A STUDY OF THERMODYNAMICS OF ELECTRON CORRELATIONS IN A MAGNETIC FIELD

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ABSTRACT

High magnetic fields, combined with low temperatures, can quench the kinetic energy of two-dimensional electron systems, leaving the Coulomb interaction between electrons as the dominant force. We will begin by reviewing the properties of the noninteracting electron gas, developing its Greens functions, analyzing its thermodynamics, Pauli paramagnetism, and Landau diamagnetism. We will recall how its thermodynamics is qualitatively different from those of Boltzmann and Bose gases. We simulate the Hubbard–Hofstadter model using the Deterministic Quantum Monte Carlo (DQMC) algorithm. We report the field and Hubbard interaction strength dependences of charge compressibility, fermion sign, local moment, magnetic structure factor and specific heat. The gross structure of the magnetic Bloch bands and band gap determined by the non-interacting Hofstadter spectrum is preserved in the presence of U. The fermion sign is improved in the incompressible regions of the phase diagram.

Keyword: - *DQMC, Electron, Moment, and Heat etc.*

1. INTRODUCTION

Electronic correlation is the interaction between electrons in the electronic structure of a quantum system. Correlation energy is a measure of how much the motion of an electron is affected by the presence of all other electrons. The s electrons, which to a good approximation are free electrons, will shield the interaction between two d electrons to a great extent when the d' electrons are on different atoms. In the present paper it is assumed that the interaction between two d electrons vanishes unless they are on the same atom. Interactions within the same atom will not be appreciably conserved. When the Bohm–Pines theory is applied to Ni which has 0.6 4s electrons per atom, the shielded interaction changes its sign depending on the distance between nearest neighbor lattice sites. Although this result cannot be taken up for quantitative verification, the above assumption can be considered a semi-quantitatively correct simplification to make the calculations feasible. In calculating the matrix elements of interactions, we will ignore the overlap between atomic orbitals belonging to neighboring atoms. In other words, the atomic orbitals are replaced by the corresponding Wannier functions. This last assumption may be reasonable for a non-degenerate band in the limit of tightly bound electrons. This will be re-examined later, when the distortion of the D band will be taken into account.

The properties of non-interacting electrons in a two-dimensional periodic lattice under the influence of a strong magnetic field are fairly well understood. In this system, competition between the lattice and magnetic length scales leads to a fractal Hofstadter butterfly spectrum with recalcitrant magnetic subband structure[1,2], which generalizes the idea of Landau levels in a free electron gas. The Chern number integers associated with these magnetic subbands provide an elegant interpretation of the quantum Hall effect[3]. Experimentally, the Hofstadter Hamiltonian has been realized in ultra-cold atoms loaded on optical lattices[4], and direct observation of the Hofstadter spectrum has been reported in Moiré superlattices in graphene with high resolution[5,6].

Deterministic Quantum Monte Carlo (DQMC) [7,8,9] is an unbiased and numerically accurate algorithm to study quantum systems at finite temperatures. It employs a discrete Hubbard–Stratnovich transformation to reduce the quaternion Hubbard interaction term to a quadratic at the expense of introducing a fluctuating auxiliary field. This auxiliary region is then sampled using the Metropolis-Hastings algorithm. DQMC has been successfully employed in (zero-field) Hubbard models to study spin and charge excitations [10,11] and superconducting fluctuations [12], as well as fluctuating stripes [13] and T Evidence has also been found for -linear resistance [14]. The DQMC method is particularly powerful at half-filling in the absence of kinetic frustration36, where the fermion sign

problem is absent even in the presence of a magnetic field due to particle-hole symmetry. This allows simulations to be performed at much lower temperatures, giving access to properties more reflective of the ground state.

