# Enhancing *T*<sub>c</sub> in a composite superconductor/metal bilayer system: A dynamical cluster approximation study

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It has been proposed that the superconducting transition temperature  $T_c$  of an unconventional superconductor with a large pairing scale but strong phase fluctuations can be enhanced by coupling it to a metal. However, the general efficacy of this approach across different parameter regimes remains an open question. Using the dynamical cluster approximation, we study this question in a system composed of an attractive Hubbard layer in the intermediate coupling regime, where the magnitude of the attractive Coulomb interaction |U| is slightly larger than the bandwidth W, hybridized with a noninteracting metallic layer. We find that while the superconducting transition becomes more mean-field-like with increasing interlayer hopping, the superconducting transition temperature  $T_c$  exhibits a nonmonotonic dependence on the strength of the hybridization  $t_{\perp}$ . This behavior arises from a reduction of the effective pairing interaction in the correlated layer that outcompetes the growth in the intrinsic pair-field susceptibility induced by the coupling to the metallic layer. We find that the largest  $T_c$ inferred here for the composite system is comparable to the maximum value currently estimated for the isolated negative-U Hubbard model.

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# I. INTRODUCTION

An early and curious observation of the underdoped cuprate superconductors is that they host a remarkably low carrier density and correspondingly low superfluid stiffness; yet, they have a large pairing scale characterized by the superconducting gap and correspondingly short coherence length [1,2]. These properties give rise to a situation where Cooper pairing and long-range phase coherence occur at different temperatures, and the superconducting transition temperature  $T_c$  is significantly lower than the corresponding mean-field temperature scale  $T_c^{MF}$  [2–7]. This behavior is in contrast to metallic superconductors, where pairing and long-range phase coherence happen simultaneously and  $T_c^{MF} = T_c$  [3].

Kivelson [8] proposed that the  $T_c$  of a superconductor with low superfluid stiffness could be raised closer to its mean-field value by coupling it to a metallic system. Using a disconnected (i.e., no in-plane hopping  $t_1$ ; see Fig. 1) negative-UHubbard layer coupled to a metallic layer by single-particle tunneling  $t_{\perp}$ , this proposal was originally studied perturbatively [9] for |U| and  $t_{\perp}$  much smaller than the metallic bandwidth W, and later using quantum Monte Carlo (QMC) up to values of |U| larger than the bandwidth [10]. In this model, the pairing layer has zero superfluid stiffness and the corresponding critical temperature vanishes when the interlayer tunneling is switched off (i.e.,  $t_{\perp} = 0$ ). For small and increasing  $t_{\perp}$ , phase coupling between pairing sites is enabled by Josephson tunneling through the metallic layer [9,10] and  $T_c$  increases; however,  $T_c$  is eventually suppressed by the same delocalization effects beyond intermediate values of  $t_{\perp}$ . The numerical results obtained by Watchel *et al.* [10] further suggest that phase fluctuations exponentially suppress  $T_c$  for small  $t_{\perp}$ . Moreover, they found that the highest  $T_c$  that can be achieved by varying  $t_{\perp}$  were quite modest. For example,  $T_c$  is three to four times smaller than  $T_c^{MF}$  for small and intermediate |U|/t, where t is the hopping amplitude in the metallic layer ( $t_2$  in our model). Moreover,  $T_c$  remains below the highest  $T_c$  in the isolated 2D negative-U Hubbard model for large |U|/t.

The intermediate coupling regime  $|U| \sim W$ , where W is the bandwidth in the negative-U layer, but with intraplane hopping in the negative-U layer restored was later addressed using QMC [11]. In that case, the correlated layer has a small but nonzero superfluid stiffness, even when  $t_{\perp} = 0$ , and the superconducting transition follows the Berezinskii-Kosterlitz-Thouless (BKT) universality class of the XY model. For increasing  $t_{\perp}$ , Ref. [11] observed a proximity effect-induced suppression of the pairing correlations in the correlated layer, while the metallic layer exhibited nonmonotonic behavior with a maximum in the pairing correlations at intermediate  $t_{\perp}$ . In other words, pairing is layer (or orbital) dependent for small  $t_{\perp}$ , an observation that is reminiscent of the orbital selective behaviors seen in many multiorbital Hubbard models [12,13]. Eventually, the pairing in both layers is suppressed simultaneously beyond a critical value of  $t_{\perp}$ .

