The Semimetal-Mott Insulator Quantum Phase Transition of the Hubbard Model on the Honeycomb Lattice

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The Hubbard model on a honeycomb lattice is known to exhibit a semimetal-insulator quantum phase transition into an antiferromagnetic Mott insulating phase at a critical on-site coupling of $U_c \approx 3.8$, with critical exponents thought to fall into the universality class of the Gross-Neveu model. We present a novel analysis of this transition by means of grand canonical Hybrid Monte Carlo simulations. For the first time we control all the systematics of the single-particle gap, extrapolating to the temporal continuum and thermodynamic limits. The critical coupling and exponents are determined by a finite-size scaling analysis in the inverse temperature, which gives a critical exponent of $\beta = 1.232^{−0.069}_{0.069}$ and a critical coupling of $U_c = 3.844^{−0.044}_{0.044}$. The strong anti-correlation between $\beta$ and $U_c$ is carefully accounted for. We discuss the implications of our findings for carbon-based nano-materials, such as graphene, carbon nanotubes and fullerenes. We also comment on the computational scaling of our Hybrid Monte Carlo algorithm.

I. INTRODUCTION

Strongly correlated electron-electron interaction effects in carbon-based nano-materials \cite{1,2} is an emerging topic in both the condensed matter \cite{3,4} and nuclear physics communities \cite{5,6}. The two dominant theoretical frameworks applied to this problem are density functional theory (DFT) and the Hubbard Model. The latter is a Hamiltonian approach which is directly related to the familiar tight-binding description of the atomic orbitals in a lattice of carbon ions \cite{7,8,9,10}, as well as to problems of current interest in atomic and nuclear physics, such as nuclear lattice effective field theory (NLEFT) \cite{11,12,13,14}, and the unitary Fermi gas. The properties of the Hubbard Model on a honeycomb lattice are thought to closely resemble those of graphene. The electronic properties of graphene are then determined by the relative strength of the on-site electron-electron interaction $U$ and the nearest-neighbor hopping amplitude $\kappa$. For small values of $U$, the honeycomb Hubbard model is in a semimetallic phase, which exhibits the two familiar Dirac points of graphene. At a critical coupling of $U_c/\kappa \approx 3.8$, a second-order phase transition occurs into a (gapped) anti-ferromagnetic Mott insulating (AFMI) phase. The critical properties of this transition, the possible existence of a spin-liquid phase at intermediate couplings \cite{15,16}, and whether the AFMI phase could be observable in nature (for instance in samples of suspended graphene or graphene with biaxial strain applied) are important questions both from the point of view of fundamental and applied physics, and have thus been much studied with a variety of experimental and theoretical methods. According to current knowledge, the physical value of $U/\kappa$ is likely to be less than the critical value, thus rendering the actual opening of a single-particle gap due to the AFMI transition unobservable in realistic graphene samples (although the Fermi velocity at the Dirac points may still be significantly renormalized due to interaction effects) \cite{17,18}.

The consequences of the relatively strong on-site electron-electron interaction are also likely to be more prominent in fullerenes and carbon nanotubes, due to the reduced dimensionality of such systems \cite{19}. While $\kappa$ is relatively well constrained from DFT and experiment \cite{20}, the on-site coupling $U$ is more difficult to determine theoretically \cite{21}. The effects of long-range interactions in graphene have also been studied, and are thought to frustrate the AFMI transition, as the nearest-neighbor (or Coulomb tail) interactions favor the charge-density wave (CDW) symmetry breaking \cite{22,23}. The critical exponents of the AFMI transition are thought to fall into the universality class of the Gross-Neveu (GN) model, though such conclusions remain tentative \cite{5}.

This paper is organized as follows. We describe our formalism and summarize our algorithm in Section \cite{24}. In Section \cite{25} we give details of how we measure the single-particle correlation function using the Hybrid Monte Carlo (HMC) algorithm in the grand canonical ensemble. We extract the gap at finite temporal and spatial lattice extends and remove discretization as well as finite-volume artifacts. Finally we obtain continuum, infinite-volume, finite-temperature values for the gap $\Delta_0$. In Section \cite{26} we analyze those results using finite-size temperature scaling and find a second-order zero-temperature quantum phase transition into a Mott insulating state, believed to be antiferromagnetic, with critical coupling $U_c/\kappa = 3.844^{−0.044}_{0.044}$ and critical exponent $\beta = 1.232^{−0.069}_{0.069}$, carefully accounting for their strong (anti)correlation. Our final result is summarized in Figure \cite{27}. We expect that our method can be straightforwardly applied to systems such as nanotubes and topological insulators.
II. FORMALISM

The Hubbard Model is a model of fermions that can hop between definite sites and interact. The fermions are described by the Hamiltonian

\[ H = - \sum_{xy} (a_x^\dagger h_{xy} a_y + b_x^\dagger h_{xy} b_y) + \frac{1}{2} \sum_{xy} \rho_x V_{xy} \rho_y \]

(1)

where \( a^\dagger \) (\( b^\dagger \)) and \( a \) (\( b \)) are the creation and annihilation operators for an electron (hole), respectively. Here we have used the signed particle/hole transformation to change from electrons with spins \( \uparrow \) and \( \downarrow \) to spinless particles \( a \) and holes \( b \), and dropped constant terms. The hopping matrix \( h_{xy} = \kappa \delta_{xy} \) encodes nearest-neighbor hopping while \( V \) is the potential between particles on different sites and \( \rho = b^\dagger b - a^\dagger a \) is the charge operator. In this work we study the usual Hubbard model with only on-site interactions \( V_{xy} = U \delta_{xy} \) so that \( U \) characterizes the interaction strength. We focus on the two-dimensional honeycomb lattice, which can be bi-partitioned into \( A \) sites and \( B \) sites.

Hamiltonian theories such as the Hubbard Model have for a long time been studied with lattice Monte Carlo methods [22, 23], as this allows for a fully \textit{ab initio} stochastic evaluation of the Grassmann path integral. There is a large freedom of choice in the construction of lattice Monte Carlo algorithms, including the discretization of the theory, the choice of Hubbard-Stratonovich (or auxiliary field) transformation, and the algorithm used to update the auxiliary field degrees of freedom. This freedom is often exploited in order to optimize the algorithm with respect to a particular computational challenge. These pertain to the efficient scaling of the computational effort with system (lattice) size \( L \), inverse temperature \( \beta \), number of time slices \( N_t = \beta / \delta \), interaction strength \( U/\kappa \), and electron number density (away from half filling). In the condensed matter and atomic physics communities, Hamiltonian theories are typically simulated with an exponential (or compact) form of both the kinetic and potential energy contributions to the partition function (or Euclidean time projection amplitude), and with random Metropolis updates of the auxiliary field degrees of freedom (which may be either discrete or continuous). These features are summarized in the Blankenbecler-Sugar-Scalapino (BSS) algorithm [24].

In the field of Lattice QCD the high dimensionality of the theory and the need to precisely approach the continuum limit have led to the development of an array of specialized algorithms, which seek to optimize the computational scaling with \( L \). These efforts have culminated in the Hybrid Monte Carlo (HMC) algorithm, which combines elements of the Langevin, Molecular Dynamics, and Metropolis algorithms [25]. The application of HMC to the Hubbard Model has proven to be surprisingly difficult, due to problems related to ergodicity, symmetries of the Hamiltonian, and the correct approach to the (temporal) continuum limit. For a thorough treatment of these from the point of view of HMC, see Refs. [19, 26, 27]. In order to provide the expected \( V^{5/4} \) computational scaling, a suitable conjugate gradient (CG) method has to be found for the numerical integration of Hamilton’s equations of motion. The Hasenbusch preconditioners [25] from Lattice QCD has recently been found to work for the Hubbard Model as well [29]. The resulting combination of HMC with the Hubbard Model is referred to as the Brower-Rebbi-Schaich (BRS) algorithm [30, 31], which is closely related to the BSS algorithm—the main differences are the linearized kinetic energy (or nearest-neighbor hopping) term, and the purely imaginary auxiliary field, which is updated using HMC moves.