1.1 Thermodynamics of electron correlations

The Hofstadter–Hubbard model captures the physics of strongly correlated electrons in an applied magnetic field, which is relevant to many recent experiments on Moiré materials. Few large-scale, numerically accurate simulations exist for this model. Based on state-of-the-art quantum Monte Carlo simulations, we investigate the metallic states of a one-dimensional T-J model and a disordered Kondo lattice model in two dimensions. In the one-dimensional case, it is known that correlation effects invalidate the Fermi liquid picture and the primary excitations are spinons and holons that carry the charge and spin of the electron separately. In this dimension we will present new results on the single particle spectral function and discuss the implications of spin-charge separation on this quantity. The Kondo lattice model describes heavy fermion materials that have the usual Fermi liquid ground state but have effective masses up to three orders of magnitude larger than the bare electron mass.

1.2 Magnetic Field

Magnetic field is the area around a magnet in which the effect of magnetism is felt. We use magnetic fields as a tool to explain how magnetic forces are distributed around and within a magnetic object in nature. The basic view is that magnetism is one of the manifestations of electron–electron interaction, and its treatment should be part of the general discussion of electron correlation effects. Although the text is mainly theoretical, a large number of illustrative examples are brought from the experimental literature.

2. THE ONE-DIMENSIONAL T - J MODEL AT FINITE DOPING

In the Fermi liquid theory, the metallic state can be viewed as a gas of non-interacting electrons where correlation effects are hidden in a renormalized mass. The primary excitations are carrying quantum numbers of the bare electron: unit charge and spin 1/2. The success of the Fermi liquid theory is based on two facts: (i) due to Fermi statistics, the phase space available for Coulomb repulsion vanishes at low energies and (ii) Coulomb repulsion is investigated. One of the important issues in the theory of correlated electron systems is to understand under what conditions the Fermi liquid ground state will or will not be realized. From an experimental point of view materials such as high temperature superconductors point to the failure of the Fermi liquid theory. Heavy fermion materials like CeCu6, on the other hand, generally have a Fermi liquid ground state, but the effective mass is up to three orders of magnitude greater than that of the bare electron.

For a better understanding of the T-J model it is useful to make a canonical transformation rather than studying it in its standard formulation (Equation 1). In this way, without introducing approximations and without expanding the Hilbert space of the system, we obtain a Hamiltonian bilinear in fermion fields that is very suitable to investigate through a new QMC algorithm, the hybrid loop algorithm, which we developed Is and will be described. In detail in the following section. The canonical transformation is as follows [1]

$$H_{t-J} = -t \sum_{<i,j>,\sigma} \tilde{c}^{\dagger}_{i,\sigma} \tilde{c}_{j,\sigma} + J \sum_{<i,j>} \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{1}{4} \tilde{n}_i \tilde{n}_j \right). \qquad (1)$$

$$c^{\dagger}_{i\uparrow} = \gamma^{+}_i f_i - \gamma^{-}_i f^{\dagger}_i \,, \quad c^{\dagger}_{i\downarrow} = \sigma^{-}_i (f_i + f^{\dagger}_i) \,, \qquad (2)$$

3. METHODS

In simple terms, the molecular orbitals of the Hartree–Fock method are optimized by evaluating the energy of an electron in each molecular orbital rotating in the average field of all other electrons, rather than involving instantaneous repulsion between electrons.

To take electron correlation into account, there are several post-Hartree–Fock methods, including: Configuration Interaction (CI) One of the most important methods to correct missing correlation is the configuration interaction (CI) method. Starting from the Hartree–Fock wavefunction as the ground determinant, one takes a linear combination of the ground and excited determinant AI as the correlated wavefunction and optimizes the weighting factors.

CI according to variational theory. When taking all possible excited determinants, one speaks of the full-CI. In the full-CI wave function all electrons are perfectly correlated. For non-small molecules, full-CI is computationally very expensive. One truncates the CI expansion and obtains well-correlated wave functions and well-correlated energies according to the level of truncation.

Moller–Plesset perturbation theory (MP2, MP3, MP4, etc.)