While the work in Ref. [11] provided a finite-size analysis of the pairing correlations above  $T_c$ , it did not determine  $T_c$  as a function of  $t_{\perp}$ . Estimating the latter is crucial, however,



FIG. 1. A cartoon depiction of the two-layer (two-orbital) model studied in this work. Each layer consists of a square lattice. The dashed arrows exemplify the possible hoppings  $t_1$ ,  $t_2$ , and  $t_{\perp}$ , and black arrows represent spin-up and -down electrons. Here we use  $t_2 = 2t_1$  and  $\epsilon_2 = 0.2t_1$  and treat  $t_{\perp}$  as a variable parameter and set  $-|U| = -10t_1$ .

because the strength of the pairing correlations at  $T > T_c$  can be a poor indicator for the actual  $T_c$  realized in a system [14,15]. We address this issue by studying a negative-U Hubbard model coupled to a noninteracting layer using a QMC dynamic cluster approximation (DCA). Here, we focus on the nature of the superconducting transition and determining  $T_{\rm c}$ as a function of  $t_{\perp}$  by solving the Bethe-Salpeter equation in the particle-particle channel. Since the DCA incorporates long range physics in the thermodynamic limit through a coarsegraining of momentum space, it also provides a different numerical perspective than finite cluster QMC methods. Our results show that for large clusters,  $T_c$  is enhanced for finite  $t_{\perp}$  beyond the system's  $T_{c}$  when  $t_{\perp} = 0$ . That is, an increased single-particle tunneling between the layers reduces the effects of phase fluctuations present in the negative-U layer and thus leads to an increased  $T_c$ . We also discuss how the increased interlayer coupling leads to an increase in the intrinsic pair-field susceptibility, which competes with a reduction in the effective pairing interaction, leading to a nonmonotonic dependence of  $T_c$  on  $t_{\perp}$ . These two quantities suggest signs of crossover behavior similar to the BEC-BCS crossover found in the pure negative-U Hubbard model [16–19].

# **II. MODEL AND METHODS**

## A. Two-component model

Our composite system consists of a correlated negative-UHubbard layer and a noninteracting metallic layer connected through interlayer single-particle tunneling  $t_{\perp}$  (see Fig. 1). Both layers have square lattice geometry with identical lattice spacing. The associated bilayer Hamiltonian is defined as

$$\hat{H} = -\sum_{\langle ij \rangle, \ell, \sigma} t_{\ell} (\hat{c}_{i\ell\sigma}^{\dagger} \hat{c}_{j\ell\sigma} + \text{H.c.}) - |U| \sum_{i} \hat{n}_{i1\uparrow} \hat{n}_{i1\downarrow} + \sum_{i,\ell,\sigma} (\epsilon_2 \delta_{\ell 2} - \mu) \hat{n}_{i\ell\sigma} - t_{\perp} \sum_{i,\sigma} (\hat{c}_{i1\sigma}^{\dagger} \hat{c}_{i2\sigma} + \text{H.c.}), (1)$$

where  $\hat{c}_{i\ell\sigma}^{\dagger}$  ( $\hat{c}_{i\ell\sigma}$ ) creates (destroys) an electron on the *i*th site of the  $\ell = 1$  or 2 layers with spin  $\sigma (=\uparrow, \downarrow)$  and  $\hat{n}_{i\ell\sigma} = \hat{c}_{i\ell\sigma}^{\dagger}\hat{c}_{i\ell\sigma}$ . The in-plane nearest-neighbor hoppings  $t_{\ell}$  are fixed such that  $t_1 \equiv t = 1$  and  $t_2 = 2t$ , whereas the interlayer tunneling  $t_{\perp}$  is a variable parameter. An attractive on-site Coulomb interaction -|U| in the correlated layer ( $\ell = 1$ ) is responsible for the formation of local (*s*-wave) Cooper pairs. Lastly, the noninteracting metallic layer ( $\ell = 2$ ) has an additional on-site energy term that is used to shift the van Hove singularity slightly above the chemical potential  $\mu$  (we set  $\epsilon_2 - \mu = 0.2t$ ).

#### **B.** Methods

We studied the Hamiltonian in Eq. (1) using the DCA++ code [20], a state-of-the-art implementation of the DCA method. In this formalism, the lattice problem is reduced to a finite-size cluster embedded in a mean field that is selfconsistently determined to represent the system beyond the cluster [21]. Our model is an effective two orbital model resulting in a  $N = 2N_c$ -site cluster problem for an in-plane cluster of size  $N_c$ , which is solved using a continuous-time auxiliary-field QMC algorithm [22–24]. In this work, we examine several different in-plane cluster sizes including  $4 \times 4$  $(N_c = 16)$ ,  $6 \times 6$   $(N_c = 36)$ ,  $8 \times 8$   $(N_c = 64)$ , and  $10 \times 10$  $(N_c = 100)$ .

