

**Attractive Hubbard model on a honeycomb lattice: Quantum Monte Carlo study**

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We study the attractive fermionic Hubbard model on a honeycomb lattice using determinantal quantum Monte Carlo simulations. By increasing the interaction strength  $U$  (relative to the hopping parameter  $t$ ) at half filling and zero temperature, the system undergoes a quantum phase transition at  $5.0 < U_c/t < 5.1$  from a semimetal to a phase displaying simultaneously superfluid behavior and density order. Doping away from half filling, and increasing the interaction strength at finite but low temperature  $T$ , the system always appears to be a superfluid exhibiting a crossover between a BCS and a molecular regime. These different regimes are analyzed by studying the spectral function. The formation of pairs and the emergence of phase coherence throughout the sample are studied as  $U$  is increased and  $T$  is lowered.

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The recent discovery of graphene layers, i.e., single-atom thick layers of carbon atoms arranged in a planar honeycomb structure,<sup>1</sup> has attracted considerable attention due to its interest in fundamental physics as well as for potential applications. The energy-band spectrum shows “conical points” where the valence and conduction bands are connected, and the Fermi energy at half filling is located precisely at these points as only half of the available states are filled. Around these points, the energy varies proportionally to the modulus of the wave vector and the excitations (holes or particles) of the system are equivalent to ultrarelativistic (massless) Dirac fermions since their dispersion relation is linear.<sup>2</sup> Graphene sheets then allows for table-top experiments on two-dimensional (2D) field theories with quantum anomalies, allowing us to explore the Klein paradox,<sup>3</sup> the anomalous quantum Hall effect induced by Berry phases<sup>4,5</sup> and its corresponding modified Landau levels.<sup>6</sup>

When the fermions are interacting, the peculiar nature of the Fermi surface (i.e., reduced to a finite number of Dirac points) leads to special physics at and around half filling. In a square lattice, the nesting of the Fermi surface generally leads to ordered phases even for arbitrarily small interaction strengths. On the contrary, in the honeycomb lattice and with repulsive interactions, Paiva *et al.*<sup>7</sup> have found a quantum phase transition (QPT) at half filling between a metallic and an ordered phase when the interaction strength is increased. However, since graphene is a weakly interacting system, this QPT is not accessible experimentally.

It is now known that a hexagonal optical lattice could be produced with three laser beams.<sup>8,9</sup> In a recent work, some of us have analyzed the possibility of reproducing graphene physics and of extending it to the interacting regime by creating a two-dimensional honeycomb optical lattice and loading ultracold spin-1/2 fermionic atoms, such as <sup>6</sup>Li, into it.<sup>10</sup>

The key advantage is that the relevant experimental parameters (e.g., configuration and strength of the optical potential, interatomic interaction strength tuned via Feshbach resonance) can be accurately controlled while getting rid of the inherent complexity of a solid. Following this idea, we use exact quantum Monte Carlo (QMC) simulations to study interacting ultracold fermions loaded into a honeycomb optical lattice in the absence of any external confinement. We will focus on the case of attractive interactions as it is accessible with these numerical techniques and free from the sign problem at and away from half filling.

In the continuum at zero temperature, as the interacting fermionic gas is driven from the weak to the strong attractive coupling limit, there is a crossover from a BCS regime of weakly bound delocalized pairs to a Bose-Einstein condensate (BEC) of tightly bound pairs (later called molecules for simplicity).<sup>11–13</sup> At finite but sufficiently low temperature, a similar BCS-molecule crossover is observed except that, the system being two dimensional, there is only quasilong-range order and, consequently, no true condensate but only a superfluid. In this paper, we will study interacting particles on a lattice, represented by a simple fermionic Hubbard model.<sup>14</sup> Nonetheless, some aspects of the continuum limit, such as the BCS-BEC crossover, are expected to be reproduced in the discrete model. Zhao and Paramekanti<sup>15</sup> have explored the attractive fermionic Hubbard model on a honeycomb lattice using mean-field theory and they found a QPT between a semimetal and a superfluid at half filling. Away from half filling, they recovered the crossover already observed in the continuum limit. Recently, Su *et al.*<sup>16</sup> used QMC methods to study the BCS-BEC crossover on the honeycomb lattice away from half filling and concluded that it was similar to the one obtained for the square lattice. In the present work, we use QMC simulations and large system sizes to study the pair formation at half filling and accurately determine the critical value of the coupling strength at which pairs form. We then study pairing away from half filling by analyzing several quantities, including spectral functions.

The paper is organized as follows. In Sec. I, we introduce the model, notations, and the quantities we use to characterize the different phases. In Sec. II, we show that our system at half filling can be related to the repulsive Hubbard model<sup>7</sup> and then present complementary results for this case, including the QPT point the system crosses to go from a semimetallic disordered phase to an ordered one displaying both superfluid behavior and density wave order. The location of this QPT point has been accurately determined compared to previous works and the nature of the weakly interacting phase before the transition is addressed by analyzing the behavior of the spectral function as the interaction strength is varied. Finally, in Sec. III we study the system doped away from half filling. The system is clearly shown to exhibit superfluid behavior while the density wave order present at half filling has been destroyed. We conclude our study by analyzing the formation of pairs and the emergence of global phase coherence as a function of temperature and interaction strength.

## I. FERMIONIC HUBBARD MODEL

The physics of a system of  $N_f$  spin-1/2 fermions, with attractive two-body interactions and equal spin populations,

filling up a lattice made of  $N$  sites is encapsulated in a simple tight-binding model, namely, the fermionic attractive Hubbard model (FAHM), whose grand-canonical Hamiltonian operator reads<sup>17</sup>

$$H = -t \sum_{\langle i,j \rangle, \sigma} (f_{i\sigma}^\dagger f_{j\sigma} + f_{j\sigma}^\dagger f_{i\sigma}) - U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) - \mu \sum_{i,\sigma} n_{i\sigma}. \quad (1)$$

Here  $\langle i,j \rangle$  denotes pairs of nearest-neighbor sites on the lattice,  $\sigma = \uparrow, \downarrow$  are the two possible spin states of the fermions,  $f_{i\sigma}^\dagger$  and  $f_{i\sigma}$  are the creation and annihilation operators of a fermion with spin state  $\sigma$  at site  $i$ ,  $n_{i\sigma} = f_{i\sigma}^\dagger f_{i\sigma}$  is the corresponding number operator,  $t$  is the hopping amplitude between nearest-neighbor sites,  $U \geq 0$  is the strength of the attractive interaction between fermions with opposite spin states, and  $\mu$  is the chemical potential whose value fixes the average total fermionic density  $\rho$ . With the present form of the interaction term, the system is half filled, i.e., there is on average one fermion per site ( $\rho = N_f/N = 1$ ), when  $\mu = 0$ . In the noninteracting limit  $U = 0$ , this system is known to behave like a semimetal with vanishing density of states at the Fermi level and its elementary excitations are massless Dirac fermions that obey the 2D Weyl-Dirac equation.<sup>18</sup>

The FAHM [Eq. (1)] on a bipartite lattice is particle-hole symmetric<sup>19</sup> and thus adopts the same phases for densities  $\rho$  and  $2 - \rho$ . It is then sufficient to study the system for densities  $\rho \geq 1$ . This model can also be mapped onto the fermionic repulsive Hubbard model (FRHM) (Refs. 7 and 14) by performing a particle-hole transformation on only one of the species. Consequently, the physics of the FAHM at densities  $(\rho_\uparrow, \rho_\downarrow)$  is equivalent to that of the FRHM at densities  $(1 - \rho_\uparrow, \rho_\downarrow)$  or  $(\rho_\uparrow, 1 - \rho_\downarrow)$  but with a nonzero Zeeman-type term,  $-\mu \sum_i (n_{i\uparrow} - n_{i\downarrow})$ . Therefore, the two models are identical at half filling ( $\mu = 0$ ). We will use this equivalence in Sec. II where we concentrate on the half-filled case.