Perturbation theory gives correlated energies, but no new wave functions. PT is not variable. This means that the calculated energy is not an upper bound for the exact energy. In Möller–Plesset perturbation theory it is possible to split the energy through interacting quantum atoms (IQA) energy splitting (although correlation energies are usually

not split). It is an extension of the theory of atoms in molecules. IQA energy partitioning enables the correlation energy contributions from individual atoms and atomic interactions to be seen in detail. IQA correlation energy partitioning has also been shown to be possible with coupled cluster methods. [15] [16]

Multi-Configurational Self-Consistent Field (MCSCF)

Combinations are also possible. E.g. one has some truncated CI method for the static correlation and/or some truncated CI method for the largest part of the dynamic correlation and/or some perturbative ansatz for small perturbations (insignificant) on top of the multi-configurational self-consistent field method. There may be some approximately degenerate determinants for . Determinant. Examples of those combinations are CASPT2 and SORCI.

Explicitly correlated wavefunction (R12 method)

This approach includes a term depending on the interelectron distance in the wavefunction. This leads to faster convergence in terms of basis set size than a pure Gaussian-type basis set, but requires the computation of more complex integrals. To simplify them, the interelectron distances are expanded into a series forming simple integrals. The idea of R12 methods is quite old, but practical implementations have only recently begun to emerge.

4. RESULTS AND DISCUSSION

At half-filling, the Fermi surface of the non-interacting Hofstadter model consists of a finite number of Dirac points at isoquant rational fractions of the magnetic flux per fillet. Thus the ground state of the Hubbard–Hofstadter model is expected to remain a Dirac semimetal up to some finite coupling strength UC. At half magnetic flux quantum per fillet, the model is also known as the π-flux model and has been extensively studied numerically. As the interaction is turned on, the π-flux model exhibits a quantum phase transition of the chiral Heisenberg Gross-Neuve universality class at Uc ≈ 5.6t in an antiferromagnetic Mott insulator (AFMI). Since the π-flux model corresponds to the threaded Hubbard–Hofstadter Hamiltonian with the maximum possible flux, we can think of the zero-field Hubbard model on a half-filled square lattice as a "0-flux model", which is a metal Emits AFMI transition with Uc = 029,30. Our simulations address the intermediate field strengths between the 0-flux and π-flux Hubbard models, which, to the best of our knowledge, have not been studied via DQMC.

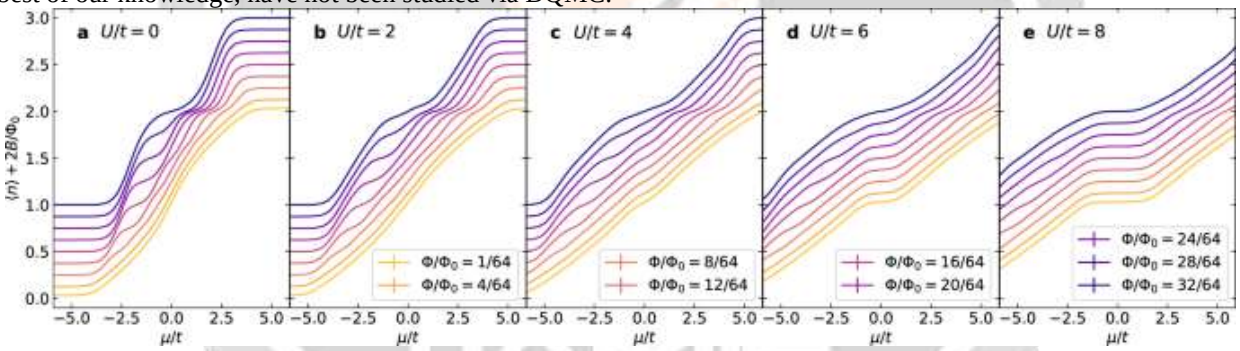

Figure 1.1: Electron density versus chemical potential[17].

