Finite temperature study of correlations in bilayer band-insulator

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We perform the finite-temperature determinant quantum Monte Carlo simulation for the attractive Hubbard model on the half-filled bilayer square lattice. Recent progress on optical lattice experiments lead us to investigate various single-particle properties such as momentum distribution and double occupancies which should be easily measured in cold-atom experiments. The pair-pair and the density-density correlations have been studied in detail, and through finite-size scaling, we show that there is no competing charge density wave order in the bilayer band-insulator model and that the superfluid phase is the stable phase for the interaction range $|U|/t = 5 - 10$. We show the existence of two energy scales in the system as we increase the attractive interaction, one governing the phase coherence and the other one corresponding to the molecule formation. In the end, we map out the full $T - U$ phase diagram and compare the $T_c$ obtained through the mean-field analysis. We observe that the maximum $T_c/t^{\alpha} = 0.27$ occurs for $|U|/t = 6$, which is roughly twice the reported $T_c$ of the single-layer attractive Hubbard model.

I. INTRODUCTION

The half-filled attractive Hubbard model (AHM), at low temperatures, shows the s-wave superfluidity with a BEC-BCS crossover along with the charge density wave (or pair density wave) [1]. In the weak-coupling regime ($U << t$), fermions of opposite spin and same momentum state form loosely bound Cooper pairs and go to the BCS state at the critical temperature $T_c$, which increases with $|U|/t$. As we go towards the strong-coupling regime ($U >> t$), the strong interactions between the particles lead to the formation of the bound pairs that condense to form a BEC state at $T_c$, which decreases as $t^2/|U|$. The fermionic pairs in the BEC state can be regarded as the hard-core bosons, and the tunneling of the pairs is dominated by the second-order tunneling $t^2/|U|$. The advancement in the field of cold atoms has generated a lot of interest in the condensed matter community due to a control over various parameters such as tuning the interaction between particles by the Feshbach resonance, tuning the hopping between lattice sites by laser intensity, and so on. The lowest temperature that has been achieved so far in experiments on the AHM is $T \sim 0.4t$ [2]. Earlier theoretical work on half-filled AHM has shown $T_c \sim 0.13t$ for $|U|/t = 8$ [3], whereas the maximum $T_c \sim 0.17t$ at density $n = 0.7$ and $|U|/t = 4$ has been reported [4, 5]. The process to lower the temperature experimentally in optical lattice systems has been hampered by the cooling problem (entropy issues) [4, 6–9]. Recent progress made in the experiments towards the realization of the attractive Hubbard model has been of great interest [2, 10]. There have been some theoretical attempts to “increase” the characteristic temperature $T_c$ which can be achieved experimentally [11, 12]. In this work, we focus on the bilayer attractive Hubbard model band-insulator model discussed in Ref. [11]. The model is a bilayer square lattice model, as shown in Fig. 1. Both layers have been hybridized by the coupling $t_h$. The hoppings in both layers were taken to be opposite to each other such that the in-plane energy dispersions in the two layers are of the opposite signs, i.e., $\epsilon_A(k) = -\epsilon_B(k) \equiv \epsilon(k)$. The idea is to start with a low entropy state and explore the possibility of realizing a superfluid. At half filling, for a finite $t_h$ and for small values of $|U|$, the system is in the normal band-insulator state. With the increase in the on-site attractive interaction $|U|$, a quantum phase transition occurs at $|U_c|$, ushering in a superfluid state. Detailed analysis including Gaussian fluctuations and variational Monte Carlo (VMC) calculations establish that there are no competing orders such as an intervening charge density wave (CDW) and confirm that the superfluid state is stable at $T = 0$ [11]. Band-insulator-superfluid transitions have been studied

\begin{figure*}[ht]
\centering
\includegraphics[width=\textwidth]{figure1}
\caption{Schematic of the bilayer band insulator. Nearest-neighbor hopping $t$ and next-nearest-neighbor hopping $t'$ in layer $A$ is opposite to that of layer $B$ of the square lattice. Both layers have been hybridized by hopping $t_h$. The right panel shows the energy dispersion for $t_h = 0$ and $t_h \neq 0$.}
\end{figure*}

