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Fermionic quantum critical point of spinless fermions on a honeycomb lattice

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Abstract
Spinless fermions on a honeycomb lattice provide a minimal realization of lattice Dirac fermions. Repulsive interactions between nearest neighbors drive a quantum phase transition from a Dirac semimetal to a charge-density-wave state through a fermionic quantum critical point, where the coupling of the Ising order parameter to the Dirac fermions at low energy drastically affects the quantum critical behavior. Encouraged by a recent discovery (Huffman and Chandrasekharan 2014 Phys. Rev. B 89 111101) of the absence of the fermion sign problem in this model, we study the fermionic quantum critical point using the continuous-time quantum Monte Carlo method with a worm-sampling technique. We estimate the transition point $V/t = 1.356(1)$ with the critical exponents $\nu = 0.80(3)$ and $\eta = 0.302(7)$. Compatible results for the transition point are also obtained with infinite projected entangled-pair states.

Keywords: quantum critical point, Dirac fermions, quantum Monte Carlo

1. Introduction
Interaction-induced quantum phase transitions of Dirac fermions are of general interest in graphene [2], $d$-wave superconductors [3], topological insulators [4], ultracold atoms [5] and high-energy physics [6]. One of the prototypical examples consists of half-filled spinless
fermions on a honeycomb lattice interacting through nearest-neighbor repulsions

\[
\hat{H} = \hat{H}_0 + \hat{H}_1,
\]

\[
\hat{H}_0 = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i) = \sum_{i,j} \hat{c}_i^\dagger K_{ij} \hat{c}_j,
\]

\[
\hat{H}_1 = V \sum_{\langle i,j \rangle} \left( \hat{n}_i - \frac{1}{2} \right) \left( \hat{n}_j - \frac{1}{2} \right).
\]

Equation (1) is arguably the simplest model exhibiting a quantum phase transition of Dirac fermions in two dimensions. However, despite its deceptively simple form, the model exhibits an unconventional quantum critical point that deserves detailed study because it may lay the foundation for understanding rich phenomena when other degrees of freedom or intertwined phases are involved.

The phase diagram of equation (1) is easy to anticipate; see figure 1. The system behaves like a classical lattice gas in the strong-coupling limit \( (V \gg t) \) and favors a staggered charge-density-wave (CDW) state. The CDW state breaks the discrete sublattice symmetry and melts through a two-dimensional (2D) Ising transition upon an increase of temperature or a quantum phase transition upon decrease of \( V/t \). The red dot represents a fermonic quantum critical point, which is the focus of this paper.

The topology of the phase diagram figure 1 resembles that of the familiar 2D transverse field Ising model [3], where quantum fluctuations induced by the transverse field destroy the Ising long-range order. However, in model equation (1), the coupling of the Ising-order...
parameter to the Dirac fermions at low energy strongly affects its quantum critical behavior. It cannot be treated by the familiar scalar $\phi^4$-theory, since integrating the Dirac fermions will lead to a singular action for the Ising fields. The low-energy physics are believed to be described by the Gross–Neveu–Yukawa theory [7–10], which features a fermionic quantum critical point. The Gross–Neveu–Yukawa theory has been studied intensively in the context of high-energy physics [11–14], and the quantum critical point scenario of the $d$-wave superconductors [15–17]; however, there is no consensus concerning the critical exponents, partially due to the uncontrolled approximations involved in various theoretic approaches.

Quantum Monte Carlo (QMC) simulations are a valuable unbiased approach to study the quantum critical behavior if the notorious fermion sign problem is absent [18]. A recent example is the study of Dirac semimetal to antiferromagnetic insulator transition in the half-filled repulsive Hubbard model on the honeycomb lattice [19–22]. Unfortunately, the seemingly simpler model equation (1) has a severe sign problem in the conventional auxiliary field QMC method [23]. Early QMC studies have thus been limited to high temperatures or small system sizes [24, 25]. The meron-cluster algorithm [26] solves the sign problem for $V \geq 2t$ and simulations using it confirm the finite temperature Ising transition of several staggered fermion models [27, 28]. However, the quantum critical point of the model equation (1) lies at $V < 2t$ and is not accessible by the meron-cluster algorithm. The Fermi bag approach [29] has been used to study the 3D lattice massless Thirring model [30] and the Gross–Neveu model [31] with two flavors of four-component Dirac fermions.