The QMC simulations utilized 6000 independent Markov chains to collect  $2 \times 10^6$  to  $5 \times 10^6$  total measurements. The model with negative-U interaction does not have a sign problem but tends to produce long autocorrelation times. To combat the latter, each of the contributing measurements was made after skipping 50–100 Monte Carlo sweeps to further ensure statistically independent sampling. A typical DCA calculation for our model (i.e., for a single set of model parameters) converges in six to eight iterations depending on the cluster size.

Throughout this work, we allow the chemical potential  $\mu$  to vary such that the filling in the correlated layer remains fixed at  $n_1 \equiv \langle \hat{n}_{i1} \rangle = 0.75$ , where  $\hat{n}_{i1} = \hat{n}_{i1\uparrow} + \hat{n}_{i1\downarrow}$ . The filling of the metallic layer is allowed to take whatever value is necessary to satisfy thermodynamic equilibrium as a result. This choice of filling avoids any complications that might stem from a perfectly nested Fermi surface as seen at half filling and it still gives us access to the superconducting transition in the negative-U model.

For the isolated  $(t_{\perp} = 0)$  2D negative-*U* Hubbard model away from half filling, the system has an *s*-wave superconducting ground state [16–19,25–27]. When  $|U|/t \ll 1$ , the system adopts a weak coupling BCS state and eventually crosses over to a Bose-Einstein condensate (BEC) of hardcore on-site bosons for  $|U|/t \gg 1$  [16–19]. Consequently,  $T_c$ is a nonmonotonic function of |U|/t that peaks at intermediate  $|U|/t \approx 4 - 6$  and gradually tapers off in the presence of increasingly stronger phase fluctuations at larger values of |U|/t [18,26,27]. We are interested in the question of whether the reduction in  $T_c$  due to phase fluctuations can be reversed in the composite system. We therefore set -|U| = -10t in the correlated layer and vary the interlayer hopping  $t_{\perp}$  to study its effects on the  $T_c$  of the composite system. We estimate  $T_c$  by solving the Bethe-Salpeter equation [28,29] as an eigenvalue problem:

$$-\frac{1}{N_{\rm c}}\sum_{k'}\sum_{\ell_3,\ell_4,\ell_5,\ell_6}\Gamma^{\rm pp}_{\ell_1\ell_2\ell_3\ell_4}(k,k')G_{\ell_3\ell_5}(k')G_{\ell_4\ell_6}(-k')\phi^{\alpha}_{\ell_5\ell_6}(k') = \lambda_{\alpha}\phi^{\alpha}_{\ell_1\ell_2}(k).$$
(2)

Here the eigenvalues and corresponding eigenvectors are given by  $\lambda_{\alpha}$  and  $\phi_{\ell\ell'}^{\alpha}$ , respectively;  $G_{\ell\ell'}(k)$  is the dressed single-particle propagator and  $\Gamma_{\ell_1\ell_2\ell_3\ell_4}^{\text{pp}}(k, k')$  is the irreducible particle-particle vertex, both obtained from the DCA and written compactly using the notation  $k \equiv (\mathbf{k}, i\omega_n)$ , where  $\mathbf{k}$  is the momentum and  $i\omega_n$  is a fermionic Matsubara frequency  $\omega_n = (2n + 1)\pi T$ . The index  $\alpha$  ranges over the entire set of eigensolutions, but we will limit our discussion to the solution corresponding to the largest eigenvalue denoted  $\lambda_s$ . A superconducting transition occurs when the leading eigenvalue  $\lambda_s(T_c) = 1$ . In our case, we find that the leading eigenvector has *s*-wave symmetry for all the values of  $t_{\perp}$  we consider.

## **III. RESULTS**

#### A. Temperature dependence of the pairing correlations

We first examine the temperature dependence of  $1 - \lambda_s(T)$  for several values of  $t_{\perp}$  plotted in Fig. 2 for  $N_c = 16$ . Starting from high-temperature (T/t = 2), we cool the composite system down to  $T \leq T_c$ , which is identified by the temperature at which  $1 - \lambda_s(T = T_c) = 0$ . The family of curves plotted in Fig. 2 represents different values of the interlayer hopping between 0 and 2.5*t* but with all other model parameters identical (except  $\mu$ , which varies as to fix  $n_1 = 0.75$ ). All curves for  $t_{\perp}/t \leq 1$  are denoted by filled circles and solid lines (to guide the eye) and the remaining curves with  $t_{\perp}/t > 1$  are depicted with filled squares and dashed lines.