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various single-particle quantities such as the momentum $\mu$. Hence, at half filling, we have $\tilde{\mu} = 0$. We calculate various single-particle quantities such as the momentum in the presence of the on-site Hubbard interaction ("$-U$"). The first term $\mathcal{H}_K$ represents the hopping (kinetic energy) of the fermions and the latter represents the interaction energy when the two fermions occupy the same site. We choose the nearest-neighbor hopping $t = 1$ to set our unit of energy. We express all other energy scales $t_b, U, T$ and $\mu$ in terms of the energy scale $t$. We fix the hybridization hopping $t_b/t = 0.6$ throughout this work and studied the properties of our model at half-filling on a bilayer square lattice with $N = 2 \times L^2$ sites with periodic boundary conditions. Here $L$ represents the number of sites in each direction of the square lattice. At half-filling (one fermion per site), due to particle-hole symmetry in our system, $\mu = 0$.

In the DQMC simulations, we chose the imaginary-time interval $\Delta \tau = 1/20$. Following the steps of the DQMC algorithm [20, 21], we perform the Trotter-Suzuki decomposition to separate the kinetic and interaction energy exponentials. For the proposed bilayer band-insulator model, the kinetic and the interaction exponentials will have the following expressions:

$$e^{-\Delta \tau K} = \prod_{\sigma} e^{-\Delta \tau \sum \alpha, \gamma \sum_{<ij>, \sigma} (c^{\dagger}_{\alpha \sigma} K_{ij\alpha\gamma} c_{\gamma\sigma} + \text{h.c.})}$$

$$e^{-\Delta \tau V} = e^{-\Delta \tau \sum_i \sum_{\alpha, \gamma} (U n_i^\alpha n_i^\gamma + \mu (n_i^\alpha + n_i^\gamma))}$$

where $(\alpha, \gamma)$ correspond to the layers of the bilayer system and $c_{\alpha \gamma}(c^{\dagger}_{\alpha \gamma})$ is equivalent to the operators $a(a^{\dagger})$ and $b(b^{\dagger})$ for $\alpha = 1$ and 2, respectively. $K$ is the kinetic energy matrix whose elements are given by

$$K_{ij\alpha\gamma}^\sigma = t_{ij\alpha\gamma} - \mu \delta_{ij} \delta_{\alpha\gamma},$$

with

$$t_{ij\alpha\gamma} = \begin{cases} 
-t & \text{if } i \text{ and } j \text{ are the } nn \text{ for } (\alpha, \gamma) = (1, 1) \\
-t' & \text{if } i \text{ and } j \text{ are the } nnn \text{ for } (\alpha, \gamma) = (1, 1) \\
t & \text{if } i \text{ and } j \text{ are the } nn \text{ for } (\alpha, \gamma) = (2, 2) \\
t' & \text{if } i \text{ and } j \text{ are the } nnn \text{ for } (\alpha, \gamma) = (2, 2) \\
-t_h & \text{if } i \text{ and } j \text{ are the } nn \text{ for } (\alpha, \gamma) = (1, 2) \text{ or } (2, 1) \\
0 & \text{otherwise.}
\end{cases}$$

where $nn$ represents the nearest neighbors, while $nnn$ represents the next-nearest neighbors. After applying the Hubbard-Stratonovich transformation for the bilayer band-insulator model, the elements of the matrix $V$ and the chemical potential in the kinetic energy term are modified to

$$\lambda \Delta \tau \sum_{ij} \delta_{ij} \delta_{\alpha\gamma},$$

$$\tilde{\mu} = \mu + \frac{|U|}{2}.$$
III. SINGLE PARTICLE PROPERTIES

The mean-field analysis and the Gaussian fluctuation theory suggest that the bilayer band-insulator model undergoes a second-order phase transition at some critical value of the attractive interaction $|U_c|$. The fermions start to form pairs as we tune the on-site attractive interaction through Feshbach resonance. In the strong-coupling limit ($|U| >> t$), these pairs get tightly bound, forming a molecule (boson). Thus, by tuning the interaction, we go from a band-insulating state to a loosely bound state of Cooper pairs and then to a tightly bound molecule-forming state, implying that there is a smooth $BCS - BEC$ crossover extending from a small to a large value of the interactions. Hence, 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 $BEC$ state of bosonic molecules (where fermions with opposite spin form tightly bound pairs) when $|U|$ is increased beyond $|U_c|$.