To calculate the equilibrium properties of this model at finite but low temperatures  $T$ , we used the standard determinant quantum Monte Carlo (DQMC) algorithm.<sup>20–24</sup> The partition function is expressed as a path integral with the help of Suzuki-Trotter decomposition ( $\Delta\tau = 0.125$ ). The interaction term is decoupled through discrete Hubbard-Stratonovich (HS) transformation.<sup>20</sup> The fermionic degrees of freedom are traced out analytically and the summation over the HS field is done stochastically. Metropolis algorithm is used to perform local moves which flip the HS variables at a given site and a given imaginary time. For each data points (temperature, interaction strength, lattice, and density), 20 simulations of different random seeds are performed, each with 1000 warm-up sweeps and 2000 measurement sweeps. Statistical average of the 20 simulations are reported. The cases under our consideration (namely, attractive interactions and equal densities of spin-up and spin-down fermions) are free of the sign problem<sup>23</sup> that used to plague numerical simulations of fermionic systems. This will allow us to reach the low temperatures needed to study pairing and superfluidity. In the following, the reciprocal of the thermal energy (also called

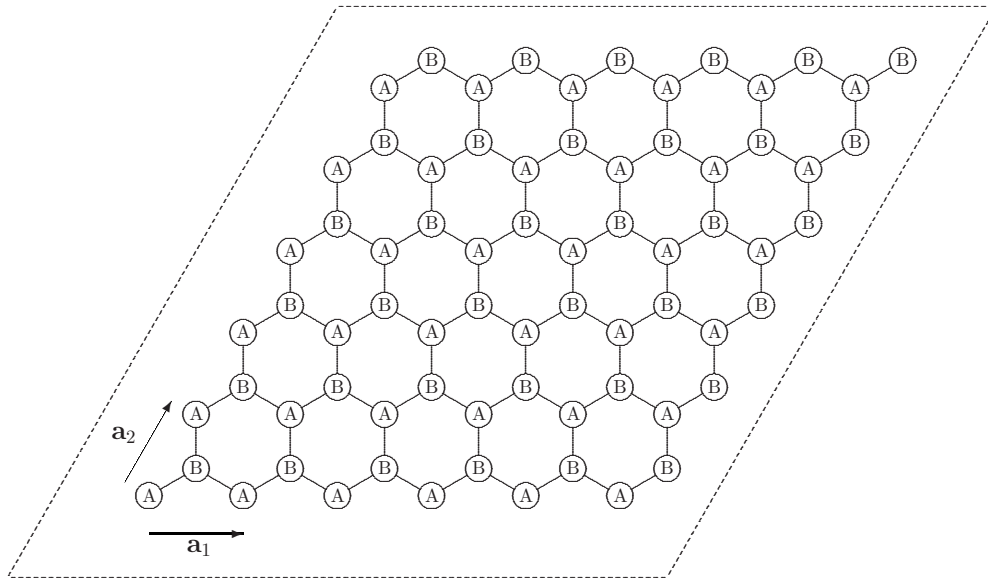


FIG. 1. Finite honeycomb lattice of linear dimension  $L=6$ . The total number of sites is  $N=2L^2=72$ .

the inverse temperature) is denoted as usual by  $\beta=1/k_B T$ , where  $k_B$  is the Boltzmann constant.

In the DQMC simulations, we have used the honeycomb lattice depicted in Fig. 1 with periodic boundary conditions. The primitive vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  delineate a diamond-shaped primitive cell of the Bravais lattice which contains two non-equivalent sites (A and B) separated by  $\overline{AB}=(\mathbf{a}_1+\mathbf{a}_2)/3$  and each producing upon tiling a hexagonal sublattice. A finite honeycomb lattice of side  $L$  then contains  $N=2L^2$  sites. In the noninteracting case, the energy levels are given by<sup>2,10</sup>

$$\epsilon_{\pm}(k_1, k_2) = \pm t |1 + e^{i2\pi k_1/L} + e^{i2\pi k_2/L}|,$$

where  $k_1, k_2 \in \{0, 1, \dots, L-1\}$ . When  $L$  is a multiple of three, there always exist pairs  $(k_1, k_2)$  such that  $\epsilon_{\pm}(k_1, k_2)=0$ , i.e., there are four states (two per spin state) located exactly at the Fermi level and only two of these states will be occupied if  $\rho=1$ . This does not happen when  $L$  is not a multiple of three. As a consequence, on small finite-size systems, a small gap of order  $1/L$  appears around half filling when  $L$  is not a multiple of three (see Fig. 2). To avoid confusion between

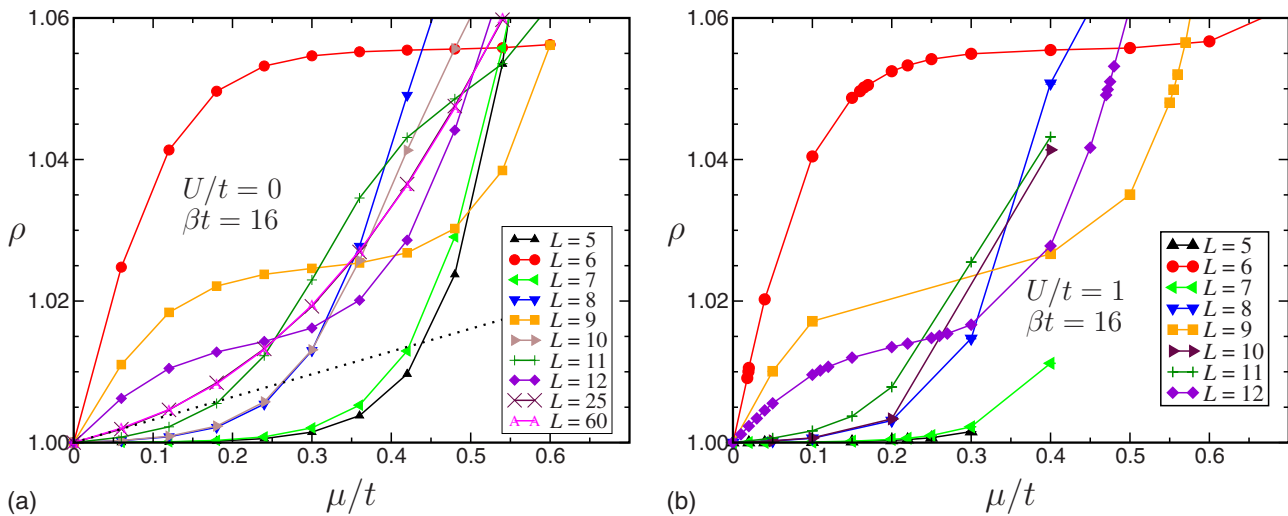


FIG. 2. (Color online) Total average density  $\rho$  vs chemical potential  $\mu$  for  $U/t=0$  (top) and  $U/t=1$  (bottom) at  $\beta t=16$  and different lattice sizes  $L$ . The top figure is obtained by analytical calculation at  $U=0$ . The bottom figure is obtained from numerical data generated by DQMC. For sizes that are not multiples of three, there is no state at half filling and a small gap appears for small system sizes. There is no such gap when  $L$  is a multiple of three. For sizes that are multiples of three, plateaus appear away from half filling. These plateaus are also finite-size effects and they disappear when  $L \rightarrow \infty$ . The dotted line in the top figure is obtained by an exact evaluation of the derivative  $\partial\rho/\partial\mu|_{\mu=0}$  in the noninteracting limit when  $L \rightarrow \infty$ . The two figures show that the “magic number 3” effect is present even when the interaction strength  $U$  is comparable to the hopping parameter  $t$ .