The projection Monte Carlo (PMC) method within the canonical ensemble has preferentially been used with the BSS algorithm [16, 15]. In PMC calculations, particle number is conserved and one is restricted to particular many-body Hilbert spaces. The PMC method is highly efficient at accessing zero-temperature (or ground state) properties, especially when the number of particles is independent of the linear size \( L \) of the lattice (such as in NLEFT, where systems of \( A \) nucleons are considered). However, to simulate the Hubbard model on the honeycomb lattice at half-filling, the fully anti-symmetric trial wave function must encode the \( 2 \times L^2 \) electrons to be propagated in Euclidean time. This scaling in \( L^2 \) negates many of the computational advantages that PMC algorithms typically have over grand canonical ones. The PMC and grand canonical versions of the BSS algorithm both exhibit \( V^3 \) scaling (with random, local Metropolis updates).

In contrast, the grand canonical version of the BRS algorithm has been successfully combined with HMC updates. The formalism then resides in the full Fock space, and no trial wave function is used. One extracts Boltzmann-weighted thermal expectation values for observables; at low temperatures and large Euclidean times, spectral observables are measured relative to the ground state of the Fock space, which is the half-filling state (an explicit example is given in Section [11]). With HMC updates, such an algorithm scales as \( V^{5/4} \) [29, 32]. The drawback of working within the grand canonical ensemble is the explicit finite temperature \( T \), and thus the need to take the limit \( T \to 0 \) by extrapolation. While the \( T \)-dependence may be considerable (though observable-dependent), it should be noted that PMC simulations are also not free of effects due to contamination from excited state contributions at finite Euclidean projection time, even though such effects are typically less severe due to the absence of backwards-propagating states in Euclidean time.

Typically within the grand canonical BRS algorithm auxiliary field configurations, once thermalized, are stored.
With these thermalized configurations observables can be measured separately, and new observables can be computed as interests and understanding develops. As the grand canonical BRS algorithm can also be successfully combined with HMC updates, it is arguably preferable if the scaling of the algorithm to very large systems, such as multi-walled nanotubes or nano-ribbons at macroscopic scales, is to be given precedence over other issues. However, in spite of the considerable $T$-dependence of our MC results for the single-particle gap, we shall find that we are nevertheless able to determine the critical properties of the AFMI transition with high accuracy.

HMC updates have proven difficult for the BSS algorithm. The main reason for this is the exponential form of the fermion operator, which causes the fermion determinant to factorize into regions of positive and negative sign. Though this does not imply a sign problem at half filling (the action is proportional to the absolute square of a fermion determinant), it does introduce boundaries in the energy landscape of the theory which HMC trajectories in general cannot cross (without special and very computationally expensive methods \cite{22,25}). Moreover, at low temperatures this fragmentation effect increases dramatically. This means that HMC simulations of BSS are not expected to be ergodic. While this problem can be circumvented by introducing a complex-valued auxiliary field, the resulting “complexified” HMC algorithm showed poor (roughly cubic) scaling with system size \cite{22}. It is interesting to note how the BRS algorithm avoids this ergodicity problem. Due to the linearization of the hopping term in the fermion operator (with imaginary auxiliary field), the boundaries impassable to HMC are reduced in dimension and can be avoided \cite{26}. Naturally, in the temporal continuum limit, the BSS and BRS formulations become equivalent, such that the ergodicity problem would eventually reassert itself in the continuum limit (where MC simulations are in any case not practical). A particular drawback of the BRS formulation is that spin symmetry is explicitly broken at finite temporal lattice spacing, due to the linearization of the hopping term \cite{20}. Hence, it is fair to say that the choice of BSS versus BRS represents a tradeoff between the retention of more symmetries at finite temporal lattice spacing and faster convergence to the continuum limit (BSS), or improved ergodicity and superior computational scaling with system size (BRS).

Here we adopt the BRS approach and leverage HMC for a stochastic evaluation of Hubbard Model path integrals. Leveraging the Hubbard-Stratanovich transformation one finds a theory with auxiliary fields $\phi$ whose action depends on the discretization-dependent fermion matrix $M$. Ref. \cite{19} used a mixed differencing operator, where $A$ sites had a forward differencing in time while $B$ sites had a backward differencing, avoiding the doublers that higher-order schemes allow. In the non-interacting case this mixed differencing gives $O(\delta^2)$ discretisation errors and it has been observed numerically that it still leads to much better results than only forward or only backward differencing if the interaction is non-zero. As we discuss in Appendix \ref{sec:appb} to ensure that we correctly capture the effects of a marginal seagull term as we approach the continuum limit, we use a slightly different diagonal operator,

\begin{equation}
M_{(x,t)(y,t')}^{AA} = \delta_{x,y} \left( \delta_{t+1,t'} - \delta_{t,t'} \left( e^{-i \tilde{\phi}_{x,t}} \right) \right) \\
M_{(x,t)(y,t')}^{BB} = \delta_{x,y} \left( \delta_{t,t'} - \delta_{t-1,t'} \left( e^{i \tilde{\phi}_{x,t}} \right) \right) \\
M_{(x,t)(y,t')}^{AB} = M_{(x,t)(y,t')}^{BA} = -\kappa \delta_{(x,y)} \delta_{t,t'}, \tag{2}
\end{equation}

which ensures we do not generate a staggered mass in the continuum limit, while maintaining the sparseness that an unexponentiate hopping matrix on the time diagonal provides. We denote all quantities multiplied by $\delta$ with a tilde.

Finally, we emphasize that all the $O(\delta^2)$-errors are local errors and we have to integrate over a path with $N_t$ terms so that we expect global errors of order $O(\delta)$.

\section{The Gap}

\subsection{The single particle correlator}

The operators $a$ and $a^\dagger$ destroy and create a negatively-charged particle, while $b$ and $b^\dagger$ destroy and create a positively-charged hole. We can create and destroy these quasiparticles at different locations and different times and compute their correlation,

\begin{equation}
C_{xy}(t) = \langle a_x,t a_{y,0}^\dagger \rangle = \frac{1}{Z} \int \mathcal{D}\phi \ M_{x,y,0}^{-1} e^{-S} = \langle M[\phi]_{x,t,y,0}^{-1} \rangle 
\end{equation}

where we used Wick contraction to replace the ladder operators with the fermion propagator. We can Fourier transform the spatial locations $x$ and $y$ to (lattice) momentum space $k$ and $p$. To compute $M[\phi]_{x,t,y,0}^{-1}$ one creates a plane wave source $\eta$ with momentum $p$ on timeslice $0$, solves

\begin{equation}
M[\phi]_{y,0,x,t} \psi_{x,t} = \eta_{y,0} \tag{4}
\end{equation}
for \( \psi \) and takes its dot product with a plane-wave sink with momentum \( k \) on timeslice \( t \). Repeating this procedure yields measurements whose ensemble average estimates \( C_{kp}(t) \). There are two Dirac points \( K \) and \( K' \) and by symmetry we have:

\[
C_{KK}(t) = C_{K'K'}(t),
\]

in expectation value, but not configuration-by-configuration. These correlation functions may be written as a thermal trace

\[
C_{xy}(t) = \left\langle a_{xt} a_{y0}^\dagger \right\rangle = \frac{1}{Z} \Tr \left[ e^{-\beta H} a_{xt} a_{y0}^\dagger e^{-\beta H} \right] = \frac{1}{Z} \Tr \left[ e^{-H(\beta-t)} a_{x} e^{-Ht} a_{y}^\dagger \right],
\]

where we have moved to the Heisenberg picture. Inserting the identity resolved in the interacting eigenbasis, one arrives at the spectral decomposition

\[
C_{xy}(t) = \sum_{mn} e^{-\beta E_m} e^{-(E_n-E_m)t} z_{mxn} z_{myn}^*,
\]