Recently, in [1] it was discovered that the sign problem of the model equation (1) is absent in the continuous-time quantum Monte Carlo (CTQMC) formalism [32, 33]. This allows us to access the quantum critical point in the CTQMC simulation. Using a standard finite size scaling (FSS) analysis we estimate the critical point $V/t \approx 1.356$ and the critical exponents $\nu \approx 0.8, \eta \approx 0.3$. Our results are summarized in table 1. We believe these results not only apply to the specific microscopic model equation (1), but also hold for many intriguing problems, including the chiral symmetry breaking of Dirac fermions [6] and the quantum critical point in the $d$-wave superconductors [3]. Future theoretical or experimental advances in either field [2–6] will be able to test our predictions.

<table>
<thead>
<tr>
<th>L = 6, 9, 12, 15</th>
<th>L = 9, 12, 15</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_c$</td>
<td>1.356(1)</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.80(3)</td>
</tr>
<tr>
<td>$\eta$</td>
<td>0.302(7)</td>
</tr>
<tr>
<td>$\tilde{\beta}$</td>
<td>0.52(2)</td>
</tr>
<tr>
<td>$\chi^2$/d.o.f.</td>
<td>1.23</td>
</tr>
</tbody>
</table>

Table 1. The critical point and critical exponents determined using data collapse of $M_2$ and $M_4$ for all system sizes ($L = 6, 9, 12, 15$) and excluding the smallest one ($L = 9, 12, 15$). The critical exponent $\tilde{\beta}$ (to avoid confusion with the inverse temperature $\beta$) is calculated using $\tilde{\beta} = \frac{1}{2}(z + \eta)$. The estimated uncertainty [37] of the last digit is shown in the brackets. The $\chi^2$/d.o.f. listed in the last row shows the quality of the data collapse.
The paper is organized as follows. In section 2.1 we briefly review the CTQMC method focusing on the absence of the sign problem [1]. In section 2.2 we introduce the worm sampling technique in the Monte Carlo calculation [33–35] to improve the efficiency of the simulation. Section 3 contains our main results and discussions, as well as comparisons with results obtained by infinite-projected entangled-pair states (iPEPS) calculations. In section 4 we briefly anticipate several future research directions based on this work. In the appendices, we provide technical details of our numerical calculation (appendix A) and additional results obtained on the π-flux square lattice (appendix B).

2. Method

Two properties of the model (1) are essential for the absence of the sign problem in the CTQMC simulation. First, the filling is fixed at 1/2 per site because of the model’s particle-hole symmetry. Second, the hopping amplitudes are real and the hopping matrix \( K \) defined in equation (2) satisfies

\[ K_{ij} = -\eta_i K_{ij} \eta_j, \tag{4} \]

where the ‘parity index’ \( \eta_i = 1(-1) \) for a site \( i \in \{A,B\} \) sublattice. In fact, equation (4) together with the hermiticity property implies \( K_{ij} = 0 \) if sites \( i \) and \( j \) belong to the same sublattice, i.e. the bipartite condition.

2.1. Interaction expansion CTQMC and the sign problem

We expand the partition function of the system in terms of the interaction vertices of equation (3) [32, 33]

\[
Z = Z_0 \sum_{k=0}^{\infty} \frac{(-V)^k}{k!} \sum_{\{i_1,i_2\}} \cdots \sum_{\{i_{2k-1},i_{2k}\}} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \cdots \int_0^\beta d\tau_{2k} \delta(\tau_1 - \tau_2) \cdots \delta(\tau_{2k-1} - \tau_{2k})
\times \left\langle \left( \hat{n}_{i_1}(\tau_1) - \frac{1}{2} \right) \left( \hat{n}_{i_2}(\tau_2) - \frac{1}{2} \right) \cdots \left( \hat{n}_{i_{2k-1}}(\tau_{2k-1}) - \frac{1}{2} \right) \left( \hat{n}_{i_{2k}}(\tau_{2k}) - \frac{1}{2} \right) \right\rangle_0
= Z_0 \sum_{k=0}^{\infty} \frac{(-V)^k}{k!} \sum_{\{i_1,i_2\}} \cdots \sum_{\{i_{2k-1},i_{2k}\}} \int_0^\beta d\tau_2 \int_0^\beta d\tau_4 \cdots \int_0^\beta d\tau_{2k} \det(G^k), \tag{5}
\]

