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# Auxiliary-Field Quantum Monte Carlo Simulations of Strongly-Correlated Systems, the Final Report

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## Disclaimer



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## I. OVERALL OBJECTIVE

In this final report, we present preliminary results of ground state phases of interacting spinless Dirac fermions. The name "Dirac fermion" originates from the fact that low-energy excitations of electrons hopping on the honeycomb lattice are described by a relativistic Dirac equation. Dirac fermions have received much attention particularly after the seminal work of Haldale[1] which shows that the quantum Hall physics can be realized on the honeycomb lattice without magnetic fields. Haldane's work later becomes the foundation of topological insulators (TIs). While the physics of TIs is based largely on spin-orbit coupled non-interacting electrons, it was conjectured[2] that topological insulators can be induced by strong correlations alone.

Motivated by the idea of topological Mott insulators, we study the physics of interacting spinless Dirac fermions. The system is arguably the simplest model that can possibly realize the topological Mott insulator.[2] The model is defined by the Hamiltonian

$$\hat{H} = -t\sum_{\langle ij\rangle}\left(\hat{c}_i^\dagger\hat{c}_j + \hat{c}_j^\dagger\hat{c}_i\right) + V_1\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j + V_2\sum_{\langle\langle ij\rangle\rangle}\hat{n}_i\hat{n}_j. \quad (1)$$

Here $\hat{c}_i^\dagger$ ($\hat{c}_i$) creates (destroys) a spinless fermion at site $i$, and $\hat{n}_i$ is the number operator. $t$ is the uniform hopping integral between near-neighbor sites $i$ and $j$. The parameter $V_1$ and $V_2$ represent the strength of near-neighbor (NN) and next-next-neighbor (NNN) interactions. The notation $\langle ij\rangle$ and $\langle\langle ij\rangle\rangle$ denote the summation is carried out over NN and NNN sites respectively. We use $t$ as the unit of energy and set $t = 1$.

In this report, focus will be on the physics induced by the NN interaction $V_1$. As such, the NNN interaction will be set to $V_2 = 0$. At half-filling and $V_1 > 0$, exact QMC calculations[3,4] have shown that the system will undergo a quantum phase transition at $V_1^c \sim 1.36(3)$. The ground state is a semimetal for $V_1 < V_1^c$, and a charge density wave at $V_1 > V_1^c$. There is no QMC data for $V_1 < 0$ to date due to the sign problem. We use the AFQMC approach developed for generalized Hartree-Fock orbitals and extend the algorithm for spinless fermions. Trial wave functions are generated using a mean-field theory that allows both diagonal $\langle\hat{c}_i^\dagger\hat{c}_i\rangle$ (density order) and off-diagonal $\langle\hat{c}_i^\dagger\hat{c}_j\rangle$ (bond order) order parameters. The previous report has given results of the attractive $V_1$ model at half-filling. In this case, the ground state phase separates into particle-rich and hole-rich regions when the interaction strength $V_1 \lesssim -1.7$. Here we will report preliminary data of the model when it is doped with holes.

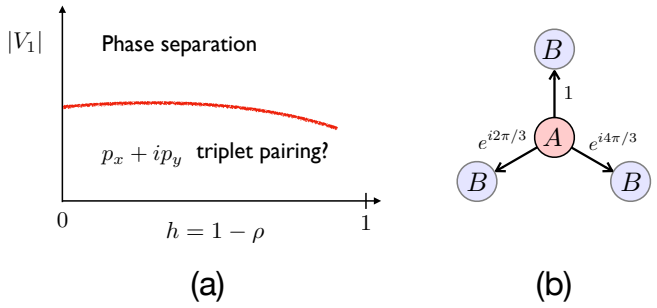


FIG. 1. (a) Schematic ground state phase diagram of doped Hubbard model for spinless fermions on the honeycomb lattice. $h$ and $\rho$ are hole and particle density respectively. (b) Real-space near-neighbor $p_x + ip_y$ pairing symmetry. $A$ and $B$ are the two sublattice indices of the honeycomb lattice. The complex number attached to each arrow is the pair-field operator form factor.

## II. PRELIMINARY RESULTS

Density distribution: The results at half-filling suggest that the ground state of doped Hubbard model for spinless Dirac fermions will phase separate at sufficiently large $|V_1|$. In order to verify this conjecture, we will first be looking at real space density distribution $\rho(\mathbf{r})$ and hole-hole correlation function. The latter quantity is defined as

$$N(\mathbf{q}) = \frac{1}{L}\sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\,\langle(1-\hat{n}_i)(1-\hat{n}_j)\rangle. \quad (2)$$

