation functional was obtained. The method is simple and gives post-processing corrections that can be applied to any many-body calculations. Applications to a model insulator, to semiconducting Si, and to metallic Na showed that the method delivers greatly improved finite-size corrections. The method has recently been implemented by Dario Alfe in the open-source PWSCF package [17] (and used in calculations of solid iron [18].)

F What is the Hartree-Fock ground state in the electron gas?

In 1962, Overhauser showed that within HF the electron gas is unstable to a spin density wave (SDW) state. Determining the true HF ground state has remained a challenge. Using numerical and analytic techniques, we obtained the HF ground state of the three-dimensional electron gas. At high density, we found a number of novel states characterized by nearly constant charge density but broken spin symmetry, with an SDW wave vectors differing from the Overhauser states. We showed that the broken-symmetry state originates from pairing instabilities at the Fermi surface, and proposed a model to explain its properties [19] (Fig. 2).

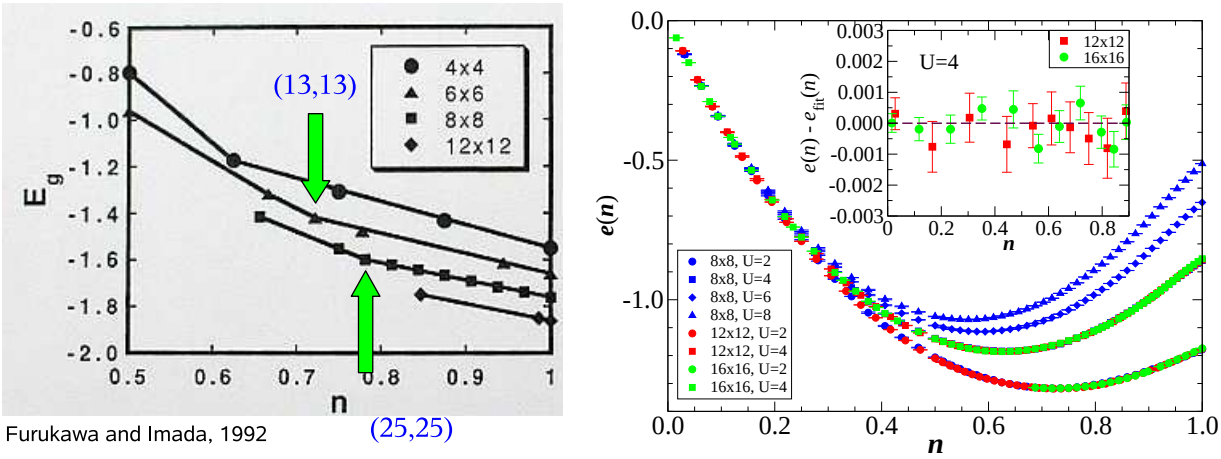

Figure 4: Accurate calculations of the equation of state (EOS) in the 2-D repulsive Hubbard model. This was made possible by recent advances in using twist-averaging boundary conditions (TABC) [22] and in controlling the phase problem[23, 24, 1], which eliminated shell effects (see kinks on the left from a typical prior calculation [25]) and drastically reduced finite-size effects. EOS curves on the right are smooth and different lattice sizes are indistinguishable. A fit for the EOS was obtained. From the inset on the right, it is seen that the quality of the fit is excellent.

G Two-dimensional optical lattices with repulsive interaction – equation of state.

We have determined the equation of state in the ground state of the two-dimensional repulsive single-band Hubbard model at intermediate interactions. Shell effects are eliminated and finite-size effects are greatly reduced by boundary condition integration. Spin-spin correlation functions and structure factors are also calculated. In lattice sizes up to 16×16, the results show signal for phase instability. Upon doping, the energy in these finite systems is larger than it would be if the system were to separate into two phases: one of density $n = 1$ (hole-free) and the other at density n_c (~ 0.9). The long-range antiferromagnetic order is coupled to this process, and is lost below n_c. This suggests that in the thermodynamic limit, either the system truely phase separates, or there exists long wavelength collective modes whose wavelength is comparable to or larger than the system size we are able to simulate. The question is addressed in the next part.

H Spin-density wave states with long wave length modulation in the ground state of the doped Hubbard model.

What happens to the antiferromagnetic (AF) order in the Hubbard model when it is doped? This is a long-standing fundamental question not only for understanding the magnetic properties, which the Hubbard model was originally designed to describe, but also in the context

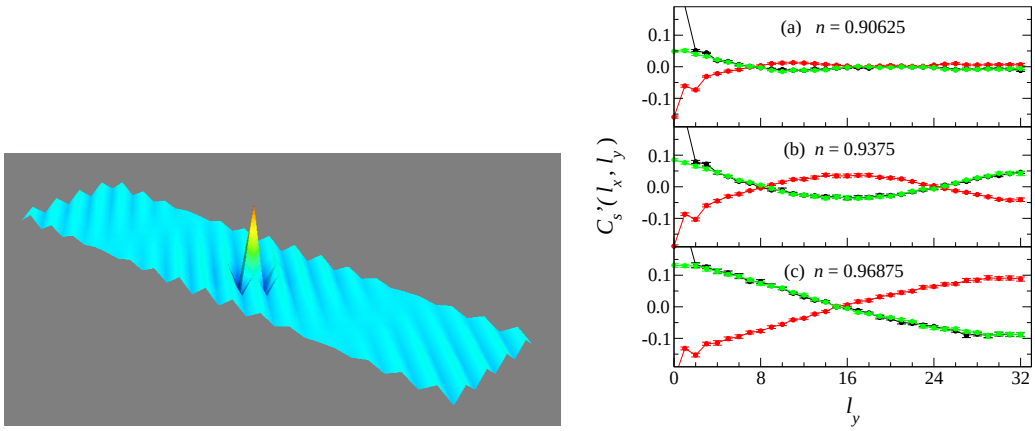

Figure 3: SDW states with long wavelength modulation in the 2-D Hubbard model [26]. The **left panel** is a 3-D plot of the spin-spin correlation function in the ground state of 8×32 lattice with 240 electrons ($n = 0.9375$) and $U/t = 4$. Anti-ferromagnetic order can be seen from the diagonal "lines." Phase shifts occur at the nodal lines, across which there is a mismatch of the diagonal lines. The **right panel** examines the doping dependence. The staggered spin-spin correlation function is plotted, at three different densities. Calculations are done using *free-electron* trial wave function. The long wavelength modulation and nodal lines (two colors crosing) are clear. As doping is increased, the wavelength of the modulating wave decreases, as does the amplitude of the SDW.

of high-T_c, which shares the same parameter regime and is believed to be closely related to AF fluctuations. We have calculated the ground-state equation of state [24, 26] and the magnetic correlations [26], using the phaseless AFQMC method (which reduces to the constrained path method [27] with on-site interaction). Twist-average boundary conditions were used, a common algorithmic development with electronic structure calculations [7]. An accurate equation of state was obtained for the paramagnetic phase (doping $>\sim 0.15$). With smaller doping, an incommensurate SDW state is found at intermediate interaction strengths, with antiferromagnetic order and essentially homogeneous charge correlation. The wavelength of the collective mode decreases with doping, as does its magnitude. As the interaction is increased, the holes go from a wave- to a particle-like state, and charge ordering begins to develop which eventually evolves into stripe states [28].

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