The indices \( i, m, \) and \( n \) run over interacting eigenstates, \( E \) is their energies, and \( z \) are overlap factors. At low temperatures the exponential decay allows us to isolate, in the long-time limit,

\[
\lim_{t \to \infty} \lim_{\beta \to \infty} C_{xy}(t) = e^{-(E_1-E_0)t} z_{0x1} z_{0y1}^*
\]

where 0 and 1 label the ground and first excited states, as long as the overlap factors are non-zero. By Fourier transforming \( x \) and \( y \) to a Dirac point we can exactly change the overlap factors so that the first excited state is a Dirac-point quasiparticle, and \( E_1 - E_0 \) is that particle’s energy cost. We call this difference the effective mass,

\[
m_{\text{eff}} = E_1 - E_0
\]

which can be extracted from the correlator

\[
m_{\text{eff}}(t) = \lim_{\beta \to \infty} -\partial_t \ln C_{xy}(t),
\]

again, as long as the overlap factors are nonzero. The finite-volume finite-discretization gap in the spectrum is then, simply,

\[
\Delta = 2m_{\text{eff}};
\]

we discuss extrapolation to the continuum, infinite volume gap in the next two subsections.

By symmetry, the two Dirac points are indistinguishable and the correlators are symmetric in time around \( \beta/2 \) (or \( N_t/2 \) in dimensionless units), in expectation value. We therefore average and fold the correlator configuration-by-configuration

\[
C(t) = \frac{1}{4} \left( C_{KK}(t) + C_{K'K'}(t) + C_{KK}(\beta-t) + C_{K'K'}(\beta-t) \right)
\]

to increase our precision without generating additional configurations.

Figure 1 shows the plots of two effective masses and the corresponding fits. In practice, because of the finite temperature and the quasiparticle effective masses being so light, we cannot suppress thermal effects due to backwards-propagating states to completely isolate an exponential decay. Instead, the effective mass is obtained for each timeslice \( \tau = t/\delta \) by a numerical solution of

\[
\frac{\cosh \left( m_{\text{eff}}(\tau) \delta \left( \tau - \frac{N_t}{2} \right) \right)}{\cosh \left( m_{\text{eff}}(\tau) \delta \left( \tau + 1 - \frac{N_t}{2} \right) \right)} = \frac{C(\tau)}{C(\tau + 1)}
\]

\footnote{Because of the underlying sublattices \( A \) and \( B \), there are in principle two independent correlators for each momentum \( k \) \cite{19}. However, these two correlators are degenerate at each Dirac point \( K \) and \( K' \); we average them to construct \( C_{KK} \) and \( C_{K'K'} \), respectively.}
Figure 1. Effective mass of representatively chosen single particle correlators from our ensembles. Blue line and band give $m_{\text{eff}}$ and statistical error obtained from a cosh effective mass (14). Their extent corresponds to the fitting region. A direct, constant fit to the effective mass (11) is depicted by the dashed orange line, whereas the dot-dashed red line shows the estimation of the systematic error as explained in Appendix B. Red and orange lines have been extended outside of the fitting region for clearer visibility. Left: $\kappa \beta = 8$, $L = 15$, $N_t = 64$, $U/\kappa = 3.55$. Right: $\kappa \beta = 12$, $L = 6$, $N_t = 72$, $U/\kappa = 3.85$. The timeslice $\tau$ is an integer; the effective mass $m_{\text{eff}}$ is in units of $\kappa$.

where $C(\tau)$ is the folded, symmetrized correlator (13). This cosh-formulation is preferable over the more common exponential formulation (11) because the masses are so light and the backward-propagating contributions are non-negligible. The values of the effective mass are used to find the optimal fit region (for details see Appendix B). Subsequently we fit the correlator in this region using

$$C(\tau) = a \cosh \left( m_{\text{eff}} \delta \left( \tau - \frac{N_t}{2} \right) \right)$$

(15)

with the two fit parameters $a$ and $m_{\text{eff}}$. Note that this is not the same as fitting a constant to $m_{\text{eff}}(\tau)$ because the latter can gain a positive bias for small effective masses and a high noise level. We show the difference in Figure 1 where the blue line denotes the cosh-fit with its statistical error and the orange dashed line visualises the direct fit of $m_{\text{eff}}(\tau)$. An estimation of the systematic error due to the choice of the fit range as explained in Appendix B is depicted by the dot-dashed red line.

We obtained the statistical error via bootstrap. The total error has then been estimated as the sum in quadrature of statistical and systematic uncertainties.

The data analysis described in this and the following sections has mostly been performed in R [36], a significant part using the hadron package [37].

B. Lattice artefacts

To obtain robust and statistically relevant thermodynamic properties, we have to systematically remove the discretization and finite-volume effects by extrapolation. To determine zero-temperature properties we must also remove finite-temperature effects.

To our knowledge, only Ref. [18] performed a thorough temporal continuum limit, by refining their discretization until their numerical results stabilized. However, they use a discretisation very different from the form we employ. As demonstrated in Appendices B and D of Ref. [26], discretization errors can bias even those results formulated with a compact kinetic operator rather than the linear operator used in this work, and to make any confident claim about the continuum limit one must extrapolate.

Refs. [16, 17] (for the single-particle gap and the staggered magnetic moment), Ref. [18] (for the squared staggered magnetic moment) and Ref. [21] (for the square of the total spin per sublattice) assume a finite volume dependence of the form $a + bL^{-1} + cL^{-2}$, but find that manifestly positive quantities have a negative infinite-volume extrapolation.
In contrast to the polynomial assumptions, Ref. [38] finds a plateau of the conductivity, though their approach substantially differs from our line of attack.

We show in Appendix C that the leading-order deviation of the gap in the spatial lattice extent behaves as $L^{-3}$. However, this dependence does not hold for all observables, but only those that fulfil two conditions: First, the observable must not have larger than cubic errors on single MC trajectories that are not cancelled by averaging. This is the case for the correlation functions located at the Dirac points, but not in general for (squared) magnetic or other locally defined quantities. The problem with, for example, the squared magnetisation is that its $L^{-2}$ fluctuations are positive on every MC trajectory and the average of the positive contributions does not vanish and thus the remaining error is still quadratic.

The second condition is that the deviations are dominated by the discretisation in momentum space, not by changes of the physical state due to finite size. This implies a correlation length much smaller than the lattice size. Thus we expect the scaling to hold far from phase transitions, but not in their vicinity, where we expect spatial correlations to diverge. Our relatively small values of $\beta \kappa \leq 12$ however limit correlation lengths by the inverse minimum Matsubara frequencies $\pi/\beta$, so that the cubic scaling holds if

$$L \gg \frac{\beta \kappa}{\pi}. \quad (16)$$

Numerically our results support this observation since our fits starting at $L = 9 \gg 4 > \beta \kappa/\pi$ are completely governed by the cubic finite size scaling (see Figs. 2 and 7).

Section II and Appendix A discuss the continuum limit and the discretisation artefacts. The latter are expected to vanish with $\delta$ (or $N^{-1}_f$).