Here $\langle\ldots\rangle$ denotes the ground state expectation value, and $\mathbf{q}$ is the allowed wave vectors within the first Brillouin zone. $L$ is the linear dimension of the $L\times L\times 2$ honeycomb lattice. Fig. 2 summarizes the data acquired on the $L = 6$ lattice at $V_1 = -1.6$ and $-1.8$. At $\rho = 5/12$, which is close to half-filling $\rho = 6/12$, the density distribution already shows some degree of inhomogeneity at $V_1 = -1.6$. Recall that at $\rho = 6/12$ the critical $V_1$ for phase phase separation is roughly $V_1 = -1.7$. As a result, the slight inhomogeneity observed in the slight doped case is very likely a precursor of phase separation. Indeed, at $V_1 = -1.8$, the doped ground state phase separates, as shown in Fig. 2(c). This is also demonstrated by the structure factor $N(\mathbf{q})$ Fig. 2(d) which clearly peaks at the smallest (in length) wave vector. Turning to the heavily doped case $\rho = 3/12$, the density distribution is quite homogeneous at $V_1 = -1.6$. Here again, Fig. 2(g) and (h) strongly indicate that the system is phase separated at $V = -1.8$. To better contract the behavior of $N(\mathbf{q})$ near the phase separation critical point, we plot in Fig. 3 the charge structure factor along high symmetry