It monotonically decreases as the magnetic field increases, which is consistent with previous accurate diagonalization results. The same trend can be seen in the "correlated Hofstadter butterfly" plot, as shown in Supplementary Figure 1.1 and described in Supplementary Note 2. We will discuss in more detail later, the behavior of the Mott gap. It is instructive to plot our data as a Wannier diagram, i.e., a color intensity plot of charge compressibility $\chi = \partial \langle n \rangle / \partial \mu$ as a function of electron density $\langle n \rangle$ and magnetic field strength B. Charge compressibility, or thermodynamic density of states, is directly measurable in experiments 9,13. In a non-interacting system, at zero temperature, the charge compressibility is equal to the single-particle density of states.

Fermion symbol[17]

An important quantity in QMC simulations of interacting fermions is the fermion sign. The Hubbard–Hofstadter model is sign-problem-free on half-fillings on bipartite lattices. But the fermion sign problem45 fundamentally prevents us from obtaining high quality simulation data at low temperatures and far from half filling. Thus, any insight into the factors influencing the severity of the signal problem is valuable. Since the fermion sign problem is NP-hard46, we do not expect any general solution to the fermion sign problem. Nevertheless, since the sign problem is representation-dependent, it is possible to reduce or completely remove the sign problem for specific classes of non-generic Hamiltonians. In this work, we find a correlation between the fermion sign and the charge compressibility. In Figure 1.2, we show the fermion sign $\langle s \rangle$ and the charge compressibility χ, both plotted against $\langle n \rangle$ for a representative set of parameters. In this interacting system the local minima of charge compressibility correspond exactly to the local maxima of the fermion sign. At these local maxima, the fermion sign

can be an order of magnitude better than the value for other electron densities and the standard zero-field Hubbard model. For an extended figure showing that this correspondence is general in our parameter space and not a finite-size artifact, see Supplementary Figure 1.2 and Supplementary Note 3. Our results may mean that although the Hubbard model, in general, suffers from a sign problem, it is possible to obtain good results when we precisely locate the integer quantum Hall plateau. Since similar signal-compression correspondences have been reported, it appears that fermion sign rectification is quite common in insulating phases, which is consistent with our intuition that fermionic statistics become less important in localized states. Our results also relate to recent work that suggests that the fermion sign is not just a coincidental barrier to access to low temperature physics, but may reflect the intrinsic physics of the model Hamiltonian.