C. Simultaneous continuum and thermodynamic limit extrapolations

The usual method for extracting thermodynamic quantities at a fixed temperature is to first take the (temporal) continuum limit, holding the physical (spatial) volume fixed, followed by an infinite-volume extrapolation.

This procedure has several weaknesses. The largest problem is that in general the functional dependence on the finite size and discrete time artefacts is not known. Thus the only check if the extrapolation makes sense is the quality of that individual fit. However, with all but the simplest fits, the number of fit parameters quickly exhausts a limited dataset. Then, the fit quality cannot be estimated reliably if the number of data points is not much larger than the number of fit parameters. In many cases—such as with four data points—a linear fit may fail to describe the data while a quadratic fit might overfit features created by outliers. Both fit functions might be sufficient for interpolation but cannot be trusted on extrapolation.

In contrast, we can construct a two-dimensional fit that describes the data as a function of both the discretization scale $\delta$ and the finite volume $L$ at the same time. This dramatically increases the degrees of freedom in relation to the number of fit parameters and can distinguish between or falsify different functional dependences much more readily. In addition, it gives a handle to identify outliers. Moreover, a two-dimensional fit can incorporate data points where a one-dimensional extrapolation might be too costly—such as a large-volume continuum limit. Using this strategy one can also sample the parameter space more efficiently, without the limitation of requiring a rectangular grid in $L$ and $\delta$.

The error on the fits has been calculated via parametric bootstrap. This means that the bootstrap samples have been generated by drawing from independent normal distributions defined by every single value of the gap and its error.

D. Results

Using the discretization described in Section II we used Hasenbusch-accelerated HMC to generate a large number of ensembles at different temperatures $\kappa \beta$, discretizations $\kappa \delta = \kappa \beta N^{-1}_f$, couplings $U/\kappa$, and lattice sizes $L$. We simulated at six inverse temperatures $\beta \kappa \in \{3, 4, 6, 8, 10, 12\}$ and we scanned a large parameter space to provide reliable results in the physical limit for several coupling strengths $U/\kappa \in [1, 5, 5]$. The parameters range from $L = 3$ to $L = 102$ and from $\delta \kappa = 1/4$ down to $\delta \kappa = 1/40$. We always pick lattices where $L \equiv 0 \pmod{3}$, so

\[2\] These correspond to a highest temperature $T \approx 1.04 \times 10^4$ K and a lowest temperature $T \approx 2.6 \times 10^3$ K. According to Ref. [39] our entire temperature range is well below the critical temperature $T_c \approx 1.3 \times 10^4$ K at which one should expect qualitatively different behaviour because sublattice symmetry is not broken any more.

\[3\] We generated several very large lattices to provide a check of the convergence behaviour, and not for every parameter set. As we observe a nearly flat dependence of $\Delta$ on $L \gtrsim 12$, we did most of the analysis with medium sized lattices ($L \leq 21$) to save computation time.
that the non-interacting, tight-binding solution has a Dirac point and we can be sure any gap we observe is due to interactions rather than geometry—that is, we pick the geometry to ensure we measure a Mott gap, rather than a gap that combines interactions and a non-interacting band gap.

As described, we calculated the single particle correlator as an expectation value of the inverse fermion matrix at both independent Dirac-points and averaged over them to increase our statistics. We fit those correlators to extract a gap for each set of parameters. Finally, we take a simultaneous infinite-volume and continuum limit, employing the functional form

$$\Delta(L, N_t)^2 = \Delta_0^2 + a \cdot N_t^{-2} + b \cdot L^{-3},$$

(17)

fitting the infinite-volume continuum gap $\Delta_0$ and leading discretization corrections $a$ and finite-volume corrections $b$. We are aware of the fact that this formula does not describe the lattice artefacts exactly, but over our set of parameters it describes our data well with only a minimal set of fitting parameters. In the relevant regime of dominant discretisation artefacts and subdominant finite size effects it reproduces the $O(\delta)$ and $O(L^{-3})$ convergence as explained in Section III.B.

An example of such a fit is shown in Figure 2. We find that the fit form (17) describes our data well. Note that lattices as small as $L \leq 6$ have been omitted from the fit because they do not always lie in the scaling region. In the case of Figure 2 they do approximately, as can be seen in red in the right panel.

We perform this two-dimensional fit and extrapolation for many different couplings $U/\kappa$ and inverse temperatures $\kappa\beta$. We show all of the continuum, infinite-volume gaps in Figure 3. There we also show a zero temperature ($\beta = \infty$) extrapolation with corresponding error band. For details as to how the zero temperature gap has been calculated see Section IV.

IV. ANALYSIS

Let us now interrogate the gap as a function of coupling and temperature, shown in Figure 3, for signs of a quantum phase transition. This is most reliably done using a data collapsing procedure [40, 41] as performed in, for example, Refs. [17, 18]. The idea behind this approach is to leverage the finite-size scaling behavior of observables [41, 42] to ultimately eliminate their finite size effects; in our case we aim to eliminate the finite size of the thermal circle, i.e.
the finite temperature. To this end we define a universal—not explicitly $\beta$-dependent—smooth function $f$ such that

\[ u := \beta^\mu (U - U_c), \]
\[ g := \beta^\zeta \Delta_0, \]
\[ g \overset{!}{=} f(u) \] (18)

analogously to but not identical to what was done in Ref. [18]. The parameters $U_c, \mu$ and $\zeta$ have to be determined such that all points of the appropriately scaled gap $\Delta$ lie on a single line in a $u$-$g$-plot.

The imposed functional dependence leads to the scaling properties

\[ \Delta_0 \propto \beta^{-\zeta} \] (19)

for $U = U_c$ and

\[ \Delta_0 \propto \begin{cases} 0 & U \leq U_c \\ (U - U_c)^{\frac{\zeta}{\mu}} & U > U_c \end{cases} \] (20)

for $\beta = \infty$. The critical exponent $\frac{\zeta}{\mu}$ is usually denoted by $\beta$, but we avoided reusing that symbol, as it already denotes the inverse temperature.

The first property [19] is easy to see by plugging $U = U_c$ and therefore $u = 0$ into the relation (18). As $f(u)$ is then independent of $\beta$, the left hand side $g$ has to be constant as well. Thus $\Delta_0$ is inversely proportional to $\beta^\zeta$. The second property [20] follows if we additionally impose the condition that $f(u \to -\infty)$ is finite. The physical gap has to converge to a finite value for $\beta \to \infty$. For $U < U_c$ this value approaches zero as $\Delta_0 \sim \beta^{-\zeta}$. Non-zero values of $\Delta_0$ can only be obtained if $f(u) \sim \beta^\zeta$ for large beta and $U > U_c$. This implies $f(u) \sim u^{\zeta/\mu} = \beta^\zeta (U - U_c)^{\zeta/\mu}$ which shows the proportionality (20).

It turns out that $U_c$ and $\zeta$ are very strongly (anti)correlated and a direct fit of all three variables using a data collapse is therefore highly unstable. For this reason we fitted $\zeta$ first by means of equation (19). The quantity $g$ (18) is only constant for $U = U_c$, as explained above, and therefore there is only one value of $\zeta$ for which all $U$-$g$-lines cross at a single point. In order to find this value we minimise the standard deviation of the pairwise crossing points in a $U$-$g$-system. Note that the usage of the coupling $U$ instead of $u$ reduces the fitting problem to one dimension.
We obtain $\zeta = 1.054^{+0.024}_{-0.042}$ and visualise the corresponding crossing in Figure 4. The average of all the crossing points yields a first estimate of the critical coupling $U_c^1/\kappa = 3.894^{+0.068}_{-0.087}$, too. Parametric bootstrap is again employed for the error estimation.