where \( \hat{n}_{i_1}(\tau) = e^{\hat{H}_0 \tau} \hat{n}_{i_1} e^{-\hat{H}_0 \tau} \) and \( Z_0 \) is the partition function of the noninteracting system. \( \langle \ldots \rangle_0 = \mathcal{T} \text{Tr} (e^{-\beta \hat{H}_0} \ldots)/Z_0 \) denotes the average over the noninteracting Hamiltonian equation (2) and \( \mathcal{T} \) is the time ordering operator. The interaction vertices \( \{i_1, i_2\}, \ldots, \{i_{2k-1}, i_{2k}\} \) consist of \( k \) pairs of neighboring sites. The delta functions in the first line of equation (5) indicate that the interactions are instantaneous. \( G^k \) is a \( 2k \times 2k \) matrix

\[
G^k_{pq} = G^0_{i_1,i_j}(\tau_p - \tau_q) - \delta_{pq}/2, \tag{6}
\]

where \( G^0_{i_1,i_2}(\tau) = \langle \hat{c}_i(\tau) \hat{c}_j^\dagger \rangle_0 \) is the noninteracting Green’s function. The particle–hole symmetry ensures that \( G^0_{ii}(0^+) = 1/2 \), and therefore the diagonal element of \( G^k \) vanishes. In addition, one has
\[ G^0_{i,i_0}(\tau > 0) = \left( \frac{e^{-K\tau}}{1 + e^{-\beta K}} \right)_{i,i_0}, \]  
while using the antiperiodicity of the Green’s function and equation (4) one has
\[ G^0_{i,i_p}(-\tau < 0) = -\left( \frac{e^{-K(-\tau + \beta)}}{1 + e^{-\beta K}} \right)_{i,i_p} = -G^0_{i,i_0}(\tau > 0)\eta_{i_p}\eta_{i_0}. \]

Equations (6)–(8) show that the Green’s function matrix satisfies \( G_{ij}^k = -\eta_{i_p}G_{j_0}^{\ell_k}\eta_{i_0}. \) Introducing a diagonal matrix \( D^k = \text{diag}(\eta_{i_1}, \eta_{i_2}, \ldots, \eta_{i_{2k}}) \), it can be written as
\[ (G^kD^k)^T = -G^kD^k. \]

In other words, the matrix \( G^kD^k \) is skew-symmetric and its determinant is non-negative because it equals the square of the Pfafian of the matrix. We will see in a moment that this ensures the absence of a sign problem in the CTQMC simulation.

We write equation (5) in a form suitable for Monte Carlo sampling
\[ Z = Z_0 \sum_C w(C), \]
where \( C = \{i_1, i_2; \tau_1\}, \{i_3, i_4; \tau_4\} \ldots \{i_{2k-1}, i_{2k}; \tau_{2k}\} \) denotes a configuration with \( k \) vertices. Equation (9) ensures that the weight \( w(C)^3 \) is always positive [1]
\[ w(C) = (-V)^k\text{det}(G^k) = (-V)^k\text{det}(D^k)\text{det}(G^kD^k) \]
\[ = V^k\text{pf}(G^kD^k)^2 \geq 0. \]

In the second line, we have used \( \text{det}(D^k) = \prod_{\ell=1}^{k} \eta_{i_{2\ell-1}}\eta_{i_{2\ell}} = (-1)^k. \) The absence of a sign problem allows us to simulate fairly large systems at low temperatures to access the quantum critical point. In this paper, we simulate clusters with \( L \times L \) unit cells with periodic boundary conditions. The number of sites is \( N = 2L^2 \). Close to the quantum critical point, nonrelativistic corrections are irrelevant and the dynamical critical exponent \( z = 1 \) [10]. We thus scale the inverse temperature linearly with the system length \( \beta = L^{43}. \) Because of the \( \beta^3 \) scaling of the CTQMC algorithm [32, 33], the largest system size \( L = 15 \) considered in this paper is smaller than the one used in the projective auxiliary field QMC studies of the Hubbard model [20–22].

To detect the onset of the CDW order, we measure the density–density correlation function
\[ C(R) = \frac{1}{N^2 N^R} \sum_i \sum_{|i-j|=R} \left( \left\langle \hat{n}_i - \frac{1}{2} \right\rangle \left( \hat{n}_j - \frac{1}{2} \right) \right). \]

where \( \langle \ldots \rangle = \text{Tr}(e^{-\beta H\ldots})/Z \) denotes the average over the full Hamiltonian equation (1). The second summation in equation (12) runs over all sites \( j \) (in total, \( N^R \) of them) whose graph distance to the site \( i \) is \( k \). Two sites with even (odd) graph distance have the same (different) parities. The other two important observables are the square and quartic of the CDW order parameter