this gap, which is a finite-size effect and Mott gaps generated by interactions that are expected to appear in ordered phases, we used (especially at half-filling) sizes  $L$  that are multiples of three. This limits strongly the sizes that can be studied. In the most favorable cases, we went up to  $L=15$ , that is,  $N=450$  sites.

In the strong-coupling regime ( $U \gg t$ ), we expect the system to form pairs (hereafter called molecules) of fermions with opposite spins on the same site. These pairs can show two different ordering phenomena: establishment of a phase coherence order or of a solid (crystal-type) order. A solid of pairs would exhibit a density wave typical of a crystal and would reveal itself through spatial oscillations in the density-density correlation function,

$$D_{ij} = \langle n_i n_j \rangle, \quad (2)$$

where  $n_i = \sum_{\sigma} n_{i\sigma}$  is the total number of fermions on site  $i$  and where  $\langle \cdot \rangle$  denotes the quantum statistical average at temperature  $T$ . At half filling and zero temperature, we expect to observe a phase where alternate sites are empty and where only the A or the B sublattice is occupied. Such a density wave is signaled by a structure factor  $S_{\text{dw}}$  diverging linearly with the total number of sites  $N$  of the system, where

$$S_{\text{dw}} = \frac{1}{N} \sum_{i,j} (-1)^{i+j} D_{ij} \quad (3)$$

with the site index  $i$  being even on A sites and odd on B sites.

In a Bose condensed phase, the phase coherence between pairs is signaled by long-range order (or quasilong-range order for a superfluid at finite temperature) in the pair Green's function,

$$G_{ij}^p = \frac{1}{2} \langle \Delta_i^\dagger \Delta_j + \Delta_i \Delta_j^\dagger \rangle, \quad (4)$$

where  $\Delta_i^\dagger = f_{i\uparrow}^\dagger f_{i\downarrow}^\dagger$  creates a pair on site  $i$ . In a way similar to the density correlations, we define a pair structure factor  $P_s$ ,<sup>25</sup>

$$P_s = \frac{1}{N} \sum_{i,j} G_{ij}^p. \quad (5)$$

This pair structure factor diverges linearly with  $N$  when long-range order is achieved. Finally, in the absence of any order, the system is expected to be a semimetal at half filling due to the peculiar nature of the Fermi surface (no gap but a vanishing density of states at the Fermi level). To distinguish between metallic, semimetallic, or gapped (solid or superfluid) states, we calculate the spectral function  $A(\omega)$  which essentially reflects the one-particle density of states. To obtain this quantity, we first calculate the (imaginary) time-displaced on-site Green's function  $G(\tau) = \sum_i \langle f_i(\tau) f_i^\dagger(0) \rangle / N$  and then extract  $A(\omega)$  by inverting the following Laplace transform:

$$G(\tau) = \int d\omega \frac{e^{-\tau\omega}}{e^{-\beta\omega} + 1} A(\omega)$$

using the analytic continuation procedure of Sandvik<sup>26</sup> in which the spectral function is parameterized as  $N$   $\delta$  functions

on a uniform grid of frequencies  $\omega_l$ . The amplitudes  $A_l$  of the  $\delta$  functions are sampled from a probability distribution  $p(A) \sim \exp[-\chi^2 / \Theta + \alpha S]$ . Here  $\chi^2$  is the deviation of the  $G(\tau)$  computed from  $A(\omega)$  from the values  $\tilde{G}(\tau)$  produced by the QMC simulation,  $S$  is the entropy, and  $\alpha$  is chosen to have an optimal value given by Bayesian logic. An annealing procedure is used starting from large  $\Theta$ , which is then slowly reduced.

## II. HONEYCOMB LATTICE AT HALF FILLING

At half filling, the system can be mapped onto the FRHM.<sup>27-30</sup> Defining a hole creation operator  $h_{i\downarrow}^\dagger$  for the down spin through

$$(-1)^i h_{i\downarrow}^\dagger = f_{i\downarrow}, \quad (6)$$

the kinetic term is left unchanged in the spin-down holes representation. The number operator  $n_{i\downarrow}$  is accordingly transformed into  $1 - n_{i\downarrow}^h$ , where  $n_{i\downarrow}^h = h_{i\downarrow}^\dagger h_{i\downarrow}$  is the number operator for holes and up to a redefinition of the chemical potential  $\mu$ , the sign of the interaction term is reversed. The FRHM has SU(2) spin-rotation symmetry at half filling, which translates into the SU(2) pseudospin symmetry of FAHM.<sup>31</sup> Hence the spin-spin correlations are the same along the three coordinate axes,

$$\langle \sigma_i^x \sigma_j^x \rangle = \langle \sigma_i^y \sigma_j^y \rangle = \langle \sigma_i^z \sigma_j^z \rangle, \quad (7)$$

where  $x$  and  $y$  are the in-plane axes and  $z$  the axis orthogonal to the lattice plane. More specifically,

$$\sigma_i^x = f_{i\uparrow}^\dagger h_{i\downarrow} + h_{i\downarrow}^\dagger f_{i\uparrow},$$

$$\sigma_i^y = i(h_{i\downarrow}^\dagger f_{i\uparrow} - f_{i\uparrow}^\dagger h_{i\downarrow}),$$

$$\sigma_i^z = n_{i\uparrow} - n_{i\downarrow}^h. \quad (8)$$

At large interaction, the FRHM is known to be equivalent to a Heisenberg model and it develops a long-range antiferromagnetic order on the honeycomb lattice at zero temperature.<sup>7</sup> The correlation functions in Eq. (7) then show oscillations from site to site. Translated into the attractive model language, these functions become<sup>19,32</sup>

$$\langle \sigma_i^z \sigma_j^z \rangle = \langle n_i n_j - n_i - n_j - 1 \rangle, \quad (9)$$

$$\langle \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \rangle = 2(-1)^{i+j} \langle \Delta_i^\dagger \Delta_j + \Delta_i \Delta_j^\dagger \rangle. \quad (10)$$

The spin antiferromagnetic correlations along the  $z$  axis in the FRHM are then reproduced in the density-density correlations  $D_{ij}$  of the FAHM, which develops a density wave with alternating occupied and empty sites. The spin correlations in the  $xy$  lattice plane translate into long-range order for the Green's function  $G_{ij}^p$  and phase coherence of a Bose-Einstein condensate. The antiferromagnetic phase of the FRHM is thus mapped onto a peculiar phase for the FAHM since it exhibits at the same time phase coherence *and* density wave orders. In the following we will denote this phase as the density-wave-superfluid (DW-SF) phase. Moreover it is easy to show from Eqs. (9) and (10) that  $2P_s = S_{\text{dw}}$  as is



TABLE I. Comparison of  $P_s$  and  $S_{\text{dw}}/2$  for  $L=12$ ,  $\beta t=20$ ,  $U/t=3$ , and different values of  $\mu/t$ . At half filling, those quantities are equal within statistical error bars as a consequence of the SU(2) pseudospin symmetry of the FAHM.  $S_{\text{dw}}$  and  $P_s$  are small because  $U < U_c$  and the system is in its semimetallic phase. This symmetry is broken when  $\mu \neq 0$  and this is confirmed by the numerical data showing that the two quantities are indeed unequal.  $S_{\text{dw}}$  remains small but  $P_s$  is large due to the presence of quasilong-range order.