A. Momentum Distribution

The Green’s function is a fundamental quantity in DQMC where it is used in various updation processes. The momentum distribution can be obtained directly from the Green’s function via Fourier transform of the equal-time Green’s function $G_{ij\alpha\beta} = \langle c_{i\alpha\sigma} c_{j\beta\sigma}^\dagger \rangle$ as

$$n_\alpha(q) = 1 - \frac{1}{2N} \sum_{ij\sigma} e^{i \mathbf{q} \cdot \mathbf{r}_{ij}} \langle c_{i\alpha\sigma} c_{j\sigma}^\dagger \rangle$$

where $l_{ij}^\alpha = l(i, \alpha) - l(j, \alpha)$ and $N_\alpha(= L^2)$ represents the number of sites in the $\alpha$th layer.

Figure 2 shows the momentum distribution of our bilayer square lattice around the irreducible part of the Brillouin zone (BZ) for various system sizes [Fig. 2(a)], at different temperatures [Fig. 2(b)], and for different interactions $|U|$ [Figs. 2(c) and 2(d)]. At $|U| = 0$ and at half filling, $n_1(q)$ $n_2(q)$ $= 1(0)$ inside and $n_1(q)$ $n_2(q)$ $= 0(1)$ outside a square with vertices $(\pi, 0), (0, \pi), (-\pi, 0)$, and $(0, -\pi)$ within the BZ. Figure 2(a) shows that the momentum distribution has a weak lattice size dependence and its resolution increases with $L$. In Fig. 2(b), we show that the $n(q)$’s converge to their respective low-temperature values as $\beta t > W/t$. Here, $|U|/t = 5$ and the system size $L = 16$. (c) The momentum distributions for various attractive interactions ranging from $|U|/t = 1$ to $8$; (d) the enlarged region, cut perpendicular to the Fermi surface at $(\pi/2, \pi/2)$, of (c). We see a sharp Fermi surface at weak interaction $|U|$ as the momentum cuts across the Fermi surface at $q = (\pi/2, \pi/2)$ and it broadens out as $|U|/t$ increases.

B. Pair Formation

The existence of the molecule formation along the $BCS - BEC$ crossover with the increase in the interaction strength $|U|$ comes from the evolution of the double occupancy (density of on-site pairs), which can also be measured in experiments with ultracold fermions [22]. The double occupancy $D$ can be defined as

$$D = \frac{1}{N} \sum_{i=1}^{N} \langle n_{i\uparrow} n_{i\downarrow} \rangle$$

where the summation $i$ runs over the number of sites for layer $\alpha$ for both layers $\alpha = 1$ and $2$, and $N(= 2L^2)$ represents the total number of sites.

In the noninteracting limit ($|U|/t = 0$), both spin-up and spin-down particles are uncorrelated so $\sum_{i=1}^{N} \langle n_{i\uparrow} n_{i\downarrow} \rangle/N = \sum_{i=1}^{N}(n_{i\uparrow})^2/n_{i\uparrow}^2/N = 1/4$ at half filling. As we increase the attractive interaction by tuning the scattering rate, the spin-up and spin-down particles...
molecules (tightly bound pairs of fermions of opposite spins). In the high-temperature limit \( T/t >> 1 \), independent of the interaction strength, the double occupancy approaches the noninteracting values, i.e., 0.25 in the half-filled case. As we decrease the temperature, the fermions start to pair up due to the increasing effect of the attractive interaction. Hence the double occupancy increases with the decrease in temperature \( T \). We observe a local maxima as we go from the high-temperature to the low-temperature regime, implying the increase in the double occupancy with the decrease in the temperature. We see the local maxima at the intermediate temperature scale \( T/t \sim 1 \), where the kinetic energy competes with the on-site interaction and destabilizes the double occupancy in the weak- and intermediate-coupling regimes. So the double occupancy decreases a little and saturates in the weak-coupling regime, after reaching its ground-state value as \( T/t \to 0 \). But after a certain critical interaction strength \( |U_c| \), we observe that as we decrease the temperature further, the double occupancy increases again after a critical temperature \( T_c \) and then saturates to its low-temperature value. This indicates that the system goes into a superfluid phase from the band-insulating phase at this critical interaction strength and temperature. We estimate these critical values through the scaling analysis discussed at the end of this paper.