3 The \( 1/k! \) factor has been canceled by the \( k! \) permutations of the vertices.
4 Strictly speaking, these sites may not be symmetrically related and may have slightly different correlation functions.
\[ M_2 = \frac{1}{N_s^2} \sum_{i,j} \eta_i \eta_j \left\{ \left( \hat{n}_i - \frac{1}{2} \right) \left( \hat{n}_j - \frac{1}{2} \right) \right\}, \quad (13) \]

\[ M_4 = \frac{1}{N_s^4} \sum_{i,j,k,l} \eta_i \eta_j \eta_k \eta_l \left\{ \left( \hat{n}_i - \frac{1}{2} \right) \left( \hat{n}_j - \frac{1}{2} \right) \left( \hat{n}_k - \frac{1}{2} \right) \left( \hat{n}_l - \frac{1}{2} \right) \right\}. \quad (14) \]

The Binder ratio [36] is calculated as:

\[ B = \frac{M_4}{(M_2)^2}. \quad (15) \]

### 2.2. Worm algorithm

Measuring \( M_2 \) and \( M_4 \) using the conventional approach [32] requires explicit loops over the \( i, j, (k, l) \) indices, and the measurements will dominate the runtime of the Monte Carlo simulations. This is especially inefficient when noticing that each term in the summation of equations (13)–(14) may differ by orders of magnitude. In addition, it is not guaranteed that the configurations sampled according to the weight of the partition function equation (5) make a significant contribution to the physical observables. A mismatch in the two distributions will lead to large fluctuations in the Monte Carlo signal. To overcome these difficulties, we extend the configuration space and use the worm algorithm [33–35] to sample the partition function and the observables on equal footing. In this way, we greatly reduce variance in the Monte Carlo simulation and avoid the explicit sum over multiple site indices in the measurement of equations (13)–(14).

Notice the similarity between the partition function equation (5) and the observables equations (13)–(14)

\[
\int \cdots \int \sum \left( -V \right)^k \sum_{\{i,k\}} \cdots \sum_{\{i,2-k\}} \int_0^\beta \cdots \int_0^\beta \cdots \int_0^\beta \cdots \int_0^\beta \\
\times \int_0^\beta \cdots \int_0^\beta \sum \eta_i \eta_j \text{det}(G^{ki;ij}), \quad (16)
\]

\[
\int \cdots \int \sum \left( -V \right)^k \sum_{\{i,2-k\}} \cdots \sum_{\{i,2-k\}} \int_0^\beta \cdots \int_0^\beta \cdots \int_0^\beta \cdots \int_0^\beta \\
\times \int_0^\beta \cdots \int_0^\beta \sum \eta_i \eta_j \eta_k \eta_l \text{det}(G^{ki;ijkl}), \quad (17)
\]

where \( G^{k;ij} \) extends \( G^k \) to the following \( (2k + 2) \times (2k + 2) \) matrix:

\[
G^{k;ij} = \begin{pmatrix}
G_{ij|p}(\tau - \tau_q) - \delta_{pq}/2 & G_{ij|p}(\tau - \tau) & G_{ij|p}(\tau_p - \tau) \\
G_{ji|p}(\tau - \tau) & 0 & G_{ij|p}(0^-) \\
G_{ij|q}(\tau - \tau_q) & G_{ij|p}(0^+) & 0
\end{pmatrix}. \quad (18)
\]
Similar to equation (9), $G^{k;i,j}$ satisfies the following equation

$$ (G^{k;i,j}D^{k;i,j})^T = -G^{k;i,j}D^{k;i,j} \quad (19) $$

where the diagonal matrix $D^{k;i,j} = \text{diag}(\eta_{i}, \eta_{j})$ extends $D^{k}$ in a similar manner. Similarly, $G^{k;i,j,l}$ is a $(2k+4) \times (2k+4)$ matrix. We define $W_2 = \xi_2 \beta N_2^2 Z M_2$, $W_4 = \xi_4 \beta N_4^2 Z M_4$ and enlarge the configuration space into

$$ Z + W_2 + W_4 = Z_0 \sum_c W(C). \quad (20) $$

Now the configurations $C$ may contain a two-site worm $\{i, j; \tau\}$ or a four-site worm $\{i, j, k, l; \tau\}$ in addition to the vertices described in equation (10); see figure 2 for an example. By sampling the extended configuration space, we can treat the summation over $i, j, k, l$ in equation (16)–(17) and the summations over the vertices on an equal footing. Here, $\xi_2$ and $\xi_4$ are two positive numbers we can choose freely to balance the configurations in different sectors. We have devised several Monte Carlo updates and describe them in appendix A. We use the following notation to denote the relative time spend in each sector [35]