$\mu/t$	$\rho$	$S_{\text{dw}}/2$	$P_s$
0	1.0	$1.125 \pm 0.005$	$1.127 \pm 0.001$
0.9202	1.5	$0.3356 \pm 0.0004$	$10.5 \pm 0.1$

numerically checked in Table I. As the order parameter is here of dimension 3 and the lattice is of dimension 2, we do not expect any transition to an ordered phase at finite temperature.<sup>33</sup>

Paiva *et al.*<sup>7</sup> have studied the ground state of FRHM on a honeycomb lattice a few years ago. They found a QPT from an antiferromagnetic phase at large coupling to a metallic phase at low coupling, the critical coupling strength being bounded by  $4 \leq U_c/t \leq 5$ . We use finite-size scaling and larger system sizes  $L$  to improve the numerical accuracy and narrow down the region of this QPT. Spin wave theory applied to Heisenberg models implies that the structure and pair structure factors at  $T=0$  scale with the number of lattice sites  $N=2L^2$  like<sup>7,17,34,35</sup>

$$2P_s(N) = S_{\text{dw}}(N) \approx aN + b\sqrt{N} + c,$$

where  $a, b, c$  are  $U$ -dependent non-negative constants. In the disordered phase  $S_{\text{dw}}(N)$  is expected to reach a constant finite value as  $N$  goes to infinity, meaning that the coefficients  $a$  and  $b$  should then vanish. In the ordered phase,  $a$  should be strictly positive so that both  $P_s$  and  $S_{\text{dw}}$  diverge linearly with  $N$  signaling the emergence of density and phase coherence orders. Using system sizes as large as  $L=15$  and using the vanishing of coefficient  $a$  to define the onset for the DW-SF phase, we have been able to infer the critical interaction strength  $U_c$  to be in the range  $5.0 < U_c/t < 5.1$  (Fig. 3).

In the study by Paiva *et al.*, the metallic phase appearing at low  $U$  was not studied in detail. In particular, the question of the metallic or semimetallic nature of the system was not addressed. Calculating the spectral function  $A(\omega)$  for different values of  $U$  (Fig. 4), we find that the system is always a semimetal when it is not in an ordered phase. The density of states drops around the Fermi level (located at  $\omega=0$ ) for  $U/t < 5$  but without forming a gap. On the contrary, we observe a tiny metallic peak at the Fermi level. This peak is a finite-size effect due to the four states per spin located exactly at the Fermi level (in the noninteracting limit) when the system size is a multiple of three. On the contrary, using sizes that are not multiples of three, we do observe a small gap. Both this gap and the peak are finite-size effects that are reduced when we increase the size of the system. We then conclude that  $A(\omega)$  is zero (or very small) only at the Fermi level but without the formation of a gap. This is the signature of a semimetallic phase. Indeed, a metal would be signaled

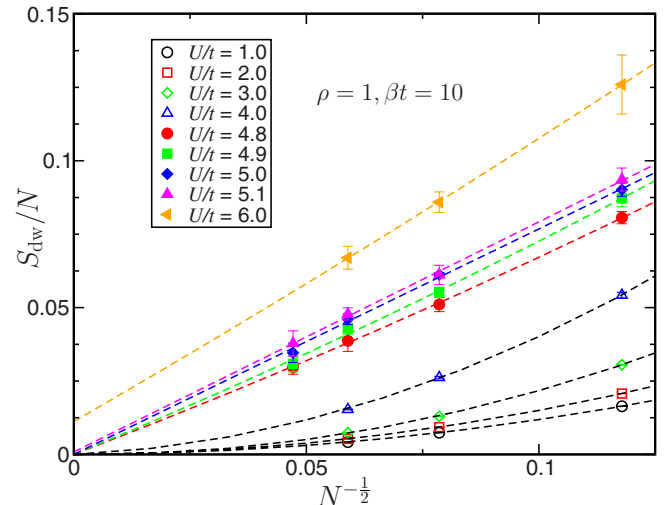


FIG. 3. (Color online) Scaling of the density wave structure factor  $S_{\text{dw}}$  with lattice size  $L$  at half filling (the total number of lattice sites is  $N=2L^2$ ). We have checked that for few coupling strengths and lattice sizes, the results remain (almost) unchanged for  $\beta t=16$ . Therefore, the value  $\beta t=10$  is sufficiently large to distinguish the semimetallic and the superfluid phases. The dashed lines are a fit of the form  $S_{\text{dw}}/N = a + b/\sqrt{N} + c/N$ . Close to or above the transition ( $U/t \gtrsim 5.0$ ), the coefficients  $a$  and  $b$  take on finite positive values implying that both density and phase coherence orders emerge in the thermodynamic limit  $N \rightarrow \infty$ . As it is seen,  $S_{\text{dw}}/N$  then essentially scales linearly with  $1/\sqrt{N}$  and achieves the finite value  $a$  when  $N \rightarrow \infty$ . Below the transition ( $U/t \lesssim 5$ ), the coefficients  $a$  and  $b$  vanish, meaning that the system reaches its disordered phase in the thermodynamic limit  $N \rightarrow \infty$ . As it is seen,  $S_{\text{dw}}/N$  then essentially scales as  $1/N$  and goes to zero when  $N \rightarrow \infty$ . The QPT point is thus signaled by the vanishing of the coefficient  $a$ , from which we can infer that the critical interaction strength lie in the range  $5.0 < U_c/t < 5.1$ .

by a persistent peak at the Fermi level (or at least a large nonzero density). The transition to the DW-SF ordered phase is signaled by the opening of the gap in  $A(\omega)$  for  $U/t \geq 5$ , which corresponds to the value for the transition previously obtained by the finite-size scaling analysis of  $S_{\text{dw}}$ .