![Figure 4](image)

Figure 4. The infinite-volume, continuum-limit gap for different inverse temperatures $\beta$ at different couplings $U$ in units of the hopping parameter $\kappa$ scaled by $\zeta$. Here $\zeta = 1.054^{+0.024}_{-0.042}$ is chosen thus as to obtain the optimal crossing. Due to relatively large errors the data for $\beta = 12$ has been omitted from both plot and fit. The average of all the crossing points $U_1^c$ has been marked.

Now that $\zeta$ is fixed, we can safely perform the data collapse by approximating the curves corresponding to individual temperatures using smoothed cubic splines and minimising the summed integrals of the squared pairwise differences. The result can be seen in Figure 5. This yields $\mu = 0.856^{+0.064}_{-0.049}$, and thus $\zeta/\mu = 1.232^{+0.069}_{-0.097}$, and $U_c/\kappa = 3.844^{+0.061}_{-0.044}$ with the correlation matrix:

$$
corr(U_c, \mu, \zeta, \zeta/\mu) = \begin{pmatrix}
1.0000 & -0.2470 & -0.9539 & -0.3087 \\
-0.2470 & 1.0000 & 0.1809 & -0.8298 \\
-0.9539 & 0.1809 & 1.0000 & 0.3946 \\
-0.3087 & -0.8298 & 0.3946 & 1.0000
\end{pmatrix}
$$

(21)

clearly showing the aforementioned anti-correlation between $\zeta$ and $U_c$. The latter result for $U_c$ is compatible with the previous one, as one would have expected, but has smaller errors because it does not rely on a local but on a global property. We discuss the values of our critical exponents in our conclusions.

In this stage we use a mixed error propagation scheme consisting of a parametric bootstrap part as above and an additional influence due to a direct propagation of the bootstrap samples of $\zeta$. For every $\zeta$-sample we generate a new data set following the parametric sampling system. Then the variation of the composite samples mirrors the total uncertainty of the results.

**A. Zero temperature extrapolation**

Finally we can extrapolate the gap to zero temperature and visualise the quantum phase transition. This is done by assuming the scaling as in equation (19) to hold approximately for $U$ slightly above $U_c$ up to a constant shift $\Delta_0^\infty$.

---

4 The gap vanishes at $U = 0$ regardless of the temperature, thus $\Delta_0(u = -\beta U_c) = 0$ and therefore data points with small $\beta$ and $U$ do clearly not follow the universal behaviour $f(u)$ any more. These deviations can be cured by introducing sub-leading order terms in $\beta$ to equation (18) as has been done in Ref. [18]. We, however, decided to simply omit points outside of the scaling region because, together with additional fit parameters, they do not increase the significance of the fit. As a cutoff we chose $\beta U < 8$.

5 We give enough digits to yield percent-level matching to our full numerical results when inverting the correlation matrix.
Figure 5. $g$ against $u$ according to equation (18) with the parameters yielding optimal data collapse. All quantities are expressed in appropriate units of $\kappa$.

the zero temperature gap. Thus we fit

$$\Delta_0 = \Delta_0^{\infty} + c_\beta \beta^{-\zeta}$$

with $\zeta$ fixed as above at constant $U/\kappa = 4$. The resulting value of $\Delta_0^{\infty}/\kappa = 0.057(23)$ allows us to determine the missing coefficient $c_U = 0.562^{+0.049}_{-0.105}$ (in appropriate units of $\kappa$) of equation (20), which we then use to make the solid black line with error bands in Figure 3. This extrapolation is, of course, only valid in the vicinity of the phase transition as for larger couplings the mean field [43] result $\Delta_0^{\infty} \propto (U - U_c)^{1/2}$ is approached. We do not aim for a quantitative determination of the region of validity in this work, but we note that an inflection point has been observed in Ref. [17] at $U/\kappa \approx 4.1$.

The error estimation for the coefficients follows the same scheme as the one for the data collapse. We obtain the error band in Figure 3 as the area enclosed by the two lines corresponding to the lower bound of $U_c$ and the upper bound of $\zeta$ (on the left) and vice versa (on the right). This method conservatively captures the high correlation between the different parameters.

V. CONCLUSIONS

In this paper we have investigated the expected semimetal-insulator transition of the honeycomb Hubbard model into an anti-ferromagnetic Mott insulating (AFMI) phase, by computing the single-particle gap as a function of $U/\kappa$. We have presented a rigorous analysis of the temporal continuum, thermodynamic and zero-temperature limits, together with a determination of the critical coupling and exponents of the AFMI transition. As far as we are aware, our work represents the first fully systematic treatment of the various limits of significance for an accurate determination of the critical properties. Moreover, our work represents the first instance where the grand canonical BRS algorithm has been applied to the honeycomb Hubbard model (beyond mere proofs of principle), and we have found highly encouraging results. In particular, previously encountered issues related to the computational scaling and ergodicity of the HMC updates have been solved.

Let us summarize our conclusions about the zero-temperature ($\beta = \infty$) critical coupling $U_c$ and critical exponent $\beta = \zeta/\mu$, and compare with Ref. [17] and Ref. [18]⁶. As expected, the differences in $\beta$ are the most pronounced.

⁶ In what remains, $\beta$ always represents the critical exponent, not the inverse temperature.
Our result $\beta > 1$ is strongly suggestive of the lattice MC data of Ref. [17], which reported an inflection point in the single-particle gap and AFMI order parameter close to $U/\kappa \simeq 4.1$, and that the behavior of both resembled the mean-field result $\beta = 1/2$ when $U \gg U_c$. However, Ref. [17] did not attempt to determine $\beta$ directly from lattice MC results. Instead, $U_c$ was determined by taking the value of $\beta/\nu \simeq 0.90$ (where $\nu$ is the correlation length exponent) to coincide with that of the Gross-Neveu model to $O(\epsilon)$ in the $\epsilon$-expansion. They then found an acceptable data collapse in $L$ using the similarly-determined value $\nu \simeq 0.88$ of the correlation length exponent.

On the other hand, Ref. [18] found $\beta \simeq 0.8$, which appears inconsistent with our result $\beta \simeq 1.2$. However, $\beta < 1$ is also inconsistent with the conclusion of Ref. [17] about the existence of an inflection point for $U/\kappa \simeq 4.1$, above which the gap and other order parameters approach mean-field-like behavior. One way to reconcile these findings is to assume that Ref. [18] lacks the necessary resolution in the immediate vicinity of $U_c$ to detect the inflection point of Ref. [17]. To be fair, the focus of Ref. [18] was on verifying or refuting the earlier tentative observation of an intermediate spin-liquid phase [10], by considering the discontinuity of the momentum distribution function at the Fermi level (or the quasiparticle weight) as an "order parameter" for the semimetallic phase. The study of AFMI order in Ref. [14], which considered both contact and long-ranged interactions, found a rather large value of $U_c \simeq 3.94$ and $\beta \simeq 0.75$, which differ significantly from our findings. In this situation, our next objective should be the combination of our present work on the single-particle gap with a systematic analysis of the various order parameters for the AFMI phase which appear in the literature. While Ref. [17] speculated that the inflection point at $U/\kappa \simeq 4.1$ could be due to systematical errors in the extrapolation $L \to \infty$, our present result for the critical exponent $\beta > 1$ strengthens the case for the inflection point being a physical feature. As a side note, Ref. [17] observed (in addition to the unexpected inflection point) that the single-particle gap appeared at slightly smaller $U/\kappa$ than the AFMI order parameter.