FIG. 2. Temperature dependence of  $1 - \lambda_s(T)$  for the composite bilayer system on a  $N_c = 16$  site cluster for several different values of the interlayer hopping in the interval  $t_{\perp}/t \in [0, 2.5]$ . Filled circles (squares) with solid (dashed) lines depict results for  $t_{\perp}/t \leq 1$  ( $t_{\perp}/t > 1$ ).

As noted, the superconducting transition in this model is expected to follow the BKT universality class. Since the DCA embeds the finite-size cluster in a mean field, the calculated temperature dependence will cross over to mean-field behavior when the correlation length exceeds the cluster size [21]. But at higher temperatures, when the correlations are still contained within the cluster, the DCA results will exhibit the true temperature dependence of the system in the thermodynamic limit. For small  $t_{\perp}/t < 1$ , the curves display convex behavior, indicating the presence of phase fluctuations and BKT behavior [7]. For larger  $t_{\perp}/t > 1$ , the temperature dependence of  $1 - \lambda_s(T)$  changes qualitatively to a more BCS-like behavior, exhibiting logarithmic  $\ln(T/T_c^{MF})$  dependence. The change in curvature around  $t_{\perp} = 1$  is similar to what is observed for the repulsive Hubbard model with increasing hole doping [7]. It reflects a change in the nature of the superconducting phase transition and the decreasing strength of phase fluctuations as  $t_{\perp}$  increases. The results in Fig. 2, therefore, suggest that coupling to the metallic layer makes the superconducting transition more mean-field-like.

## B. Transition temperature vs interlayer coupling

Figure 3 plots the estimated  $T_c$  values for  $N_c = 16, 36, 64$ , and 100. Unfortunately, the long autocorrelation times affecting the small  $t_{\perp}$  calculations prevent us from obtaining  $T_c$ estimates for larger clusters. Moreover, we observe significant cluster size dependence in the extracted values of  $T_c$ , particularly when  $t_{\perp}/t < 1$ . This occurs because larger clusters are needed to account for the long-range spatial fluctuations that suppress  $T_c$  in this regime. (This observation agrees with recent DQMC studies, which found that large clusters were needed to accurately estimate  $T_c$  for the negative-U Hubbard model [26,27].) Despite these limitations, we are able to draw some general conclusions about the pairing tendencies in the model, which we now address.

The results from the two smallest cluster sizes ( $N_c = 16$ , 36) are qualitatively similar in that the coupling  $t_{\perp}$  to the metallic layer suppresses  $T_c$  in this parameter regime. For  $N_c = 64$ , however,  $T_c(t_{\perp})$  displays nonmonotonic behavior with a maximum  $T_c$  near  $t_{\perp}/t = 1.5$ . Interestingly, the maximum occurs near the crossover between the BEC and the BCS behaviors observed in the temperature dependence of  $\lambda_s(T)$  in Fig. 2. We will further discuss this point in Sec. D below. This result suggests that  $T_c$  can indeed be optimized by adjusting the interlayer coupling; however, to determine the precise magnitude of this enhancement, we must contend with the finite-size effects in the small  $t_{\perp}$  regime.

The most recent estimates for the negative-*U* Hubbard model [27], based on DQMC and extrapolated to the thermodynamic limit, place  $T_c/t \approx 0.12$  for our model parameters, as indicated in Fig. 3. We therefore expect the estimated  $T_c$  from DCA to continue to decrease for larger cluster sizes ( $N_c > 64$ ) and  $t_{\perp}/t \ll 1$  until it is on par with this value. Conversely,



FIG. 3. Superconducting critical temperature  $T_c/t$  as a function of interlayer tunneling  $t_{\perp}/t$  for  $N_c = 16$ , 36, 64, and 100. For  $N_c = 16$ and 36,  $T_c$  is a monotonically decreasing function of  $t_{\perp}$ , but with strong indications of a cluster size dependence for small  $t_{\perp}$ . However, when  $N_c = 64$ ,  $T_c$  is nonmonotonic as a function of  $t_{\perp}$ , suggesting that large cluster sizes are required to capture the effects of phase fluctuations on  $T_c$  for small  $t_{\perp}$ . We include two points for  $N_c = 100$  to demonstrate that  $T_c$  is well captured by smaller clusters when  $t_{\perp}/t >$ 2. The red star indicates the estimate for  $T_c(t_{\perp}/t = 0)$  as  $N_c \rightarrow \infty$ stemming from a recent DQMC study (Ref. [27]) of the 2D negative-U model. The solid lines are intended to guide the eye.