### III. DOPING AWAY FROM HALF FILLING

At zero temperature, when the FAHM is doped away from the DW-SF ordered phase obtained at half filling when  $U > U_c$ , say by increasing  $\rho$  from 1, we expect the density order to disappear and the phase coherence order to persist. However, one also expects phase coherence to establish throughout the sample when the system is doped away from the semimetallic phase obtained at half filling when  $U < U_c$ . Indeed in this case the Fermi surface is no longer limited to isolated points and BCS pairing becomes possible. Therefore, we expect the phase coherence order to establish at zero temperature for all values of the interaction  $U$  as soon as  $\rho \neq 1$ . With an order parameter of dimension 2 (a phase gradient pictured as a vector lying in the  $xy$  plane), the system undergoes a Berezinsky-Kosterlitz-Thouless (BKT) (Refs. 36–38) transition at some critical temperature  $T_c$ , leading to

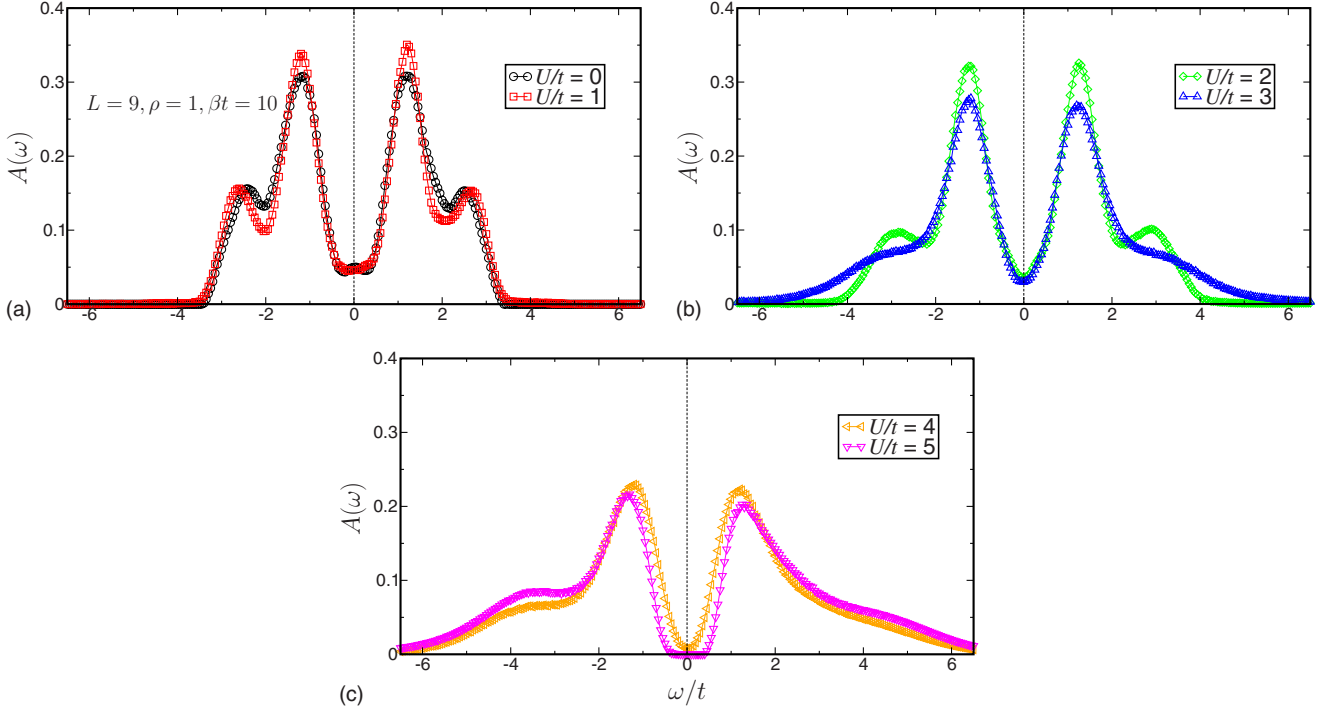


FIG. 4. (Color online) Spectral function  $A(\omega)$  at half filling ( $\rho=1$ ) for different values of the interaction strength  $U$ . The lattice size is  $L=9$  and  $\beta t=10$ . The Fermi level is located at  $\omega=0$ . For  $U/t < 5$ , the system is a semimetal as witnessed by the dip around the Fermi level. The nonvanishing density of states at the Fermi level is due to finite-size effects (see Fig. 2). For  $U/t > 5$ , a gap opens as the system enters the DW-SF ordered phase. The small peaks situated at  $|\omega| \approx 2.5t$  are also a result of finite-size effects.

a quasilong-range phase order, i.e., a superfluid phase, at  $T < T_c$  before the appearance of the Bose-Einstein condensate at  $T=0$ .

According to mean-field theory,<sup>15</sup> a superconductor exists anywhere away from half filling, albeit the superconducting gap function or, equivalently,  $\langle \Delta_i^\dagger \rangle$ , decays exponentially with respect to  $1/(U\sqrt{\rho}-1)$  in the BCS regime. In their previous study, Su *et al.*<sup>16</sup> compared DQMC results to random-phase approximation (RPA) calculations and showed that there is a so-called BCS-BEC crossover extending from small to large values of the interaction when the system is off half filling. When  $U$  is increased, the ground state of the system evolves continuously from a BCS state (where fermions with opposite spins form loose pairs of plane waves with opposite momenta) to a BEC of bosonic molecules (where fermions with opposite spin form tightly bound pairs). We have extended their study to larger lattices (up to  $L=15$ ) and lower temperatures (up to  $\beta t=20$ ) and we have also analyzed new observables.

We first studied the behavior of the pair and density wave structure factors,  $P_s$  and  $S_{dw}$ , away from half filling. To do this, we first need to obtain the low-temperature limit of these quantities by decreasing the temperature until we observe a plateau signaling that we have reached the  $T=0$  limit (Fig. 5). To extract the plateau value, we have used the three-parameter function

$$F(\beta t) = \frac{u}{1 + v \exp(-w\beta t)} \quad (11)$$

to fit our numerical data  $P_s(\beta t)$ . The plateau value  $\lim_{\beta \rightarrow \infty} P_s$  is then approximated by  $u$ . We have also observed in our

numerical simulations that this plateau is reached at lower and lower temperatures as we approach half filling. This is because the BKT critical temperature  $T_c$  goes to zero like

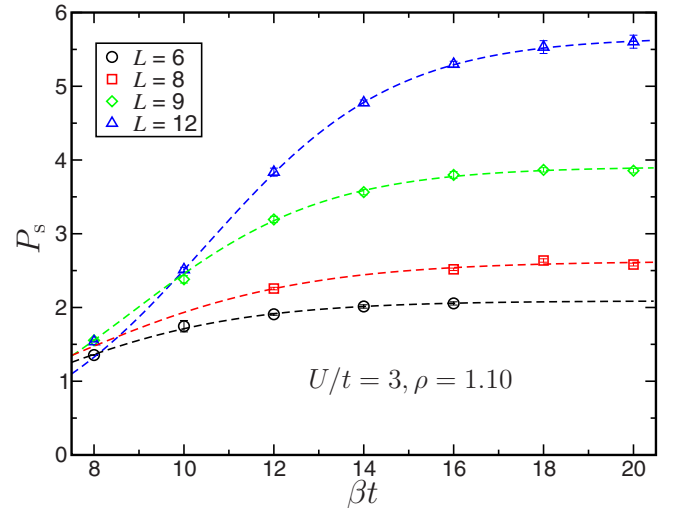


FIG. 5. (Color online) Evolution of the pair structure factor  $P_s$  as a function of the inverse temperature  $\beta t$  for several lattice sizes  $L$ . The interaction strength has been fixed at  $U=3t$  and the total average fermionic density at  $\rho=1.1$ . The dashed lines are fits using the three-parameter function  $F(\beta t)$ , Eq. (11). A plateau is reached when  $\beta t$  is much greater than the energy gap induced by finite-size effects between the ground state and the first excited state. As can be seen, the plateau is reached at larger  $\beta t$  when the lattice size increases. It is also reached at larger  $\beta t$  when  $\rho \rightarrow 1$  (not shown).