We conclude that the BRS algorithm is now applicable to realistic problems in the field of carbon-based nanomaterials. There are several future directions in which our present work can be developed. One objective is to present a systematic analysis of the various order parameters for the AFMI phase which appear in the literature. While the AFMI phase may not be directly observable in graphene, we note that tentative empirical evidence for such a phase exists in carbon nanotubes [55], along with preliminary theoretical evidence from MC simulations presented in Ref. [19]. The MC calculation of the single-particle Mott gap in a (metallic) carbon nanotube is expected to be much easier, since the physical lattice size $L$ is determined by the nanotube radius used in the experiment (as well as the number of unit cells accounted for in the longitudinal direction of the tube). As interaction (or electron-electron correlation) effects are expected to be more pronounced in the (1-dimensional) nanotubes, the treatment of flat graphene as the limiting case of an infinite-radius nanotube, would be especially interesting. Strong correlation effects could be even more pronounced in the (0-dimensional) fullerenes (or carbon buckyballs), where we are also faced with a fermion sign problem due to the admixture of pentagons into the otherwise bipartite hexagonal lattice. We note that this sign problem has the unusual property of vanishing as the system size becomes large, and that the behavior of both resembled the mean-field result $\beta = 1/2$ when $U/\kappa \gg U_c$. However, Ref. [17] did not attempt to determine $\beta$ directly from lattice MC results. Instead, $U_c$ was determined by taking the value of $\beta/\nu \simeq 0.90$ (where $\nu$ is the correlation length exponent) to coincide with that of the Gross-Neveu model to $O(\epsilon)$ in the $\epsilon$-expansion. They then found an acceptable data collapse in $L$ using the similarly-determined value $\nu \simeq 0.88$ of the correlation length exponent.

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Appendix A: Subtleties of the mixed differencing scheme

The mixed differencing scheme comes with a significant improvement of the time discretisation artefacts, if used correctly. It does not cancel the linear error term completely, but it diminishes the error as can be seen in Ref. [19]. Unfortunately the wrong form can also increase the discretisation error, up the point of a bias that does not vanish in the continuum limit.
1. Bias introduced by the naive forward differencing

Let us consider a naive form of the fermion matrix employing a forward differencing scheme

\[
M_{(x,t)(y,t')}^{AA} = \delta_{xy} \left( -\delta_{tt'} + \left( e^{i\tilde{\phi}_{x,t} - \tilde{m}_s} \right) \delta_{t+1,t'} \right)
\] (A1)

on the AA-terms, with the auxiliary field on the off-diagonal, similar to Ref. [19] and an explicit staggered mass \( \tilde{m}_s \). Again a tilde means that the corresponding quantity is multiplied by \( \delta = \beta/N_t \). Then an expansion in \( \delta \) yields

\[
M_{(x,t)(y,t')}^{AA} = \delta_{xy} \left( -\delta_{tt'} + \left( 1 + i\tilde{\phi}_{x,t} - \frac{1}{2} \partial_{x,t}^2 - \tilde{m}_s \right) \delta_{t+1,t'} \right) + \mathcal{O} \left( \delta^3 \right)
\] (A2)

\[
= \delta_{xy} \left( \delta_{t+1,t'} - \delta_{tt'} + \left( i\tilde{\phi}_{x,t} - \frac{1}{2} \partial_{x,t}^2 - \tilde{m}_s \right) \delta_{t+1,t'} \right) + \mathcal{O} \left( \delta^3 \right)
\] (A3)

\[
= \delta_{xy} \left( \delta_{tt} + \frac{1}{2} \partial_{x,t}^2 + \left( i\tilde{\phi}_{x,t} - \frac{1}{2} \partial_{x,t}^2 - \tilde{m}_s \right) \delta_{t,t'} + \delta_{t,t} \right) + \mathcal{O} \left( \delta^3 \right)
\] (A4)

\[
= \delta_{xy} \left( \delta_{tt} + \left( i\tilde{\phi}_{x,t} - \tilde{m}_s \right) \delta_{t,t'} - \delta \tilde{m}_s \delta_{t,t} \right) + \mathcal{O} \left( \delta^3 \right)
\] (A5)

where in the last step we defined

\[
\tilde{m}_s' := \tilde{m}_s - \frac{1}{2} \partial_{x,t}^2 + \frac{1}{2} \partial_{x,t}^2 - i \delta \tilde{\phi}_{x,t} \delta_{t,t}.
\] (A6)

The same calculation can be performed for the BB-elements; one finds that the effective staggered mass has the opposite sign, as expected,

\[
M_{(x,t)(y,t')}^{BB} = \delta_{xy} \left( \delta_{tt} + \left( \tilde{\phi}_{x,t} + \tilde{m}_s' \right) \delta_{t,t'} - \delta \tilde{m}_s \delta_{t,t} \right) + \mathcal{O} \left( \delta^3 \right)
\] (A7)

Note that \( \partial_{x,t}^2 \) is negative semi-definite, \( \tilde{\phi}_{x,t}^2 \) is positive semi-definite and \( i \tilde{\phi}_{x,t} \delta_{t,t} \) is indefinite, but in our experience usually \( \tilde{m}_s' \geq \tilde{m}_s \). For a vanishing bare staggered mass \( \tilde{m}_s = 0 \) this creates a non-zero bias between the sublattices introduced by the mixed differencing scheme, the sign of which prefers \( \langle m_A - m_B \rangle > 0 \). We can reproduce this bias numerically.

We consider the so called “seagull” term \( \partial_{x,t} \) separately because \( \tilde{\phi} \) scales as \( \sqrt{\delta} \) and thus this term is not in \( \mathcal{O} \left( \partial^2 \right) \) but effectively linear in \( \delta \), denoted as \( \mathcal{O}_e \left( \delta \right) \). This scaling holds because close to the continuum when the gaussian part of the action is narrow \( \tilde{\phi} \) is approximately distributed as \( \tilde{\phi} \sim \mathcal{N}(0, \sqrt{\delta} \cdot U) \). Hence, the seagull term is not suppressed in the continuum limit.

2. Field redefinition

One possibility to overcome the artefact is, following Brower et al. in Ref. [31], to absorb this term by means of a field redefinition. However, in the next section Appendix A3 we provide a numerically simple alternative approach which, by changing the forward derivative, removes the seagull term and yields the correct continuum limit, the approach we ultimately adopt.

Ref. [31] gives the field redefinition

\[
\phi_x \equiv \varphi_x - \delta \frac{1}{2} V_{x,y} \tilde{\varphi}_y \psi^*_y \psi_y
\] (A8)

introducing the field \( \psi \) on which the fermion matrix acts. The Hamiltonian then includes the terms

\[
\frac{1}{2} \sum_{t,t'} \tilde{\phi}_{x,t} \tilde{\phi}^*_{x,t} \left[ \delta_{t,t'} - \exp(-i\tilde{\phi}_{x,t}) \delta_{t-1,t'} + \tilde{m} \delta_{t-1,t'} \right] \psi_{x,t'}
\]

\[
= \frac{1}{2} \int dt \tilde{\phi}_x V_{x,y} \tilde{\phi}_y + \int dt \psi^*_x \tilde{\phi}_x \psi_x + i \int dt \psi^*_x \tilde{\phi}_x \psi_x + m \int dt \psi^*_x \psi_x
\]