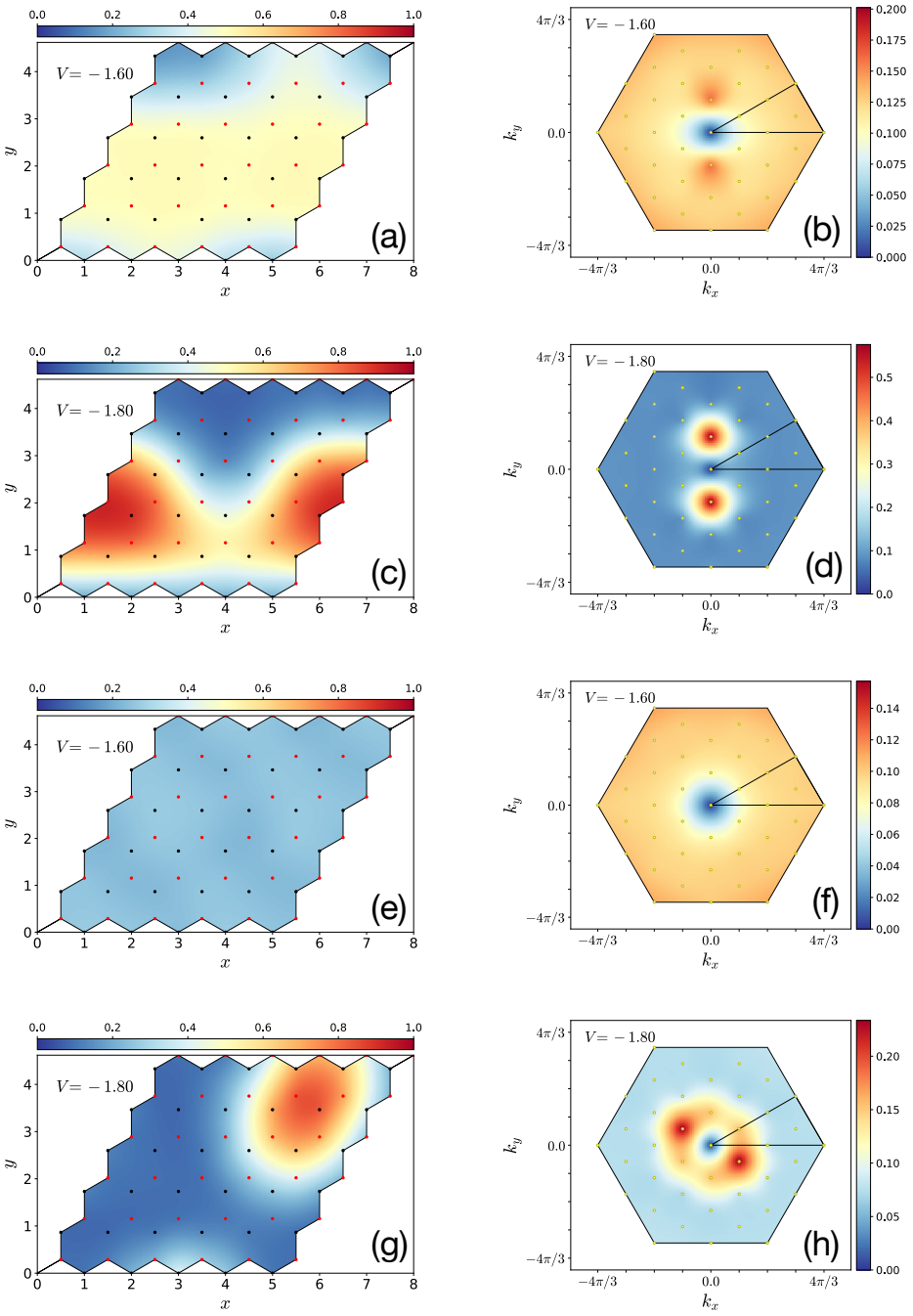


FIG. 2. Density distribution $\rho(\mathbf{r})$ (left column) and structure factor $N(\mathbf{q})$ (right column) of doped Hubbard model for spinless Dirac fermions on the $6 \times 6 \times 2$ lattice. The particle density is (a)-(d) $\rho = 5/12$, and (e)-(h) $\rho = 3/12$. The black and red dots in the density plots represent lattice sites. The yellow circles in the $N(\mathbf{q})$ plots show the allowed $\mathbf{k}$-points in the first Brillouin zone. Note that $N(\mathbf{q} = 0)$ is not plotted. At $V_1 = -1.8$, it is clear that both systems phase separate into hole-rich and particle-rich regions. In this case, $N(\mathbf{q})$ peaks at the smallest (in length) wave vector.

points $\Gamma$-$M$-$K$-$\Gamma$. It appears that, at least for $L = 6$, the ground state phase separates for $V_1 < -1.8$ regardless of doping levels.

Superconductivity: Next we move on to examine properties of the ground state before the system phase separates. In our previous report, the Bogoliubov-de Gennes calculation suggests the possibility of $p$-wave superconductivity in the doped model. To verify, we compute the uniform $p$-wave superconducting pairing structure factor

$$P_{p+ip} = \frac{1}{2L^2} \sum_{\mathbf{i} \in A} \sum_{\mathbf{j}} \langle \hat{\Delta}_{\mathbf{i}} \hat{\Delta}^{\dagger}_{\mathbf{i}+\mathbf{j}} + \hat{\Delta}^{\dagger}_{\mathbf{i}} \hat{\Delta}_{\mathbf{i}+\mathbf{j}} \rangle, \qquad (3)$$

where the pair-field operator is defined as

$$\hat{\Delta}_{\mathbf{i}} = \sum_{\delta} \mathcal{F}_{\delta}\, \hat{c}_{\mathbf{i}}\, \hat{c}_{\mathbf{i}+\delta}. \tag{4}$$

The quantity $\mathcal{F}_{\delta} = (1, e^{i2\pi/3}, e^{i4\pi/3})$ is the $p$-wave pairing form factor shown in Fig. 1(b), and $\delta$ denotes nearneighbor bonds of site $\mathbf{i}$ on sublattice $A$. Our preliminary results for the $L = 6$ lattice are plotted in the left panel of Fig. 4 at four different doping levels. The data indicate that the $p$-wave superconductivity is enhanced by increasing $|V_1|$. In all cases, the sudden drop in $P_{p+ip}$ near $-1.8 < V_1 < -1.6$ is caused by the phase separation. Interestingly, there seems to be an *optimal doping* for the $p$-wave superconductivity. In order to confirm there is a superconducting phase, we compute $P_{p+ip}$ at two different system sizes at the same density $\rho = 4/12$. The data are presented in the right panel of Fig. 4. Apart from the finite-size effect[5], $P_{p+ip}$ in fact grows with $L$. This tendency indicates the existence of a long-range $p$-wave superconducting order in the doped model.


[1] F. D. M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).
[2] S. Raghu, X.-L. Qi, C. Honerkamp, and S.-C. Zhang, Phys. Rev. Lett. **100**, 156401 (2008).
[3] L. Wang, P. Corboz, and M. Troyer, New J. Phys. **16**, 103008 (2014).
[4] Z.-X. Li, Y.-F. Jiang, and H. Yao, New J. Phys. **17**, 085003 (2015).
[5] Our preliminary data for the doped cases seem to suggest that the phase separation phase boundary depend strongly on $L$.