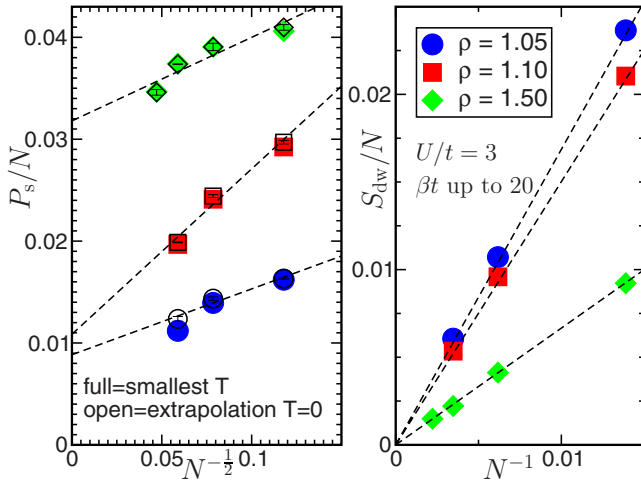


FIG. 6. (Color online) Evolution of the pair and density wave structure factors  $P_s$  and  $S_{dw}$  as a function of the number of lattice sites  $N$  for different total average fermionic densities  $\rho$ . The interaction strength has been fixed at  $U=3t$ . Full symbols have been obtained for inverse temperatures up to  $\beta t=20$  (see text). Open symbols for  $P_s$  are the plateau values at  $T=0$  as extracted from the fits in Fig. 5. The density wave structure factors  $S_{dw}$  always go to zero as the system size  $L=\sqrt{N}/2$  tends to infinity whereas the phase coherence ordering signal  $P_s$  never vanishes. The dashed lines are guides to the eyes. For the same parameters at half filling the system would be semimetallic and  $S_{dw}$  and  $P_s$  would both vanish.

$1/|\ln \delta\rho|$  as  $\delta\rho=|1-\rho|\rightarrow 0$  (Ref. 17) and lower temperatures are required to achieve phase coherence.

Figure 6 shows how  $P_s$  and  $S_{dw}$  scale with the number of lattice sites  $N$ . For each chosen lattice size  $L$  and fermionic density  $\rho$ , we have run our simulations for the lowest temperature that could be numerically achieved. The temperature range that we have been able to explore was up to  $\beta t=20$ . As expected  $S_{dw}$  always goes to zero and  $P_s$  always extrapolates to a nonzero value. We can then conclude, from direct measurement, that the BEC at zero temperature always appears as soon as the system is doped away from half filling. Even with the smallest doping that we have been studying ( $\rho=1.05$ , 5% doping), we have observed a clear persistence of the phase coherence ordering in the large size limit.

To observe the molecule formation along the BCS-BEC crossover, we have studied the density of on-site pairs

$$\rho_p = \frac{1}{N} \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle. \quad (12)$$

In the noninteracting limit ( $U/t \rightarrow 0$ ), spin-up and spin-down particles are uncorrelated. Hence  $\langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle = \rho_{\uparrow} \rho_{\downarrow}$ . Since we consider here equal spin populations  $\rho_{\uparrow} = \rho_{\downarrow} = \rho/2$ , we find  $\rho_p = \rho^2/4$ . In the molecular limit ( $U/t \rightarrow \infty$ ), fermions can only exist in pair at a site. Hence  $\langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle n_{i\uparrow} \rangle = \rho_{\uparrow}$  and  $\rho_p = \rho_{\uparrow}$ . In Fig. 7, we have plotted the rescaled density of on-site pairs,

$$\tilde{\rho}_p = \frac{\rho_p - \rho_{\uparrow}^2}{\rho_{\uparrow} - \rho_{\uparrow}^2}. \quad (13)$$

as a function of  $U/t$ . The crossover between a regime of loosely bound pairs and a regime of more tightly bound pairs

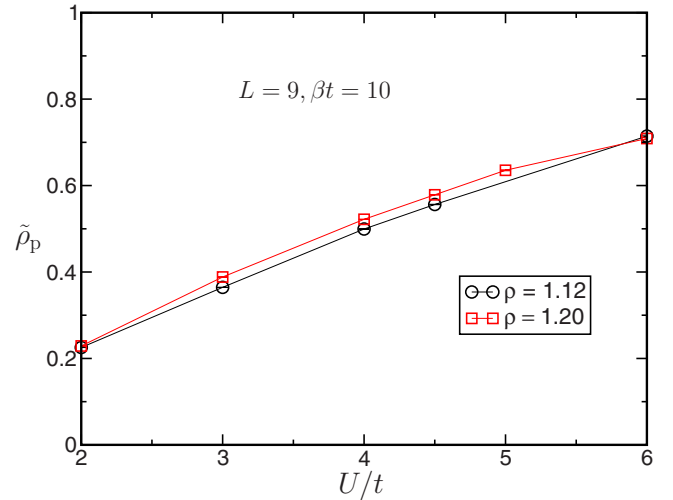


FIG. 7. (Color online) Evolution of the rescaled density  $\tilde{\rho}_p$  of on-site pairs, Eq. (13), as a function of the interaction strength  $U/t$  for two different total average fermionic densities  $\rho$ . The system size has been fixed at  $L=9$  and the inverse temperature is  $\beta t=10$ . In the noninteracting limit ( $U/t \rightarrow 0$ ), spin-up and spin-down particles are uncorrelated, hence  $\langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle = \rho_{\uparrow} \rho_{\downarrow} = \rho_{\uparrow}^2$  for equal spin populations. In this case  $\tilde{\rho}_p=0$ . In the molecular limit ( $U/t \rightarrow \infty$ ), fermions can only exist in pair at a site, hence  $\langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle n_{i\uparrow} \rangle = \rho_{\uparrow}$ . In this case  $\tilde{\rho}_p=1$ .

(molecules) is nicely evidenced by the smooth evolution of this rescaled quantity between the two limits  $\tilde{\rho}_p=0$  and  $\tilde{\rho}_p=1$  as the interaction is increased. For the intermediate values of the interactions used in our simulation, we see that the pairs are not tightly bound yet. The  $\tilde{\rho}_p=1$  limit is obtained only for extremely large values of  $U/t$ .

The second evidence for molecule formation along the BEC-BCS crossover comes from the evolution of the spectral function  $A(\omega)$  when the interaction strength  $U$  (Fig. 8) and the temperature  $T$  (Fig. 9) are varied. At large interactions ( $U \geq 4$ ), a clear gap is found at the Fermi level  $\omega=0$  provided the temperature is low enough, showing the formation of molecules. On the contrary, when the interaction is weaker ( $U \leq 3$ ), the gap does not open within the same range of temperatures. However, we observe that the value of  $A(\omega)$  at the Fermi level  $\omega=0$  decreases when the temperature is lowered (Fig. 9). We interpret this behavior as the precursor to the formation of a small BCS gap at very low temperatures. This dip in  $A(\omega)$  at the Fermi level is different from the one due to the vanishing of the noninteracting density of states at the Dirac points that was observed at half filling in the semimetal case. The Dirac dip is still present in the  $U \leq 3$  cases for  $\omega < 0$  (Fig. 8), showing that interaction strength is not large enough to strongly modify the structure of the Fermi sea, except very close to the Fermi level. This is characteristic of the BCS case. On the other hand, the Dirac dip disappears at strong interactions (Fig. 8, bottom), showing now that the original Fermi sea structure has been completely modified by interactions.