\[
+ \frac{\delta}{2} \int dt \psi^*_x \partial_{x,t} \psi_x + \mathcal{O}_e \left( \delta \right).
\] (A9)
The redefinition (A8) gives
\[
\frac{1}{2} \int dt \varphi_x V^{-1}_{x,y} \varphi_y = \frac{1}{2} \int dt \varphi_x V^{-1}_{x,y} \varphi_y - \frac{\delta}{2} \int dt \varphi_x V^{-1}_{x,z} \varphi_y \psi_y \psi_y + O_c (\delta),
\]
and along the lines of Ref. [51], we note that the seagull term in \( \varphi_x^2 \) cancels the seagull term in \( \varphi_x^2 \) to leading order in \( \delta \) in Eq. (A9). We also need to account for the Jacobian generated by the field redefinition, which is
\[
\int D\tilde{\phi} = \int D\phi \det \left[ \frac{\partial \tilde{\phi}_{x,t}}{\partial \phi_{x',t'}} \right]
\]
\[
= \int D\phi \exp \left[ \text{Tr} \log \left( \delta_{x,y} \delta_{t,t'} - \frac{\delta}{2} \tilde{V}_{x,y} \psi_y \psi_y \delta_{t,t'} \right) \right]
\]
\[
\simeq \int D\phi \exp \left( -\frac{1}{2} \int dt V_{x,x} \psi_x \psi_x \right),
\]
where in the last step we used \( \log(1 + \delta z) = \delta z + O (\delta^2) \) before taking the continuum limit. We conclude that the seagull term in the expansion of the gauge links has the correspondence
\[
\frac{\delta}{2} \int dt \psi_x^* \delta_{x,t} \psi_x \leftrightarrow \frac{1}{2} \int dt V_{x,x} \psi_x \psi_x,
\]
that is to say, the physics encoded in the normal-ordering term is captured by the seagull term in the expansion of the gauge links. Hence, as argued in Ref. [31], the normal-ordering term should be omitted when gauge links are used.

So, the mixed-difference lattice action in Ref. [19] produces a “staggered” normal-ordering term, which does not by itself correspond to the correct Hubbard Hamiltonian. Let us now suggest a simple fix to this problem. We recall that for the fully non-compact theory without any gauge links, the normal-ordering term is not automatically generated and needs to be explicitly included. Although that fermion matrix is numerically unstable due to excessive round-off error, in such a discretization we should nevertheless take
\[
\tilde{m} = \tilde{V}_{0,0} + \tilde{m}_s \quad (x \in A), \quad \tilde{m} = \tilde{V}_{0,0} - \tilde{m}_s \quad (x \in B),
\]
in order to properly reproduce the continuum theory with a normal-ordering term and a staggered mass term. On the other hand, should we decide to use the backward differencing of Eq. (A9) for both sublattices as in Ref. [58], then
\[
\bar{m} = \bar{V}_{0,0} + \bar{m}_s \quad (x \in A), \quad \bar{m} = -\bar{m}_s \quad (x \in B),
\]
would suffice, as we have found that the correct normal-ordering term is accounted for by the seagull terms of the gauge links. However, with mixed differencing (forward for sublattice A, backward for sublattice B), the normal-ordering term would be produced with the opposite sign for sublattice A. Therefore
\[
\bar{m} = \bar{V}_{0,0} + \bar{m}_s \quad (x \in A), \quad \bar{m} = -\bar{m}_s \quad (x \in B),
\]
would be required, in order to again obtain the correct Hubbard Hamiltonian with the normal-ordering and staggered mass terms.

3. Alternative forward derivative

There is a simple alternative to the redefinition from the previous section [A2]. Using
\[
M_{x,x'}^A = \delta_{x,y} \delta_{t,t'} \left( e^{-i\tilde{\phi}_{x,t} + \tilde{m}_s} \right),
\]
with the auxiliary-field term on the diagonal and the original sign in the exponent instead of the ‘+’ in the naive (A1) yields the correct sign in front of the seagull term. This definition coincides with the original up to \( O_c (\delta^2) \) and leads to the correct continuum results. Higher order terms do not agree with the backward differencing; this difference is tolerated, given that one must extrapolate to the continuum in any case. In numerical simulations we set the bare staggered mass \( \tilde{m}_s = 0 \), although when we solve we perform Hasenbusch preconditioning with finite \( \tilde{m}_s \) [28]. The spectrum of this operator lacks the conjugate reciprocity that Ref. [29] explains may create an ergodicity problem. All the considerations of the diagonal operators that suggest those operators are free from ergodicity problems carry over to the operator used here.
Appendix B: Finding a plateau

Here we present an automatised deterministic method that reliably finds the best plateau in a given data set. This means that it finds the region of least slope and fluctuations and checks whether this region really is a plateau without significant drift. If a given time series does not exhibit a plateau, the method returns this information.

Apart from the time series \( m(\tau) \) (hopefully) exhibiting a plateau, the algorithm requires two parameters that have to be chosen in advance. The first is the minimal length \( \lambda \) a plateau has to have. Secondly a window width \( \mu \leq \lambda \) has to be chosen. It decides how many points are considered in the analysis of local fluctuations. We find that

\[
\lambda = \frac{1}{6} N_t, \quad (B1)
\]

\[
\mu = \log_2 N_t \quad (B2)
\]

usually are good choices.

Algorithm 1 describes the procedure in detail. The idea is to find a balance between least statistical and systematic fluctuations. Statistical fluctuations decrease with increasing plateau length. This is why we want to choose the plateau as long as possible without running into a region with systematic deviations. But this property can also be used to our advantage in the following way. If we calculate the mean from some time \( \tau_2 \) to all the previous times, the influence of another point compatible with the mean will decrease with the distance from \( \tau_2 \). Thus the local fluctuation of the running mean decreases till it reaches a point with significant systematic deviation. This local fluctuation minimum marks the optimal \( \tau_1 \). The plateau then ranges from \( \tau_1 \) to \( \tau_2 \). We check that it does not exhibit significant drift by fitting a linear function and checking if the first order term deviates from zero within twice its error. Repeating the analysis for all possible values of \( \tau_2 \) allows to find the globally best plateau distinct by least local fluctuations of the running mean.

\[
\text{Algorithm 1: Finding a fit-range for a plateau fit.}
\]

\[
\text{input: } N_t, m[0, \ldots, N_t - 1], \lambda, \mu
\]

\[
\text{output: } \tau_1, \tau_2
\]

\[
\text{for } \tau' = \mu - 1, \ldots, N_t - 1 \text{ do}
\]

\[
\text{for } \tau = 0, \ldots, \tau' \text{ do}
\]

\[
\text{mean}(\tau; \tau') = \text{mean}(m[\tau, \ldots, \tau']);
\]

\[
\text{end}
\]

\[
\text{for } \tau = 0, \ldots, \tau' - \mu + 1 \text{ do}
\]

\[
\text{sd}(\tau; \tau') = \text{sd}(m[\tau, \ldots, \tau + \mu - 1]; \tau');
\]

\[
\text{end}
\]

\[
\text{optimal}(\tau) = \arg\min_{\tau \in \{0, \ldots, \tau' - \mu\}} (\text{sd}(\tau; \tau'));
\]

\[
\text{end}
\]

\[
\Lambda = \{(\tau, \tau') \mid \tau = \text{optimal}(\tau'), \tau' - \tau \geq \lambda\};
\]

\[
\Lambda_0 = \{(\tau, \tau') \in \Lambda \mid m[\tau, \ldots, \tau'] \text{ has no significant drift}\};
\]

\[
\text{if } \Lambda_0 \neq \emptyset \text{ then}
\]

\[
(\tau_1, \tau_2) = \arg\min_{(\tau, \tau') \in \Lambda_0} (\text{sd}(\tau; \tau'));
\]

\[
\text{else}
\]

\[
\text{No plateau of needed length exists.}
\]

\[
\text{end}
\]

As every range in the set \( \Lambda_0 \) from algorithm describes a valid plateau, it allows us to give an estimator on the systematic error due to the choice of the plateau. We simply repeat the calculation of the relevant observable for all ranges in \( \Lambda_0 \) and use the standard deviation of these values as a systematic uncertainty.