we do not observe such a strong cluster size dependence for larger  $t_{\perp}$  values. For example, the results for  $N_c = 100$  and  $t_{\perp} \ge 2$  almost lay on top of the corresponding  $N_c = 64$  data points. We therefore believe that our results are relatively well converged for larger  $t_{\perp}/t$ . Combined, the results in Fig. 3 then indicate that the  $T_c$  of the composite system is indeed larger than the  $t_{\perp} = 0$  case in the  $|U| \ge W$  regime, with the largest  $T_c$ values occurring for  $t_{\perp} \approx 1.5t - 2t$ . Moreover, given the rate of convergence observed in Fig. 3, it is clear that the maximum value of  $T_c(t_{\perp})$  is comparable to the maximum  $T_c \approx 0.16t$ value obtained in the negative-U model [27]. This  $T_c$  value is relatively constant across a range of |U|/t from 4 to 6 and electron filling  $\langle \hat{n} \rangle$  between 0.70 and 0.88.

#### C. Effective pairing interaction and pair mobility

Thus far we have demonstrated that  $T_c$  follows a nonmonotonic dependence on  $t_{\perp}$  when the DCA cluster size is sufficiently large. We now turn to the question of what drives this nonmonotonicity by examining the  $t_{\perp}$  dependence of the effective pairing interaction and the intrinsic pair-field susceptibility, both of which determine the leading eigenvalue  $\lambda_s$  of the Bethe-Salpeter equation.

The *s*-wave pair-field susceptibility  $P_s$  is given by

$$P_{s}(T) = \int_{0}^{\beta} \mathrm{d}\tau \, \langle T_{\tau} \hat{\Delta}(\tau) \hat{\Delta}^{\dagger}(0) \rangle, \qquad (3)$$



FIG. 4. Effective interaction  $V_s(t_{\perp})$  and intrinsic pair-field susceptibility  $P_{s0}(t_{\perp})$  evaluated at T = 0.2t. Results were obtained on a cluster size of  $N_c = 64$ . The solid lines are included to guide the eye.

with  $\hat{\Delta}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{i,\ell} \hat{c}^{\dagger}_{i\ell\uparrow} \hat{c}^{\dagger}_{i\ell\downarrow}$ . Its leading-order term

$$P_{s0}(T) = \frac{T}{N} \sum_{k} \sum_{\ell_1, \ell_2, \ell_3, \ell_4} G_{\ell_1 \ell_3}(k) G_{\ell_2 \ell_4}(-k)$$
(4)

defines the intrinsic pair-field susceptibility  $P_{s0}(T)$ . With these two quantities, we can then define an effective pairing interaction  $V_s$  through

$$V_s(T) = P_{s0}^{-1}(T) - P_s^{-1}(T).$$
 (5)

We note that using this definition for  $V_s$ , we find that the product  $V_s P_{s0}$  gives values very similarly to those for the leading eigenvalue  $\lambda_s$  with a difference of at most 5%. Figure 4 plots  $V_s$  and  $P_{s0}$  at a fixed temperature T/t = 0.2 across the range of  $t_{\perp}/t$  spanning the  $T_c$  "dome" in Fig. 3. As the interlayer tunneling  $t_{\perp}$  increases, the effective pairing interaction  $V_s$ decreases monotonically. Conversely, the intrinsic pair-field susceptibility increases as the coupling to the metallic layer grows. The enhancement of  $P_{s0}$  would raise  $\lambda_s$  and therefore  $T_{\rm c}$ , but it competes with the decrease in in the pairing interaction, leading to a nonmonotonic dependence of  $T_c$  on  $t_{\perp}$ . Since  $P_{s0}(t_{\perp})$  is a measure of the states available to form s-wave pairs, it provides an indirect measure of the superfluid phase stiffness. We can, therefore, conclude that the increase in  $T_{c}$ is indeed being driven by enhanced superfluid phase stiffness but that this is ultimately counteracted by a decrease in the effective pairing interaction.

We note that  $V_s$  and  $P_{s0}$  have been defined here using contributions from the entire system, i.e., the sum over  $\ell$  in Eqs. (3) and (4) runs over both layers. Although not shown, we have repeated the analysis above but restricting the sums separately over just the correlated or the metallic layer. In this case, the behavior of  $V_s$  and  $P_{s0}$  for the correlated layer is qualitatively identical to that shown in Fig. 4; however, for the metallic layer, the trends are swapped with  $V_s$  increasing and  $P_{s0}$  decreasing.