$$ \langle \delta^2 \rangle_{MC} = \frac{Z}{Z + W_2 + W_4}, \quad (21) $$

$$ \langle \delta^2 \rangle_{MC} = \frac{W_2}{Z + W_2 + W_4}, \quad (22) $$

$$ \langle \delta^2 \rangle_{MC} = \frac{W_4}{Z + W_2 + W_4}. \quad (23) $$

The observables (13)–(15) then are

$$ M_2 = \frac{1}{\xi_2 \beta N_2^2} \langle \delta^2 \rangle_{MC}, \quad (24) $$

$$ M_4 = \frac{1}{\xi_4 \beta N_4^2} \langle \delta^2 \rangle_{MC}, \quad (25) $$

$$ B = \frac{\beta \xi_2^2}{\xi_4} \langle \delta^2 \rangle_{MC} \langle \delta^2 \rangle_{MC}. \quad (26) $$

The density correlation function is measured when the configuration is in the $W_2$ space and the distance between the two worm sites $i, j$ is equal to $R$,

$$ C(R) = \frac{1}{\xi_2 \beta N_i N_j} \frac{\langle \delta^2 \rangle_{MC}}{\langle \delta^2 \rangle_{MC}}. \quad (27) $$

The weight of a configuration $C \in W_2$ with the worm at $\{i, j; \tau\}$ is

$$ w(C) = (-V)^k \eta_i \eta_j \det(G^{k;i,j}) = V^k \text{pf}(G^{k;i,j} D^{k;i,j})^2 \geq 0, \quad (28) $$
where we have used $\det(D^{ij}) = \prod_{k=1}^{V} \eta_{\eta_{i,j}} \eta_{\eta_{j}} = (-1)^k \eta_{i,j}$. One can similarly show that the weight of the $C \in W_4$ sector is positive. Therefore, there is no sign problem in the extended configuration space with worms.

3. Results

3.1. Quantum Monte Carlo results

Figure 3 shows the density–density correlations (12), which develop a staggered pattern as the interaction strength $V$ increases. The density correlation at the farthest distance $C(R_{\text{max}})$ and the CDW structure factor $M_2$ approach the square of the CDW order parameter as the system size increases. Figure 4 shows the extrapolation of $C(R_{\text{max}})$ and $M_2$ using $a/L + b/L^2$. The error bar of the extrapolation to the thermodynamic limit ($1/L = 0$) is evaluated using a jackknife analysis.

Figure 3. The density–density correlations versus distances $R$ on an $L = 12$ lattice at $\beta = 16$. The inset shows the absolute value of the correlation function on a logarithmic scale.

Figure 4. Extrapolation of the density correlations at the largest distance $C(R_{\text{max}})$ and the CDW structure factor $M_2$ using $a/L + b/L^2$. The error bar of the extrapolation to the thermodynamic limit ($1/L = 0$) is evaluated using a jackknife analysis.
using $a/L + b/L^2$. The extrapolation suggests that the quantum critical point lies between $V = 1.3$ and $V = 1.4$.\(^5\)

To better estimate the critical point, we perform an FSS analysis based on the scaling ansatz

$$M_2 = L^{-z-\eta} F \left( L^{1/\nu} (V - V_c), L^z / \beta \right)$$

(29)

$$M_4 = L^{-2z-2\eta} G \left( L^{1/\nu} (V - V_c), L^z / \beta \right)$$

(30)

$$B = G/F^2$$

(31)

where $F$ and $G$ are universal functions and $\nu$, $\eta$ are the critical exponents. This scaling ansatz holds close to the critical point. The Binder ratios of different system sizes cross at the transition point. This provides a rough estimate of the transition point $V \lesssim 1.36$, as shown in figure 5.

We next collapse the data of $M_2$ and $M_4$ to determine the transition point $V_c$ and the critical exponents $\nu$, $\eta$. The results are summarized in table 1, where we also list the estimates of the order parameter critical exponent $\beta = \frac{\nu}{2} (1 + \eta)$, which we will compare with iPEPS results in section 3.2. We have performed the data collapse using all available system sizes ($L = 6, 9, 12, 15$) and excluding the smallest system size ($L = 6$). They both give satisfactory data collapse where the $\chi^2$ per degree of freedom (d.o.f.) is close to 1. To visually examine the quality of the data collapse, figure 6(a) and (b) shows the scaled $M_2$ and $M_4$ using $\eta = 0.3$ where all the curves intersect around $V = 1.36$. Further scale the horizontal axis using $V_c = 1.356$ and $\nu = 0.8$ collapse all the data onto a single curve, figure 6(c) and (d).