A nice feature of the strongly interacting regime is the existence of two very different energy scales. One corresponds to the formation of bound pairs (molecules) and is

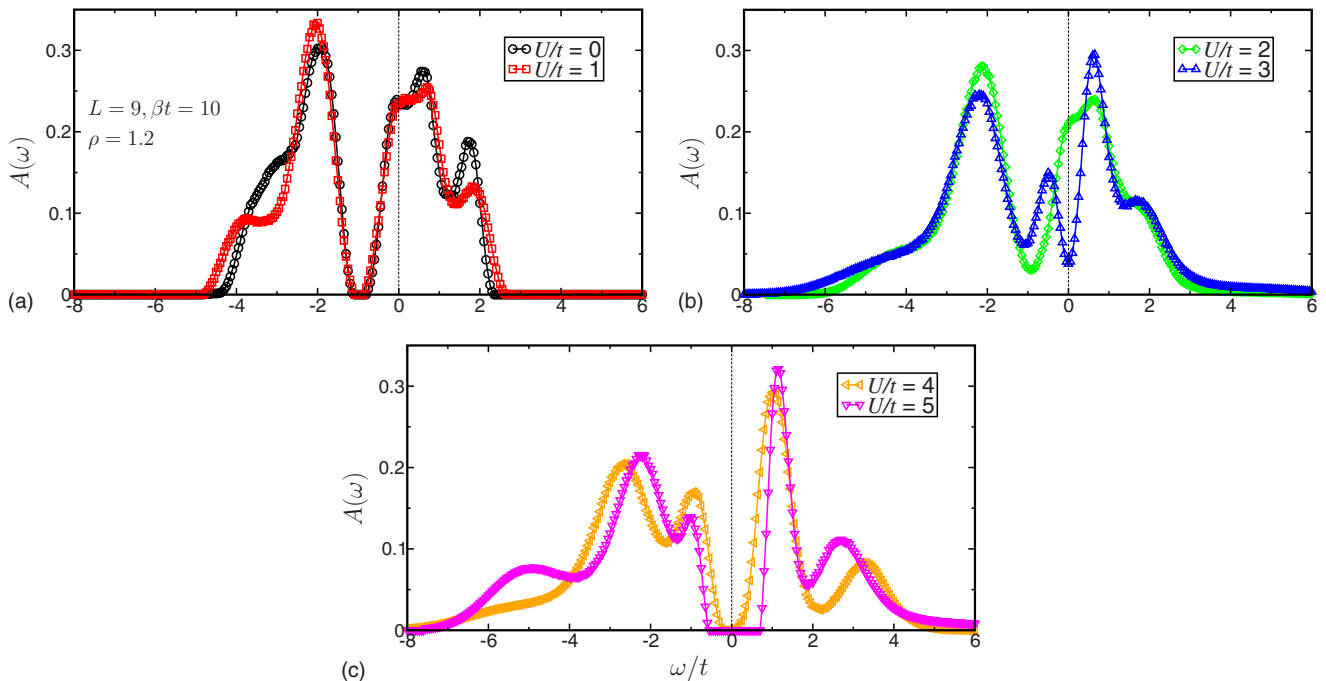


FIG. 8. (Color online) Evolution of the spectral function  $A(\omega)$  as a function of the interaction strength  $U$  at density  $\rho=1.2$ , inverse temperature  $\beta t=12$ , and lattice size  $L=9$ . When  $U=0$ , the chemical potential is numerically found to be  $\mu/t=0.8768$ , locating the Dirac points in the residual gap (due to finite-size effects and temperature rounding) around  $\omega/t=-1$ . The fact that the density of states vanishes linearly with  $\omega$  around  $\omega/t=-1$  also supports this identification of the location of the Dirac points. As  $U$  is increased, a dip develops in the spectral function at the Fermi level (located at  $\omega=0$ ) and the BCS-BEC gap eventually opens while the Dirac points are gradually destroyed.

typically on the order of  $U$  itself. The second corresponds to the emergence of phase coherence between these pairs and is of the order of the hopping parameter for pairs, typically  $t^2/U$ .<sup>39</sup> These two-energy scales are clearly identified by comparing the evolution of  $P_s$  and  $\rho_p$  when the temperature is varied, see Fig. 10. We thus can conclude that, even if the pairs are not tightly bound at the intermediate values of  $U/t$  we used (as it shown in Fig. 10), we clearly observe the formation of pairs before the emergence of phase coherence, which is expected in the BEC regime. To investigate this phenomenon further, we show in Fig. 11 the pair Green's function in Eq. (4) as a function of distance for different

temperatures. There is a range of temperatures ( $0.1 < \beta t < 5$ ) where the pair Green's function is clearly decreasing exponentially with distance (up to some boundary effects). This means that no phase coherence is achieved and the system is in a disordered regime. In other words, the corresponding temperatures are above the BKT transition temperature  $T_c$ . For this same temperature range,  $\rho_p$  has already reached its zero-temperature limit (Fig. 10). This is a clear evidence for the existence of preformed pairs which will eventually develop quasilong-range phase coherence at a much lower temperature. For temperatures  $T < T_c$ , the Green's function should decay algebraically with distance

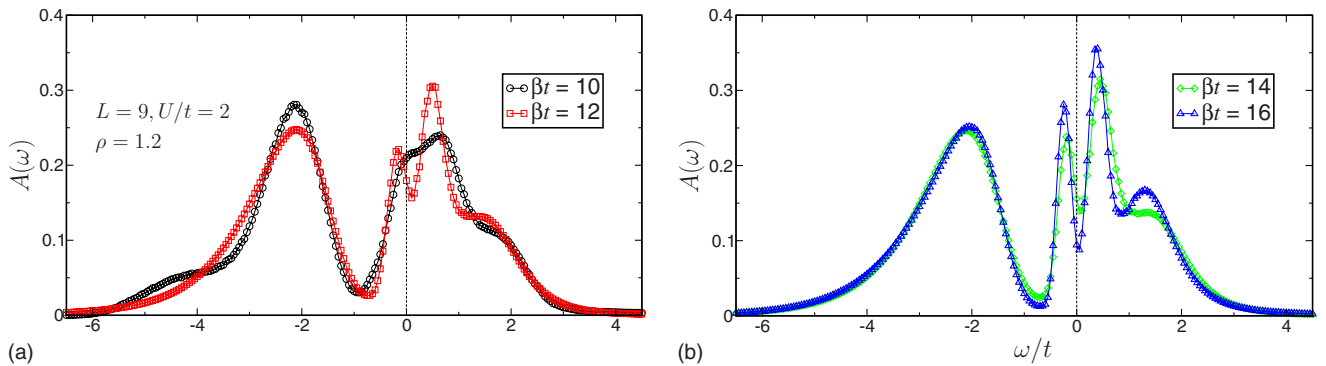


FIG. 9. (Color online) Evolution of  $A(\omega)$  as a function of inverse temperature  $\beta t$  at  $\rho=1.2$ , interaction strength  $U=2t$ , and lattice size  $L=9$ . As the temperature is lowered, a dip develops in the spectral function at the Fermi level located at  $\omega=0$ . Eventually a gap opens when the temperature is low enough (not shown). The gap opening at the Fermi level is obtained even at weak interactions, a situation characteristic of the existence of a small BCS gap.