## D. Discussion

While our DCA calculations provide direct access to the thermodynamic limit, they are also considerably more expensive than finite cluster determinant QMC (DQMC) calculations. Because of this, a shortcoming of our analysis is that it considers a narrow range of model parameters. However, a survey of the most relevant results from previous studies suggests that many of the qualitative trends we observe are likely insensitive to minor variations in model parameters. For instance, Ref. [11] examined other filling factors ( $n_1 = 0.6, 0.8, 1.0$ ) and attractive interaction strengths (U/t = -4, -6, -10). The authors found that smaller values of  $n_1$  are only marginally better for inducing pairing correlations in the metallic layer and that less negative values of U decrease pairing significantly in both layers. Thus we expect our results to be representative of the regime where the size of the interaction and the bandwidth are comparable and pairing is more significant. Although a direct comparison with Ref. [11] is not possible, their calculations (for similar parameters) show that the static pair structure factor decreases monotonically with increasing  $t_{\perp}$  in the correlated layer and peaks at finite  $t_{\perp}$  in the metallic layer. However, the strength of the induced correlations in the metallic layer is small compared with the correlated layer and not representative of a superconducting transition over the temperatures they studied. It may be, therefore, necessary to compare our results directly with those from a method like DQMC in the future. There we could better gauge the role of the mean field in the DCA method in situations where phase fluctuations are strong.

The rise and fall of  $T_c$  with  $t_{\perp}$  suggest that this composite bilayer model provides a route to enhancing  $T_c$  as discussed in Refs. [8] and [9], even for this nonperturbative case where  $t_1 \neq 0$  and  $|U| \gtrsim W$ . However, the  $T_c$  enhancement we observe is modest relative to the cases examined in previous works [9,10], which focused on models where the correlated layer has virtually no superfluid stiffness when  $t_{\perp} = 0$ . Our model has small phase stiffness in the correlated layer by tuning the interaction into a regime of increasing phase fluctuations and allowing comparable hopping amplitudes in both layers. These results suggest that the details of both the correlated and the metallic layers can play a crucial role in determining the  $T_c$  values ultimately achieved in a composite system. While this result calls for a more exhaustive study of the model space, it also indicates that opportunities for additional engineering of the layers exist.

The evolution of the superconducting transition from KTlike to BCS-like is reminiscent of the BCS-BEC crossover [30,31] discussed in the context of the 2D negative-U Hubbard model [16,17]. In the latter scenario, one goes from BEC to BCS superconductivity by systematically lowering |U| from the intermediate-strong coupling regime to the weak coupling regime. Importantly,  $T_c(|U|)$  is found to have a maximum for  $|U| \sim W$ . In the bilayer model, although |U| is kept constant, we find that the pairing interaction is effectively reduced through an increase in the interlayer tunneling amplitude  $t_{\perp}$ . Interestingly, like the purely 2D case, we find that  $T_c$  in the composite system also has a maximum with decreasing pairing interaction, i.e., when  $t_{\perp}$  is increased, near the crossover between the BEC and the BCS regimes. Based on this observation, one may speculate that the results for the composite system can be rationalized in terms of an effective single-layer negative-U model, in which the hopping amplitude has been enhanced effectively by the hopping through the metallic layer. Additional calculations are needed to determine to what extent this is indeed the case and will be the subject of future studies.

## **IV. SUMMARY AND CONCLUSION**

We have examined а composite negative-U Hubbard/noninteracting metallic bilayer system using DCA-QMC calculations to study the relationship between the superconducting  $T_c$  and the interlayer single-particle tunneling. Our work expands on previous studies [9,10] by focusing on a regime where the magnitude of the attractive interaction is comparable to the bandwidth  $(|U| \gtrsim W)$ , and both layers have finite bandwidth (i.e., nonzero intralayer hopping). Moreover, we complement Ref. [11] by estimating  $T_{\rm c}$  directly and computing the system's effective pairing interaction and superfluid stiffness as a function of  $t_{\perp}$ .