Our estimate of the correlation length exponent $\nu$ agrees with the earlier $\epsilon$-expansion result $\nu = 0.797$ [11] and functional renormalization group results $\nu = 0.738 \sim 0.927$ [12, 13]. However, our estimated anomalous dimension $\eta \approx 0.3$ is smaller than the previous estimates $\eta = 0.502 \sim 0.635$ [11–13]. We have checked that these values of $\eta$ are not consistent with our QMC data.

\(^5\) The system sizes up to $L = 15$ do not allow us to reliably pin down the critical point based on $1/L$ extrapolation [20, 21].
There can be several reasons for the discrepancy. First, we do observe drift in the Binder ratio crossings (figure 5), possibly due to subleading corrections to the scaling ansatz. Given the limited system sizes, it is unclear how much it will affect the estimated critical exponents. On the other hand, there may also be systematic error, in the field theory estimate [11–13] due to uncontrolled approximations of the analytical approaches. Last but not least, the field theory calculations [11–13] treated Dirac fermions with the same chiralities, but our lattice model contains two Dirac fermions with opposite chirality. This difference may affect the renormalization group equations and result in different critical exponents. To fully resolve these issues would require extensive simulations of larger lattices, as well as a careful examination of the previous analytical calculations. We hope our results presented in this paper provide a stimulus for this line of research. In appendix B, we present further support of our estimate of critical exponents based on results obtained on a π-flux lattice.

3.2. Comparison with iPEPS results

As an independent check of the QMC results, we have studied the model (1) with iPEPS—a variational tensor-network ansatz for 2D ground-state wave functions in the thermodynamic limit [38–41]. This ansatz is a natural extension of matrix product states (the underlying ansatz of the density-matrix renormalization group method) to two dimensions, and has been
previously applied to the same model for attractive interactions [42, 43]. Two-dimensional tensor networks were first introduced for spin models and later extended to fermionic systems [41, 44–50]. The iPEPS ansatz consists of a cell of tensors with one tensor per lattice site, which is periodically repeated on the lattice. Each tensor has a physical index of dimension $d$ which carries the local Hilbert space of a lattice site and $z$ auxiliary indices which connect to the $z$ nearest-neighboring tensors. The number of variational parameters (i.e. the accuracy of the ansatz) can be controlled by the bond dimension $D$ of the auxiliary indices, where each tensor contains $dD^z$ variational parameters, with $d = 2$ and $z = 3$ for the present model. For a general introduction to fermionic iPEPS, we refer to [41].

We simulate the honeycomb model (1) by mapping it onto a brick-wall square lattice, as done in [51]. The variational parameters of the iPEPS ansatz are optimized by performing an imaginary time evolution using a second-order Trotter–Suzuki decomposition and the full-update scheme for the truncation of a bond index (see [41] for details). To evaluate the iPEPS wave function (e.g. for the computation of expectation values) we use a variant of the corner-transfer-matrix method [52, 53] described in [54, 55]. The U(1) symmetry of the present model is exploited [56, 57] to increase the efficiency of the simulations.

Since iPEPS represent a wave function in the thermodynamic limit, symmetries of the Hamiltonian can be spontaneously broken, and the order can be measured by a local order parameter. In figure 7, the iPEPS results for the CDW order parameter $\langle \hat{n}_A - \hat{n}_B \rangle$ as a function of $V$ are shown, where $\hat{n}_A$ and $\hat{n}_B$ correspond to the particle density on sublattices A and B, respectively. Since iPEPS is an ansatz in the thermodynamic limit, there are no finite size effects. However, the finite bond dimension $D$ has a similar effect on the order parameter as a finite size system, i.e. there is no sharp transition, but the order parameter is overestimated around the critical coupling $V_c$. To obtain an estimate of the order parameter in the infinite $D$ limit we extrapolate the data linearly in $1/D$, shown by the black diamonds in figure 7. The error bar indicates the range of extrapolated values by taking into account different sets of data points. Although the analytical dependence of the order parameter on $D$ is not known\textsuperscript{6}, it has been previously found that one can get a reasonable estimate from such extrapolations (see e.g. [62]). Based on these extrapolations of the iPEPS data up to $D = 9$, we obtain a value of the critical coupling of $V_c = 1.36(3)$, which agrees with the CTQMC result.