Appendix C: Thermal gap

It proves useful to consider the influence of the finite temperature on the gap, as it provides a handle on the finite-temperature scaling.

Of course we are not able to solve the complete problem analytically, so this part considers only first order perturbation in \( U \). We assume the dispersion relation of graphene is not yet influenced by the interaction because \( U \) is
small. Then the particle density follows Fermi-Dirac statistics and an integral over the positive energy part

\[
\omega_k = \kappa \sqrt{3 + 4 \cos \frac{3ak_x}{2} \cos \frac{\sqrt{3}ak_y}{2} + 2 \cos \frac{\sqrt{3}ak_y}{2}},
\]

or the complete conduction band, gives the expectation value of the number of electrons excited from the ground state. Every excited electron contributes some energy \(E(U)\) to a thermal gap \(\Delta(\beta)\). This contribution primarily depends on the coupling and can be assumed linear in the regime of small coupling. Thus multiplying said integral by \(E(U)\) yields the following gap equation:

\[
\Delta(\beta) = \frac{3\sqrt{3}}{2} E(U) \int_{k \in \text{BZ}} d^2k \frac{a^2}{(2\pi)^2} \frac{1}{1 + e^{\beta\omega_k}}.
\]

Here \(a\) is the lattice spacing and the prefactor \(\frac{3\sqrt{3}}{2}\) simply stems from the hexagonal geometry of the first Brillouin zone (BZ).

Be aware that the thermal gap, although not distinguishable numerically, is no band gap. It can arise even if the conduction band and the valence band touch or overlap. The thermal gap measures, as explained above, the excitation above the ground state based on the number of excited states that are already occupied in thermal equilibrium.

1. Finite temperature

Now let us assume that \(\beta\) is large. Then the integrand only contributes in the region where \(\omega_k \approx 0\)—near the Dirac points \(K\) and \(K'\) which have momentum \(k_D\). In the vicinity of a Dirac-point the dispersion relation simplifies to the well-known cone \(\omega_k = \frac{3}{2} \kappa a |k - k_D|\). This allows us to approximate the integral by the sum over the two Dirac-points and perform the integral in polar coordinates

\[
\Delta(\beta) \approx 2\frac{3\sqrt{3}}{2} E(U) \int_{k \in \text{BZ}} d^2k \frac{a^2}{(2\pi)^2} \frac{1}{1 + e^{\beta\omega_k}} \approx \frac{3\sqrt{3}}{2\pi} \frac{E(U)}{(\beta\kappa)^2} \int_0^\infty dk \frac{k}{1 + e^{\beta/2\beta\kappa a k}}.
\]

Note that the error of this approximation is exponentially suppressed in \(\beta\).

We find that the prediction for the quadratic scaling in \(\beta\) and the linear approximation in \(U\) are indeed accurate. This is shown in Figure 6 where we multiplied the values of the band gap by \((\beta\kappa)^2\). In the small coupling regime the normalised points lie neatly on top of each other and on a straight line. Once they approach the critical coupling, the points separate. As expected, the linear dependence in \(U\) survives longest for small \(\beta\) because temperature effects dominate influences of the coupling. The quadratic dependence in \(\beta\) survives longest for large \(\beta\) due to its exponential convergence as stated above.

A fit of equation (C4) to our data in the region \(U/\kappa \leq 2\) under the assumption of \(E(U) \propto U\) leads to

\[
E(U) = 6.05(16) U.
\]

2. Finite lattice size

On the other hand the discretised form given by

\[
\Delta(L, \beta) = \frac{E(U)}{L^2} \sum_{k \in \text{BZ}} \frac{1}{1 + e^{\beta\omega_k}}.
\]

has a very complicated convergence behaviour. It is an effective trapezoidal approximation of the integral because of periodic boundary conditions, thus the convergence is expected to scale as \(O(L^{-2})\). A precise leading-order error estimation can be obtained as follows.

The first BZ is discretised into a regular triangular lattice. Let us denote the lattice spacing by \(h \propto L^{-1}\). We integrate a function \(f(x, y)\) over a single triangle, spanned by the coordinates \((\pm h/2, 0)\) and \((0, \sqrt{3}h/2)\),

\[
I := \frac{1}{2} \int_{-\frac{h}{2}}^{\frac{h}{2}} dx \int_{0}^{\frac{\sqrt{3}h}{2} - |x|} dy f(x, y).
\]

\[
(C7)
\]
and subtract the average of the function over the corner points, multiplied by the area of the triangle,

\[ I := \frac{1}{3} \sqrt{3} h^2 \left( f \left( \frac{h}{2}, 0 \right) + f \left( \frac{h}{2}, 0 \right) + f \left( 0, \frac{\sqrt{3}}{2} h \right) \right). \quad (C8) \]

This gives the local error

\[ I - \tilde{I} = -\frac{\sqrt{3}}{64} \left( \frac{\partial^2 f}{\partial x^2}(0) + \frac{\partial^2 f}{\partial y^2}(0) \right) h^4 + O \left( h^5 \right), \quad (C9) \]

made by discretising the integral. We obtain the global error via summation over the complete BZ

\[ \sum_{k \in \text{BZ}} \left( I(k) - \tilde{I}(k) \right) = -\frac{\sqrt{3}}{64} \sum_{k \in \text{BZ}} \left( \frac{\partial^2 f}{\partial x^2}(k) + \frac{\partial^2 f}{\partial y^2}(k) \right) h^4 + O \left( L^2 h^5 \right) \]

\[ \propto \frac{1}{L^4} \sum_{k \in \text{BZ}} \left( \frac{\partial^2 f}{\partial x^2}(k) + \frac{\partial^2 f}{\partial y^2}(k) \right) + O \left( L^{-3} \right) \quad (C10) \]

\[ \propto \frac{1}{L^2} \int_{k \in \text{BZ}} d^2 k \left( \frac{\partial^2 f}{\partial x^2}(k) + \frac{\partial^2 f}{\partial y^2}(k) \right) + O \left( L^{-3} \right) \]

\[ = \frac{1}{L^2} \oint_{k \in \partial \text{BZ}} \nabla f(k) \cdot dk + O \left( L^{-3} \right) \]

\[ \propto O \left( L^{-3} \right). \quad (C11) \]

Surprisingly one finds that the second order error term vanishes. In expression (C13) Gauss’s theorem has been applied and the projection of the gradient of \( f \) onto the normal of the BZ is integrated over the boundary of the BZ. Every momentum-periodic function takes the same values on the opposite lying edges of the BZ. Thus the integral sums up to zero. In the special case of \( f(k) \propto (1 + e^{i\beta \omega k})^{-1} \) the gradient in BZ-normal direction vanishes everywhere on the boundary and the integral (C13) does not even have to be performed.

Figure 6 shows that the cubic finite size effects are a good approximation below the phase transition, as one would expect for states with small correlation lengths. In Figure 7 we show that the approximation still works out near and above the phase transition.

Higher orders in the coupling influencing the thermal gap are not as easy to calculate but can be dealt with via diagrammatic techniques using finite temperature Matsubara formalisms [49]. We know from Ref. [50] that the Fermi
velocity is influenced only in $O(U^2)$ below some critical coupling. Thus we expect the second order term of the thermal gap to be very small as it does not arise near the Dirac-points and only the cubic correction to have a significant influence again.

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