We found that  $T_c$  displays nonmonotonic behavior and reaches a maximum at a finite value of the interlayer tunneling  $t_{\perp}$ , a trend that emerges when the DCA cluster size becomes sufficiently large (i.e., when  $N_c \gtrsim 64$ ) to capture the necessary spatial fluctuations. For smaller clusters, phase fluctuations are suppressed by the mean field and the  $T_c$  is overestimated, especially for small tunneling values. The effective pairing interaction in the correlated layer decreases monotonically with increasing  $t_{\perp}$ , thereby lowering the pairing scale. However, we see a competing increase in the intrinsic pair-field susceptibility up to a finite value of  $t_{\perp}$ , which acts to increase  $T_c$  over the same range. Our results suggest that the peak  $T_c$ may correspond to a crossover between tightly formed BEC pairs and longer range BCS pairs, much like in the negative-*U* Hubbard model.

For small interlayer tunneling, the superconducting transition displays signs of strong phase fluctuations. As the interlayer tunneling increases, we observe a shift toward a BCS-like logarithmic temperature dependence. Interestingly, this confirms that the superconducting transition in the composite system does inherit a more mean-field-like character through the interlayer hybridization. However, this partial recapture of the mean-field pairing scale produces only a modest enhancement of  $T_c$  relative to the isolated layer. We speculate that this enhancement could be further increased by considering metallic layers that can retain some degree of the large pairing interaction. For example, coupling to a metal with strong electron-phonon coupling could help counteract the reduction in  $V_s$ .

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- [1] Y. J. Uemura, G. M. Luke, B. J. Sternlieb, J. H. Brewer, J. F. Carolan, W. N. Hardy, R. Kadono, J. R. Kempton, R. F. Kiefl, S. R. Kreitzman, P. Mulhern, T. M. Riseman, D. L. Williams, B. X. Yang, S. Uchida, H. Takagi, J. Gopalakrishnan, A. W. Sleight, M. A. Subramanian, C. L. Chien *et al.*, Universal Correlations between  $T_c$  and  $\frac{n_s}{m^*}$  (Carrier Density over Effective Mass) in High- $T_c$  Cuprate Superconductors, Phys. Rev. Lett. **62**, 2317 (1989).
- [2] V. J. Emery and S. A. Kivelson, Importance of phase fluctuations in superconductors with small superfluid density, Nature (London) 374, 434 (1995).
- [3] J. Corson, R. Mallozzi, J. Orenstein, J. N. Eckstein, and I. Bozovic, Vanishing of phase coherence in underdoped Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+δ</sub>, Nature (London) **398**, 221 (1999).
- [4] Z. A. Xu, N. P. Ong, Y. Wang, T. Kakeshita, and S. Uchida, Vortex-like excitations and the onset of superconducting phase fluctuation in underdoped  $La_{2-x}Sr_xCuO_4$ , Nature (London) **406**, 486 (2000).
- [5] Y. Wang, L. Li, M. J. Naughton, G. D. Gu, S. Uchida, and N. P. Ong, Field-Enhanced Diamagnetism in the Pseudogap State of the Cuprate Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+δ</sub> Superconductor in an Intense Magnetic Field, Phys. Rev. Lett. **95**, 247002 (2005).
- [6] P. M. C. Rourke, I. Mouzopoulou, X. Xu, C. Panagopoulos, Y. Wang, B. Vignolle, C. Proust, E. V. Kurganova, U. Zeitler, Y. Tanabe, T. Adachi, Y. Koike, and N. E. Hussey, Phasefluctuating superconductivity in overdoped La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub>, Nat. Phys. 7, 455 (2011).
- [7] T. A. Maier and D. J. Scalapino, Pairfield fluctuations of a 2D Hubbard model, npj Quantum Mater. 4, 30 (2019).
- [8] S. Kivelson, Making high  $T_c$  higher: A theoretical proposal, Phys. B: Condens. Matter **318**, 61 (2002), the Future of Materials Physics: A Festschrift for Zachary Fisk.
- [9] E. Berg, D. Orgad, and S. A. Kivelson, Route to hightemperature superconductivity in composite systems, Phys. Rev. B 78, 094509 (2008).
- [10] G. Wachtel, A. Bar-Yaacov, and D. Orgad, Superfluid stiffness renormalization and critical temperature enhancement in a composite superconductor, Phys. Rev. B 86, 134531 (2012).
- [11] A. Zujev, R. T. Scalettar, G. G. Batrouni, and P. Sengupta, Pairing correlations in the two-layer attractive Hubbard model, New J. Phys. 16, 013004 (2014).