C. Kinetic Energy

Another single-particle quantity of interest is the effective hopping, defined as

\[
\beta t = \frac{1}{2} \left( \frac{W}{t} \right) \left( \frac{1}{2} + \frac{1}{4} \alpha \right)
\]

Figure 3. Color contour plot depiction of the momentum distributions. \( n_1(q) \) and \( n_2(q) \) at half filling for \( |U|/t = 1, 5, \) and 8. The lattice size is \( 2 \times 16 \times 16 \) and the inverse temperature \( \beta t = 10 \).

Figure 4. The evolution of the rescaled double occupancy with the temperature \( T/t \) for various interaction strengths \( |U|/t \). The system size is \( L = 16 \). The black arrow marks the transition temperature \( T_c/t = 0.17 \) at \( |U|/t = 5 \), estimated from the finite-size scaling analysis. The rescaled double occupancy reaches up to 0.8 at \( |U|/t = 8 \), which is an indication of the molecule (tightly bound pairs) formation. A local maxima has been observed as we go from the high-temperature to the low-temperature regime at the intermediate-temperature scale \( T/t \sim 1 \). (b) Effective hopping: as the interaction energy \( |U| \) increases, the effective hopping declines. The rate of decrease of the effective hopping with the increase in the interaction strength is the same for all \( \beta t > W/(8.8/t) \). Here we show \( t_{eff}^\beta \) for \( L = 16 \) for different values of inverse temperature \( \beta t \).
We will also discuss the density-density correlations to see the possibility of formation of the charge density wave (CDW) state at a large value of the on-site attractive interaction. We also estimate the critical strength $|U_c|$ and the critical temperature $T_c$ through the finite-size scaling analysis.

### A. Pair-Pair Correlations

We know that the long-range order (or a quasi-long-range order for a superfluid at finite temperature) in the pair-pair correlation function in the Bose-Einstein condensate state signifies a phase coherence between pairs. To study this behavior, we define the equal-time s-wave pairing $P^{s}_{\gamma}(\bf{i},\bf{j})$ for the bilayer model as

\[
P^{s\gamma}(\bf{i},\bf{j}) = \langle \Delta_s(i,\alpha)\Delta_s(j,\gamma) + h.c. \rangle
\]

where the local pair-field operator $\Delta_s(i,\alpha)$, defined as

\[
\Delta_s(i,\alpha) = c_{i,\alpha\downarrow}^\dagger c_{i,\alpha\uparrow}, \quad \text{(11)}
\]

annihilates a pair of fermions on site $i$ of layer $\alpha$ of the bilayer-square lattice. We also define the associated pair structure factor as

\[
S_s(\bf{q}) = \frac{1}{N} \sum_{\alpha,\gamma} \sum_{\bf{i,j}} e^{i\bf{q}\cdot\bf{r}\text{ij}} P^{s\gamma}_s(\bf{i},\bf{j}) \quad \text{(12)}
\]

where $P^{s\gamma}_s(\bf{i},\alpha) = P^{\alpha\gamma}(\bf{i},\bf{j})$.

The pair structure factor diverges linearly with the system size $N$ when the long-range order is achieved. As the bilayer band-insulator system undergoes a finite-temperature Berezinski-Kosterlitz-Thouless (BKT) transition into a superfluid phase [11], hence for $0 < T \leq T_c$, we expect that

\[
P_s(\bf{l}) \sim 1^{-\eta(T)}, \quad \text{(13)}
\]

with the separation $\bf{l} = |\bf{i} - \bf{j}|$, where $\bf{i,j}$ refers to sites either from layer $A$ or $B$. The critical exponent $\eta(T)$ for a BKT transition in a homogeneous system is known to increase monotonically with temperature between $\eta(0) = 0$ and $\eta(T_c) = 1/4$ [23, 24].