\textsuperscript{6} A theoretical understanding of the $D$-dependence of an order parameter has been developed for matrix product states in the case of critical one-dimensional systems (called finite entanglement scaling) [58–61]; however, in two dimensions a similar theory is still lacking.
The green crosses in figure 7 show the CTQMC data for the order parameter in the thermodynamic limit, computed as \( OR_{\text{CDW}} = \lim_{L \to \infty} 2\sqrt{M_2(L)} \), which agrees with the iPEPS data. Similar results are obtained by estimating the order parameter from \( C(R_{\text{max}}) \), i.e. \( OR_{\text{CDW}} = \lim_{L \to \infty} 2\sqrt{C(R_{\text{max}})} \). The extrapolation of QMC data close to the critical point is more difficult because the intersections at \( 1/L = 0 \) may become negative.

We also tried to extract the critical exponent \( \tilde{\beta} \) by fitting the extrapolated iPEPS data to \( k(V - V_c)^{\tilde{\beta}} \) in the range \([V_c, 1.6]\). However, due to the error bars and sensitivity of the exponent on the fitting range, we can only give a crude estimate of \( \tilde{\beta} = 0.7(15) \), which is somewhat larger than the CTQMC result \( \tilde{\beta} = 0.52(6) \), but both are smaller than the mean-field result \( \tilde{\beta}_{\text{MF}} = 1 \) [19] and consistent with the concave shape of the order parameter versus \( V \) curve.

### 4. Conclusion and outlook

We presented a sign-problem-free CTQMC study of the Dirac semi-metal to charge-density-wave transition on a honeycomb lattice and compare it with theory and iPEPS results. Our main results about the transition point and the critical exponents are summarized in table 1. Our estimate of the correlation length exponent \( \nu \) agrees with previous calculations based on the Gross–Neveu theory [11–13], but our estimate of the anomalous dimension \( \eta \) is smaller. Further numerical and theoretical investigations are needed to resolve this discrepancy.

The present study uses the static density–density correlations as the diagnosis tool for the quantum critical point. It is, however, interesting to further study the transport and entanglement properties across the phase transition. Future studies may map out the finite temperature phase diagram and especially the crossover [63] from the quantum critical point to the thermal phase transition in the 2D Ising universality class. The CDW transition of the spinful Dirac fermions [64, 65] and many-flavored fermions [66] can also be studied using a similar method. Generalization of the model to include hopping and interactions beyond the nearest neighbors may allow us to address the intriguing question about the emergence [67] and stability of the topological insulating states [68, 69] in the presence of interactions.

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### Appendix A. Monte Carlo updates

A Monte Carlo update consists of proposing a move from a configuration \( C \) to a new configuration \( C' \) with an \textit{a priori} probability of \( A(C \to C') \). The acceptance probability
The Metropolis–Hasting solution of the detailed balance equation (A.1) is

\[ R(C \rightarrow C') = \min \left\{ 1, \frac{w(C')A(C' \rightarrow C)}{w(C)A(C \rightarrow C')} \right\} \]  

(A.2)

There are three classes of configurations shown in figure A1. We devised several updates to sample the configuration space. Most updates are in complementary pairs. Within each pair, one can still fine-tune the proposed probability to enhance the acceptance rate.

A.1. Vertex add/remove

We add \( n \) vertices to a configuration with \( k \) vertices. The acceptance ratio is

\[ R_{\text{add}} = \frac{(-V)^n \det(G^{k+n})/(k+n)!}{\det(G^k)! \left( \frac{1}{\beta N_b} \right)^n} = \left( -\beta VN_b \right)^n \frac{k!}{(k+n)!} \frac{\det(G^{k+n})}{\det(G^k)}, \]  

(A.3)

where \( N_b = 3L^2 \) is the number of bonds of the honeycomb lattice. The move equation (A.3) is balanced by removing \( n \) vertices from a \( k \)-vertices configuration with the acceptance probability

\[ R_{\text{remove}} = \frac{1}{\left( -\beta VN_b \right)^n (k-n)!} \frac{k!}{\det(G^{k-n})} \frac{\det(G^k)}{\det(G^{k-n})}, \]  

(A.4)

Replace \( G^k \) by \( G^{k;i;j(k,l)\tau} \) one gets the formulas for adding/removing vertices in the worm space.