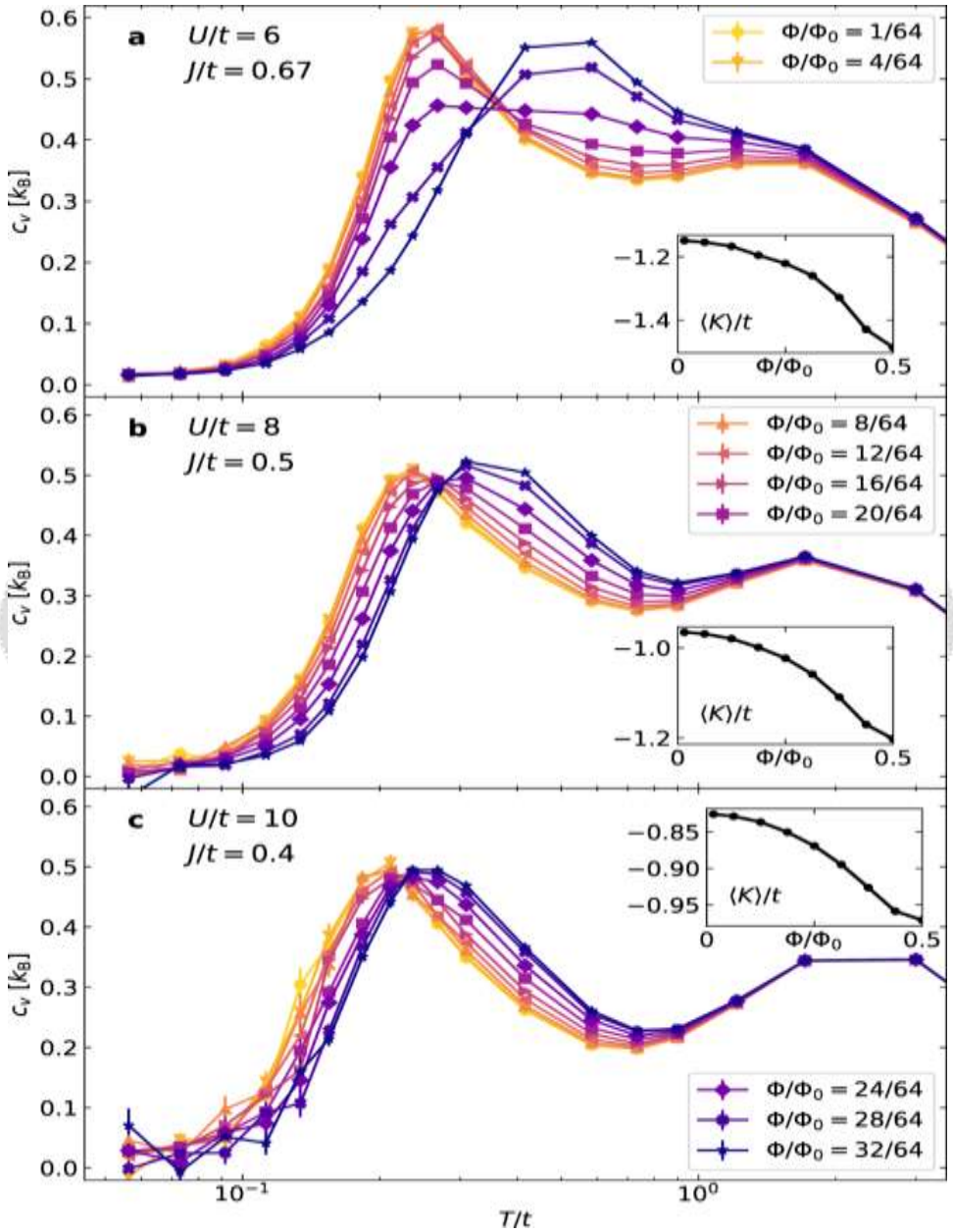

Figure 1.2: Evolution of specific heat and kinetic energy in the half-filled Hubbard-Hofstadter model[17].

5. CONCLUSIONS

In this work, we apply DQMC to simulate the Hubbard-Hoff stator model and directly investigate prototypes on the field of correlated architectural devices, specifically on charge reservoir, local amplitude, magnetic structure factor and specific heat. Attention instructions have been implemented. Did. By investigating charge compressibility, we find that the magnetic Bloch band records are being destroyed by the Hubbard, but in the presence of regional local

correlations of non-interacting bands far from the filling, the shares accessible to the DCC are created. At quasi-equality, we decide that the orbital magnetic field and the Hubbard potential act anti-correlatedly. At intermediate to strong coupling U/t [6, 10], strong orbital magnetic fields reduce the apparent width of the MOT gap, reduce the amplitude of the local amplitude and magnetic structure factors, catalog the kinetic energy, and advance Do-Changes in T typically occur from the extremes of energy to higher temperatures. Together, these phenomena indicate that an orbital magnetic field is localized to planets and the effects of U are minimized. From the algorithm parameter, we find that the fermion sign in DCMC Astron is significantly improved when the physical system is uncoupled[17]. In Co and Fe, where more than one d hole exists per atom, exchange interactions between different atomic d orbitals will contribute some to the energy difference between the ferromagnetic state and the paramagnetic state. However, discussion of these metals requires detailed knowledge of the D band and more sophisticated treatment of electron correlation. A discussion of light transition metals such as V and Ti will also not be possible, because a simple tight bond approximation employed in the present paper would not be appropriate in these metals, and interatomic interactions have been neglected in the present paper. Can play an important role.

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