Thus we can obtain the finite-size scaling behavior of the s-wave pair structure factor upon integrating $P_s(\bf{l})$ over a two-dimensional system of linear dimension $L$. Hence, $S_s(\equiv S_s(\bf{q} = 0))$ will scale as [15]

\[
L^{2-n(T_c)} S_s \sim f(L/\xi), \quad L >> 1, \quad T \rightarrow T_c^+ \quad \text{(14)}
\]

with $\xi = \exp[A/(T - T_c)^{1/2}]$ the correlation length of the infinite system where $A$ is of the order of unity. In the thermodynamic limit, one can recover $S_s \sim \xi^{7/4}$.

In Fig. 6, we have shown the dependence of the pair correlation function on the separation $l$ for two different lattice sizes $L = 14$ and 16. The separation $l$ shows a trajectory along the $x$ axis to maximal $x$ separation $(\frac{L}{2},0)$ on a lattice with periodic boundary conditions, and then to $(\frac{L}{2},\frac{L}{2})$ before returning to separation $(0,0)$. We observe that there is no pair-pair correlation when $|U|/t = 1$ as the system is still in the band-insulating state. For $|U|/t = 5$ and 8, there is a finite nonzero pair-pair correlation, implying the existence of the long-range
order at these interactions. We see that the finite-size effects are modest.

To have a clearer understanding, in Fig. 7, we show the equal-time s-wave pair structure factor \( S_s(q, \tau = 0) \) for \( |U|/t = 5 \) [Fig. 7(a)] for various temperatures \( (\beta t = 2 - 10) \) on a \( 2 \times 16 \times 16 \) lattice and [Fig. 7(b)] for various system sizes \( (L = 10 - 16) \) at \( T/t = 0.1 \). We see that the \( q = 0 \) mode becomes more and more singular in both results as we decrease the temperature or increase the system size, which is a characteristic feature of growing s-wave pairing correlations. The dependence of the \( q = 0 \) mode on the system size indicates that we need to understand the finite-size scaling behavior of \( S_s \) due to

Figure 6. The dependence of the ground-state pair-pair correlation function on the separation \( l \) for two different lattice sizes \( L = 14 \) and \( L = 16 \), in a bilayer band-insulator model. The separation \( l \) follows a trajectory along the \( x \) axis to maximal \( x \) separation \( (\hat{x}, 0) \) on a lattice with periodic boundary conditions, and then to \( (\hat{x}, \frac{L}{2}) \) before returning to separation \( (0, 0) \). The correlation functions converge to a nonzero value at large separations at \( |U|/t = 5 \) and 8, providing clear evidence for the long-range order. We see that the finite-size effects are modest.

Finite-size Scaling

To understand the finite-size scaling behavior of \( S_s \), we obtain the low-temperature limit of the pair structure factor by decreasing the temperature until we observe a plateau which signals that we have reached the \( T = 0 \) value of the pair structure factor. Figure 8(a) shows the evolution of \( S_s \) with the inverse temperature \( \beta t \) for \( |U|/t = 5 \) and for different lattice sizes. Here we see that \( S_s \) increases at low temperatures and saturates to a value which increases with the size of the lattice. For \( \beta \leq 4 \), pair correlations are short range, so the pair structure factor is independent of the lattice size. As we decrease the temperature, the point at which the pair structure factor begins to grow with the lattice size indicates the temperature at which the correlation length \( \xi \) becomes large as compared to the lattice size \( L \).

Ground State: \( |U_c| \). The important characteristic of the superfluid state in our bilayer model is that the system displays long-range order in the ground state, and hence Huse’s argument [25] of the “spin-wave scaling” is expected to hold [18],

\[
\frac{S_s}{N} = \Delta_0^2 + \frac{C(U)}{L} \tag{15}
\]

where \( \Delta_0 \) is the superfluid order parameter at zero temperature and \( C \) is a constant which depends on the interaction strength \( |U| \).

The superfluid order parameter \( \Delta_0 \) can also be extracted from the equal-time s-wave pair-pair correlation function \( P_s(l) \) for the two most distant points on a lattice, i.e., having \( R = (L/2, L/2) \) [26], with a similar spin-wave theory correction,

\[
P_s(R) = \Delta_0^2 + B(U)L. \tag{16}
\]

We expect that \( B < C \) since the structure factor includes the pair correlations at short distances which markedly
exceed $\Delta_0^2$, in addition to the finite lattice effects at larger length scales [27].