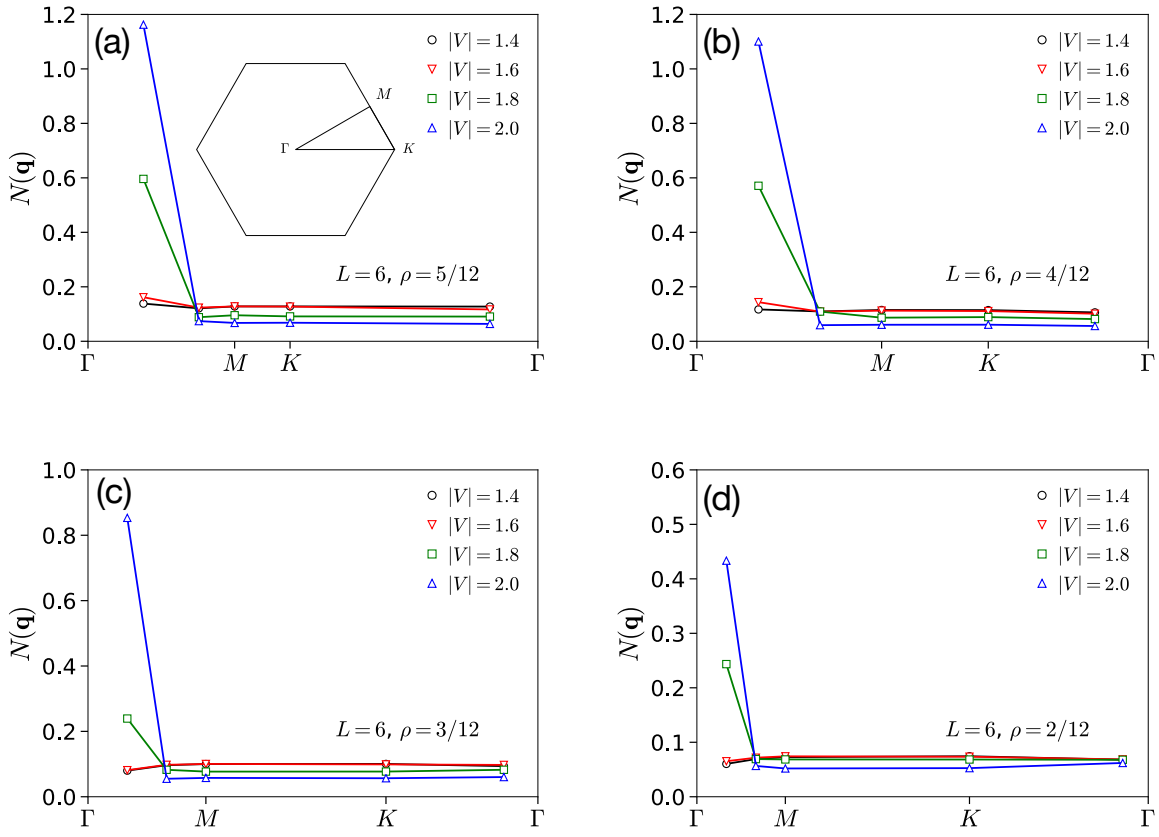


FIG. 3. Charge structure factor $N(\mathbf{q})$ plotted along high symmetry lines shown in the inset of panel (a). In all panels, there is a dramatic change in the behavior of $N(\mathbf{q})$ as we scan $|V_1|$ across $-1.60 \lesssim V_1 \lesssim -1.80$. The diverging $N(\mathbf{q})$ at $\mathbf{q} \to 0$ indicates that the ground state is phase separated at $V_1 < -1.8$.

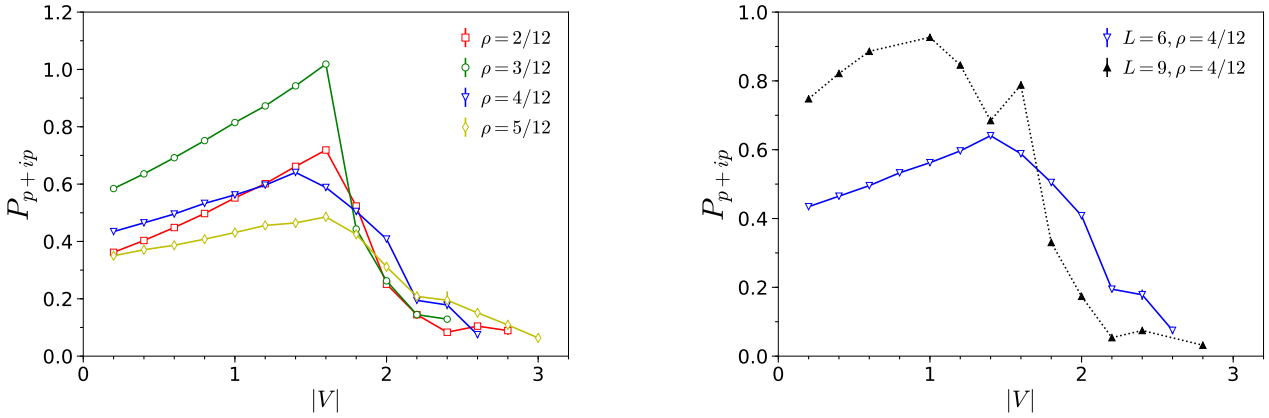


FIG. 4. Left: Uniform $p+ip$ pairing structure factor as a function of $|V_1|$ measured at 4 different doping levels. In all cases, $P_{p+ip}$ grows with the strength of attraction until the system phase separates near $-1.8 < V_1 < -1.6$. Right: Same quantity measured on two system sizes. For $|V_1| \lesssim 1.0$, $P_{p+ip}$ seems to scale with $L$, indicating the existence of a long-range superconducting order.