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- [12] P. Werner and A. J. Millis, High-Spin to Low-Spin and Orbital Polarization Transitions in Multiorbital Mott Systems, Phys. Rev. Lett. 99, 126405 (2007).
- [13] L. F. Tocchio, F. Arrigoni, S. Sorella, and F. Becca, Assessing the orbital selective Mott transition with variational wave functions, J. Phys.: Condens. Matter 28, 105602 (2016).
- [14] P. Mai, G. Balduzzi, S. Johnston, and T. A. Maier, Pairing correlations in the cuprates: A numerical study of the three-band hubbard model, Phys. Rev. B 103, 144514 (2021).
- [15] S. Karakuzu, S. Johnston, and T. A. Maier, Superconductivity in the bilayer hubbard model: Two fermi surfaces are better than one, Phys. Rev. B 104, 245109 (2021).
- [16] R. T. Scalettar, E. Y. Loh, J. E. Gubernatis, A. Moreo, S. R. White, D. J. Scalapino, R. L. Sugar, and E. Dagotto, Phase Diagram of the Two-Dimensional Negative- *U* Hubbard Model, Phys. Rev. Lett. **62**, 1407 (1989).
- [17] M. Keller, W. Metzner, and U. Schollwöck, Dynamical Mean-Field Theory for Pairing and Spin Gap in the Attractive Hubbard Model, Phys. Rev. Lett. 86, 4612 (2001).
- [18] T. Kaneko and Y. Ohta, BCS–BEC crossover in the twodimensional attractive Hubbard model: Variational cluster approach, J. Phys. Soc. Jpn. 83, 024711 (2014).
- [19] T. Hazra, N. Verma, and M. Randeria, Bounds on the Superconducting Transition Temperature: Applications to Twisted Bilayer Graphene and Cold Atoms, Phys. Rev. X 9, 031049 (2019).
- [20] U. R. Hähner, G. Alvarez, T. A. Maier, R. Solcà, P. Staar, M. S. Summers, and T. C. Schulthess, DCA + +: A software framework to solve correlated electron problems with modern quantum cluster methods, Comput. Phys. Commun. 246, 106709 (2020).
- [21] T. A. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler, Quantum cluster theories, Rev. Mod. Phys. 77, 1027 (2005).
- [22] E. Gull, P. Werner, O. Parcollet, and M. Troyer, Continuoustime auxiliary-field Monte Carlo for quantum impurity models, Europhys. Lett. 82, 57003 (2008).
- [23] E. Gull, P. Staar, S. Fuchs, P. Nukala, M. S. Summers, T. Pruschke, T. C. Schulthess, and T. Maier, Submatrix updates for the continuous-time auxiliary-field algorithm, Phys. Rev. B 83, 075122 (2011).

- [24] E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, Continuous-time Monte Carlo methods for quantum impurity models, Rev. Mod. Phys. 83, 349 (2011).
- [25] A. Moreo and D. J. Scalapino, Two-Dimensional Negative-U Hubbard Model, Phys. Rev. Lett. 66, 946 (1991).
- [26] T. Paiva, R. Scalettar, M. Randeria, and N. Trivedi, Fermions in 2D Optical Lattices: Temperature and Entropy Scales for Observing Antiferromagnetism and Superfluidity, Phys. Rev. Lett. 104, 066406 (2010).
- [27] R. A. Fontenele, N. C. Costa, R. R. dos Santos, and T. Paiva, Two-dimensional attractive Hubbard model and the BCS-BEC crossover, Phys. Rev. B 105, 184502 (2022).
- [28] T. A. Maier, M. Jarrell, and D. J. Scalapino, Pairing interaction in the two-dimensional Hubbard model studied with a dynamic

cluster quantum Monte Carlo approximation, Phys. Rev. B **74**, 094513 (2006).

- [29] T. A. Maier, M. S. Jarrell, and D. J. Scalapino, Structure of the Pairing Interaction in the Two-Dimensional Hubbard Model, Phys. Rev. Lett. 96, 047005 (2006).
- [30] A. J. Leggett, Diatomic molecules and Cooper pairs, in *Modern Trends in the Theory of Condensed Matter*, edited by A. Pękalski and J. A. Przystawa (Springer Berlin Heidelberg, Berlin, Heidelberg, 1980), pp. 13–27.
- [31] M. G. Ries, A. N. Wenz, G. Zürn, L. Bayha, I. Boettcher, D. Kedar, P. A. Murthy, M. Neidig, T. Lompe, and S. Jochim, Observation of Pair Condensation in the Quasi-2D BEC-BCS Crossover, Phys. Rev. Lett. 114, 230401 (2015).
- [32] http://energy.gov/downloads/doe-public-access-plan.