A.2. Worm creation/destruction

A.2.1. \( Z \leftrightarrow W_2 \). From the partition function sector we create a worm at \( \{i, j; \tau\} \). The corresponding new matrix is \( G^{k;i;j} \). To improve the acceptance rate, we select the site \( j \) in the neighborhood (containing \( m \) sites) of a randomly chosen site \( i \). The acceptance ratio is
\[ R_{\text{create}} = \eta_i \eta_j \xi_2 N_s \frac{\det(G^{k,ijr})}{\det(G^k)} \] (A.5)

\[ R_{\text{destroy}} = \eta_i \eta_j \frac{1}{\xi_2 N_s m \beta} \frac{\det(G^k)}{\det(G^{k,ijr})} \] (A.6)

A cheaper way to go between the partition function and the \( W_2 \) space is to randomly select a vertex and interpret it as a worm. We call this process an open update and the reverse process a close update. These two updates change the perturbation order by one. However, they are cheaper than creating/destroying the worms in equations (A.5)–(A.6) because no matrix operation is involved. The acceptance ratios are

\[ R_{\text{open}} = 2 \xi_2 \frac{k}{V} \] (A.7)

\[ R_{\text{close}} = \frac{1}{2 \xi_2 (k + 1)} \] (A.8)

The factor 2 accounts for the fact that \( \{i, j; \tau\} \) and \( \{j, i; \tau\} \) are counted as two distinct worm configurations.

**A.2.2. \( W_2 \leftrightarrow W_4 \).** In the \( W_2 \) sector, we insert another worm at \( \{k, l; \tau\} \) choosing a random site \( k \) and a nearby site \( l \) (out of \( m \) sites). The time \( \tau \) is the same as the imaginary time of the existing worm \( \{i, j; \tau\} \). Acceptance ratios are

\[ R_{\text{create}} = \eta_k \eta_l \frac{N_s \xi_2}{\xi_4} \frac{\det(G^{k,ijklr})}{\det(G^{k,ijr})} \] (A.9)

\[ R_{\text{destroy}} = \eta_k \eta_l \xi_2 \frac{N_s m \xi_4}{\xi_4} \frac{\det(G^{k,ijklr})}{\det(G^{k,ijr})} \] (A.10)

**A.2.3. \( Z \leftrightarrow W_4 \).** We create a worm at \( \{i, j, k, l; \tau\} \) in the partition function sector. To improve the acceptation ratio, we choose the sites \( j, k, l \) in the neighborhood of a randomly chosen site \( i \). The ratios are

\[ R_{\text{create}} = \eta_i \eta_j \eta_k \eta_l \frac{N_s m \beta \xi_4}{\xi_4} \frac{\det(G^{k,ijklr})}{\det(G^k)} \] (A.11)

\[ R_{\text{destroy}} = \eta_i \eta_j \eta_k \eta_l \frac{1}{N_s m \beta \xi_4} \frac{\det(G^k)}{\det(G^{k,ijklr})} \] (A.12)
A.3. Worm shift

We shift the worm to a new space–time point. To enhance the acceptance probability, we randomly choose one site in the worm and shift it to one of its neighbors. The imaginary time $\tau$ is updated to $\tau'$ by randomly by adding a random number in the range of $(-0.05\beta, 0.05\beta)$. The matrix is updated to $G^{k, ij} \tau'$ and the acceptance probability is

$$R_{\text{shift}} = \eta_i \eta_j \frac{\det(G^{k, ij} \tau')}{\det(G^{k, ij} \tau)}. \quad (A.13)$$

This process is self-balanced. The acceptance rate of worm shift in the $W_4$ space has a similar expression.

Appendix B. Monte Carlo results on the $\pi$-flux lattice

To further confirm the critical exponent found in the main text, we simulated the model equation (1) on a square lattice with $\pi$-flux inserted in each plaquette; see figure B1(a). The lattice also features two Dirac points in the Brillouin zone; see figure B1(b). The Dirac semimetal-to-CDW transition should belong to the same universality class in the honeycomb lattice. In the simulation, we use the Landau gauge for the flux and choose system sizes $L$ to be divisible by 4. The inverse temperature scales linearly with length $\beta = L$. As explained in the main text, the is no sign problem either for the $\pi$-flux lattice.

Figure B2 shows the Binder ratios, from which we infer the transition point $V_c \approx 1.3$. A data collapse analysis of $M_2$ (figure B3) gives $V_c = 1.304(2), \nu = 0.80(6)$ and $\eta = 0.318(8)$. These results indicate that the critical exponents we found for the honeycomb lattice (table 1) are universal.
Figure B2. The Binder ratio equation (15) versus $V$ for different system sizes of the $\pi$-flux lattice. Lines are linear interpolations of the data.

Figure B3. (a) and (b) The scaled $M_2$ and $M_4$ using $\eta = 0.3$. (c) and (d) data collapse using $V_c = 1.3$ and $\nu = 0.8$. 
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