In Fig. 8(b), we perform the finite-size scaling of the $s$-wave pair structure factor $S_s$ for various interaction strengths. We can approximate the superfluid order parameter by the intercept along the $y$ axis as evident from Eq. (15). Thus we observe that the zero-temperature order parameter is nonzero for the interaction $|U|/t \geq 5$. Hence the critical interaction strength $|U_c|/t \sim 5$.

Estimation of $T_c$. We can extract $T_c$ from the pair structure factor $S_s$ through a “phenomenological renormalization group” analysis [28, 29]. As we know, $\xi = \infty$ at $T_c$ and $\to \infty$ for all $0 < T < T_c$ [see Eq. (20)]. Thus, at $T_c$, $L^{-7/4} S_s(L, \beta_c)$ becomes a constant, independent of the system size. Hence all the curves for different system sizes, in the plot of the rescaled pair structure factor $L^{-7/4} S_s(L, \beta)$, should intersect at $\beta = \beta_c$, when plotted as a function of $\beta$. In Fig. 9(a), we show the rescaled pair structure factor $L^{-7/4} S_s(L, \beta)$ as a function of the inverse temperature $\beta$ for $|U|/t = 5$ for different lattice sizes. We observe that for all lattice sizes, all the curves intersect each other at a single point $\beta = 6$. This leads to a conclusion that $T_c/t \sim 0.167$.

In Fig. 9(b), we plot the rescaled pair structure factor versus the universal scaling function $f(L/\xi)$ [see Eq. (20)], where $A$ and $T_c$ are chosen such that all the data points collapse on a single curve, regardless of the system size. For $A = 0.5$ and $T_c/t = 0.17$ at $|U|/t = 5$, all data collapse onto a single curve. Hence the estimated $T_c/t = 0.17$ at $|U|/t = 5$. Similarly, we estimated $T_c$ for various interaction strengths to map out the $T-U$ phase diagram (see Fig. 13).

B. Energy Scales

In our bilayer band-insulator model, we see two different energy scales for the attractive interaction $|U|/t = 5$. One energy scale $(T^*/t)$ corresponds to the formation of molecules, while the other energy scale $(T_c/t)$ corresponds to the emergence of the phase coherence between these pairs. We can identify these two scales by comparing the evolution of the double occupancy and the $s$-wave structure factor with temperature. In Fig. 10, we show the rescaled double occupancy and the $s$-wave structure factor for $|U|/t = 5$ for the lattice size $L = 16$. We recover the two energy scales $(T^*/t \sim 0.125$ corresponding to saturation of $S_s$ and $T^*/t \sim 0.33$ corresponding to the saturation of $D$) and observe the formation of pairs be-
fore the emergence of phase coherence, which is expected in the BEC regime. Finite-size scaling gives $T_c/t \sim 0.17$.

C. Density-Density Correlation

To study the CDW order, we define the density-density correlation function as

$$C_{\sigma,\pi'}^{\sigma'}(i,j) = \langle n_i^\sigma n_j^{\pi'} \rangle - \langle n_i^\sigma \rangle \langle n_j^{\pi'} \rangle$$

(17)

where $\sigma$ and $\pi'$ correspond to $\uparrow$ or $\downarrow$ spin, respectively, $\alpha$ and $\gamma$ correspond to layer $A$ or $B$, respectively, $n_i^\sigma$ corresponds to the fermion density at site $i$ of the $\alpha$th layer, and $i$ and $j$ run over sites 1 to $N$. For $\alpha = \gamma$, $C_{\sigma,\pi'}^{\pi'}(i,j)$ corresponds to the intralayer density-density correlation, while for $\alpha \neq \gamma$, $C_{\alpha',\pi'}^{\alpha\pi'}(i,j)$ corresponds to the interlayer density-density correlation function. Similarly, we define the CDW structure factor $S_{\text{CDW}}$ as

$$S_{\text{CDW}}(q) = \frac{1}{N} \sum_{\alpha,\pi} \sum_{\sigma,\gamma} \sum_{ij} e^{i q \cdot \mathbf{l}_{ij}} C_{\sigma,\pi'}^{\sigma'}(i,j)$$

(18)

where $\mathbf{l}_{ij} = \mathbf{l}(i, \alpha) - \mathbf{l}(j, \gamma)$.