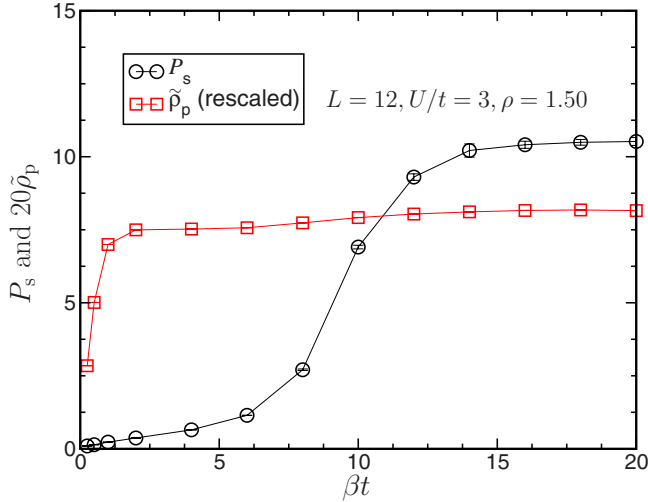


FIG. 10. (Color online) Evolution of the pair structure factor  $P_s$  (circles) and the rescaled density of on-site pairs  $\tilde{\rho}_p$  (squares) as a function of the inverse temperature  $\beta t$  at interaction strength  $U = 3t$ . The total average fermionic density is set at  $\rho = 1.5$  and the system size is  $L = 12$ . Two different energy scales are clearly identified as  $P_s$ , signaling the emergence of phase coherence, saturates at  $\beta t \approx U/t$  whereas  $\tilde{\rho}_p$ , signaling the molecule formation, saturates at  $\beta t \approx t/U$ . We recover here (in dimensionless units) the two-energy scales  $t^2/U$  and  $U$ , typical of the emergence of phase coherence and of the formation of tightly bound pairs.

with an exponent  $\eta = T/(4T_c)$ .<sup>17</sup> For  $\beta t \geq 10$ , the pair Green's function behavior is consistent with a power-law decay but it is difficult to extract the corresponding exponent due to finite-size effects.

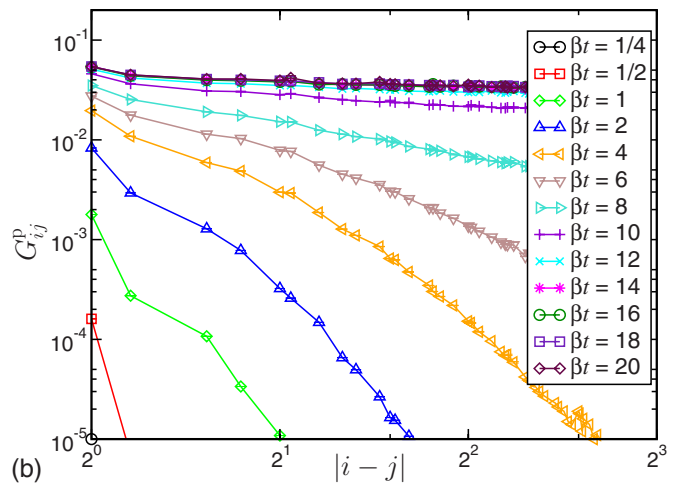
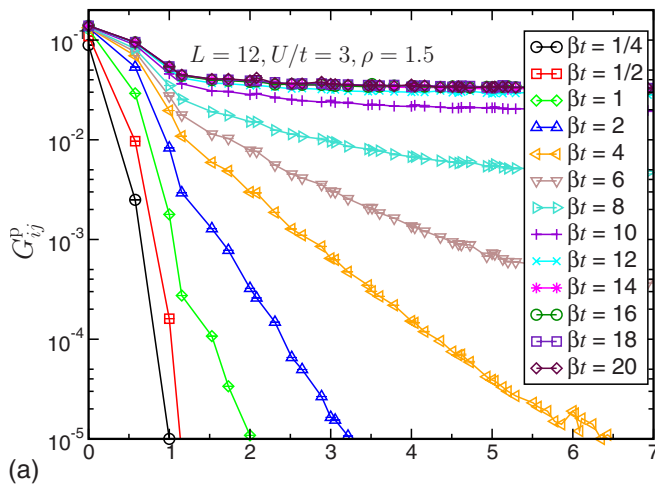


FIG. 11. (Color online) Evolution of the pair Green's function as a function of distance for different temperatures. The total average fermionic density is set at  $\rho = 1.5$ , the interaction strength at  $U = 3t$ , and the lattice size is  $L = 12$ . The vertical axes are plotted in logarithmic scale while the horizontal axes are plotted with linear (top) and logarithmic (bottom) scales. For large site separation  $|i - j|$ , we observe a transition from an exponential decay (linear behavior in the log-linear plot) at high temperature to a weak algebraic decay (linear behavior in the log-log plot) at low temperature. This is the signature of the BKT transition where the system leaves the disordered phase to enter a phase with quasilong-range order as the temperature is lowered. However, due to limited system size, the weak algebraic decay of the pair Green's function is difficult to infer unambiguously.

#### IV. CONCLUSION

We have studied the Hubbard model on a honeycomb lattice with attractive interactions. At half filling, building upon previous existing studies, we have used the mapping onto the FRHM to show that there is a quantum phase transition at  $T = 0$  between a disordered phase and a DW-SF phase exhibiting crystalline as well as superfluid orders. The critical interaction strength at which this QPT takes place is accurately bounded by  $5.0 \leq U_c/t \leq 5.1$ . We have also shown that before the transition, the system is semimetallic and that the interactions do not markedly change the nature of this phase. Away from half filling, within our numerical accuracy, the system seems to become superfluid, even for arbitrary small values of the doping. We have elucidated the presence of the BCS-BEC crossover by looking at several quantities, especially the one-particle density of states. We have clearly evidenced, for strong enough interactions, the existence of two different energy scales, one for the formation of the pairs and one for the emergence of phase coherence (the BKT transition), which is typical of the strongly interacting regime.

For weak interactions, both at and away from half filling, we have observed that the spectral function  $A(\omega)$  is qualitatively the same as in the noninteracting case. Only the states close to the Fermi level are affected by those weak interactions. As there are no available states in the half-filled case close to the Fermi level, the interactions hardly play a role and the system remains a semimetal (at half filling) up to  $U = 5t$ . It is only when the interactions are strong enough to destabilize the Fermi sea and form tightly bound pairs that the system enters a different phase. In this case, the description in terms of individual fermions and plane-wave states is no longer relevant.

We further observe that the BCS and the semimetal regimes are two phases sharing some common features. Indeed, in both phases, interactions are not strong enough to substantially modify the Fermi sea structure except around the Fermi level. This is reflected in the fact that the Dirac dip in  $A(\omega)$  is always clearly visible in these cases. By the same token, the molecular superfluid phase (BEC) and the DW-SF have in common that the description in term of individual fermions is meaningless. Indeed, for both phases, the fermionic excitations are gapped and the Dirac dip in  $A(\omega)$  has disappeared. Close to half filling, we then expect to observe the BCS-BEC crossover to happen for interaction strengths close to the value of the QPT at half filling, i.e.,  $U \approx 5t$ . The opening of a clear gap for  $U/t=4-5$  in Fig. 8 supports this interpretation.

## ACKNOWLEDGMENTS

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