In Fig. 11, we show the spatial variation of the density-density correlation function $C_{\sigma,\pi'}^{\pi'}(i,j)$. We observe that the density wave formation will start to take place for $|U|/t \geq 8$. Thus there is no competing order in the region where the superfluid state exists. To confirm this, we perform the scaling analysis.

In Fig. 12(a), we show the evolution of the CDW structure factor $S_{\text{CDW}}$ with attractive interaction $|U|$ for various temperatures. $S_{\text{CDW}}$ increases slowly in the weak-coupling regime where the system is in a band-insulating state. As the attractive interaction increases, the density wave structure factor increases. To investigate the existence of the charge density wave order in the ground state of the bilayer band-insulating model, we perform the finite-size scaling.

Finite-size Scaling

Using the Huse’s argument of the spin-wave theory, we expect that the CDW structure factor and the density-density correlation function behave as

$$S_{\text{CDW}}^N \sim \frac{C(U)}{L},$$

$$C(L/2, L/2) = \Delta_0^2 + B(U) L,$$

(19)

where $\Delta_0$ is the zero-temperature charge density wave order parameter and $C$ and $B$ are constants which depend on the interaction strength $|U|$.

Figure 12(b) shows the finite-size scaling of the CDW structure factor $S_{\text{CDW}}$ for various interaction strengths. From Eq. (19) we see that the intercept along the $y$ axis gives the square of the zero-temperature CDW order parameter $\Delta_0^2$. For the range of attractive interaction strengths (5 – 10), the finite-size scaling of the CDW structure factor confirms that the CDW phase does not exist in the bilayer band-insulator model. Even though we observe density wave formation for $|U|/t \geq 8$, to have a long-range CDW order, the CDW structure factor measured on finite lattices at the critical temperature $T_c'$ should obey

$$L^{-7/4} S_{\text{CDW}} \sim f(L (\beta - \beta_c'))$$

(20)

Hence if we plot $L^{-7/4} S_{\text{CDW}}$ as a function of the inverse temperature $\beta$, different sizes $L$ must cross at $\beta = \beta_c'$. But we could not see any crossing for different system sizes for the CDW structure factor. On the contrary, this crossing has been clearly visible for a pair-pair structure factor where long-range superfluid order is present (Fig. 9). Hence, even for $U/t = 10$, long-range CDW order is absent.

V. DISCUSSION AND CONCLUSION

In summary, we have used an unbiased and exact DQMC technique to study various single-particle
and two-particle properties of the bilayer band-insulator model. We have shown the existence of two energy scales: one scale governs the phase coherence and the other one corresponds to the molecule formation (formation of tightly bound fermionic pairs). We compare our results with the one obtained with the mean-field and the Gaussian-fluctuation theory results presented in [11]. The critical strength $|U_c|/t \sim 5$ is slightly higher than the saddle-point analysis ($|U_c|/t = 3.2$) and is close to the VMC prediction ($|U_c|/t = 4.5$). Through the finite-size scaling, we show that there is no competing CDW order in the bilayer band-insulator model for the interaction range $|U|/t = 5$–10. The saddle-point analysis suggested the maximum critical temperature $T_c(\sim 0.4)$ at $|U|/t = 5$, whereas DQMC predicted $T_c/|t|_{\text{DQMC}} = 0.17$, which is lower than the saddle-point prediction at $|U|/t = 5$. We estimated the transition temperature for various interaction strengths and map out the $T$–$U$ phase diagram shown in Fig. 13. DQMC simulation predicts the maximum $T_c/|t| = 0.27$ which occurs at $|U|/t \sim 6$. We find that the maximum $T_c$ in our proposed half-filled bilayer band insulator is twice that of the maximum $T_c/|t| \sim 0.13$ (for $|U|/t = 8$) published in Ref. [3] for the single-layer attractive Hubbard model. Thus, the studied bilayer band-insulator model has “higher” characteristic temperature $T_c$, with no competing orders as compared to earlier attempts, and is expected to be realized in cold-atom experiments.

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