The Berezinskii-Kosterlitz-Thouless (BKT) transition is a generic transition describing the loss of coherence in two-dimensional systems and has been invoked, for example, to describe the superconductor-insulator transition in thin films. However, recent experiments have shown that the BKT transition, driven by phase fluctuations, is not sufficient to describe the loss of superconducting order, and amplitude fluctuations must also be taken into account. The standard models that are extensively used to model two-dimensional superconductors are the Hubbard and \( XY \) models. Whereas the \( XY \) model allows only phase fluctuations, the Hubbard model has an extra degree of freedom: amplitude fluctuations. In this paper we compare two Hubbard models with the same critical temperature but with different interactions and deduce the role of the amplitude fluctuations in the superconducting transition. For this purpose, a novel approximation is presented and used. We derive an effective phase-only (\( XY \)) Hamiltonian, incorporating amplitude fluctuations in an explicit temperature dependence of the phase rigidity. We study the relation between amplitude fluctuations and coupling strength. Our results support existing claims about the suppression of phase rigidity due to amplitude fluctuations not present in the \( XY \) model.

DOI: 10.1103/PhysRevB.88.184510

PACS number(s): 74.78.—w, 74.25.Bt, 74.40.—n

II. MODELS AND METHODS

The Hamiltonian of the classical \( XY \) model is given by

\[
H_{XY} = -\sum_{\langle i,j \rangle} J_{ij} \cos(\theta_i - \theta_j),
\]

where \( \langle i,j \rangle \) designates near neighbors, and \( J_{ij} = J \) the bare near-neighbor coupling, which we take to be uniform in this paper. In the context of superconductivity, the classical phases \( \theta_i \in [0,2\pi) \) mimic the local phase of the superconducting order parameter. It is the thermal fluctuation of these phases which is believed to be the main mechanism for the loss of conventional superconductivity in thin films and perhaps certain cuprates. Starting from the low-temperature phase and increasing the temperature towards the transition temperature \( T_c \), the \( XY \) model undergoes a BKT transition at \( T_c \approx 0.89J \). Usually, \( T_c \) is found by use of the helicity modulus, \( \eta(T_c) \), which is expected to have a universal jump (for an infinite system) at \( T_c \). However, due to the exponentially diverging correlation length at the BKT transition, numerical calculation of the helicity modulus always suffers from finite-size effects. An alternative technique\(^{11}\) relies on the expected scaling of the correlations,

\[
\langle \cos(\theta_i - \theta_{i+L}) \rangle \sim \frac{1}{L^{n(T)}} F\left( \frac{L}{\xi} \right),
\]

with \( n(T) \) the temperature-dependent correlation exponent and \( \xi \) the (finite-size) correlation length at temperatures below the BKT transition. Taken with the universal BKT prediction \( n(T_c) = \frac{1}{2} \), this provides a numerically simple way to determine \( T_c \), as it requires only calculation of the (numerically more accessible) correlation function. In Fig. 1(a) we demonstrate how this scaling technique is used to determine \( T_c \) for the two-dimensional Hubbard model with \( U = 2 \). Similarly, when we employed this technique for the \( XY \) model, we found \( T_c \approx 0.89J \) to good accuracy, even when using only small systems.

Although the phase fluctuations and resulting BKT transition are well captured by the classical \( XY \) model, in real
FIG. 1. (Color online) (a) Deducing $T_c$ from the scaling relation [Eq. (2)]. Scaled edge-to-edge correlation functions $L^{1/4} \langle \cos(\theta_i - \theta_{i+L/2}) \rangle$ for three different-sized systems cross at $T_c \approx 0.058$. (b) Schematic of $T_c(U)$ for the Hubbard model. The dashed (blue) line is the XY model $T_c \approx 0.89J$ with $J \propto U$. The dotted (red) line shows the two values, $U = 2$ and $15$ (black arrows), having the same $T_c$ studied in this paper.

Superconductors the amplitude of the superconducting order parameter can also fluctuate. Such amplitude fluctuations, physically the breaking of a Cooper pair into two quasiparticles, cause suppression of $T_c$ compared with the purely phase (XY) scenario. To allow such amplitude fluctuations, we use the negative-$U$ Hubbard model,

$$\mathcal{H}_{\text{Hub}} = -\sum_{\langle i,j \rangle,\sigma} t C_i^{\dagger}\sigma C_j^{\sigma} - U \sum_i C_i^{\dagger}\uparrow C_i^{\downarrow} C_i^{\downarrow} C_i^{\uparrow}$$

$$- \sum_{i,\sigma} \mu_0 C_i^{\dagger}\sigma C_i^{\sigma},$$

where $(i,j)$ indicates a sum over nearest neighbors; $C_{i\sigma}^{\dagger}$ creates a spin-$\sigma$ electron on site $i$; $t$ is the homogeneous hopping integral, taken to be the unit of energy; and $-U < 0$ is the on-site attractive interaction. The chemical potential $\mu_0$ determines the average density $n$ and is fixed self-consistently so that the density $n = 0.875$ remains temperature independent.

To simulate the model without resorting to quantum Monte Carlo (MC), we use a well-established method that takes into account thermal fluctuations but ignores quantum ones. Since we wish to simulate our systems far from a (possible) quantum phase transition, we are justified in making this approximation, thus allowing us to enjoy the relative ease of a classical simulation. Our simulation technique is explained in greater detail elsewhere. We provide a brief description here for the sake of completeness and notation.

Applying a Hubbard-Stratonovic transformation to the Hubbard Hamiltonian, $(3)$, with a local complex Hubbard-Stratonovic field, $\Delta$, and ignoring the temporal dependence of these fields (quantum fluctuations), the partition function becomes

$$Z = \text{Tr}[e^{-\beta\mathcal{H}_{\text{Hub}}}] = \int D(\{\Delta_i, \Delta_i^\dagger\}) \text{Tr}_f[e^{-\beta\mathcal{H}_{\text{BdG}}(\{\Delta_i\})}],$$

with the Bogoliubov–de Gennes (BdG) Hamiltonian given by

$$\mathcal{H}_{\text{BdG}} = -\sum_{\langle i,j \rangle,\sigma} t C_i^{\dagger}\sigma C_j^{\sigma} - \sum_{\sigma} \mu_0 C_i^{\dagger}\sigma C_i^{\sigma}$$

$$+ \sum_{\sigma} (U C_i^{\dagger}\sigma C_i^{\sigma} + \Delta_i C_i^{\dagger}\uparrow C_i^{\downarrow} + \Delta^*_i C_i^{\downarrow} C_i^{\uparrow}).$$

Here $\text{Tr}_f$ traces the fermionic degrees of freedom over the single-body Hamiltonian $\mathcal{H}_{\text{BdG}}$ and can be evaluated exactly using its eigenvalues. Direct diagonalization of the Hamiltonian at each MC step is extremely time-consuming, and instead, since MC updates are local, one can use a Chebyshev polynomial expansion. The integral over the fields $\{\Delta_i, \Delta_i^\dagger\}$ can then be calculated using the (classical) metropolis MC technique. One should note that, unlike the BdG approximation, which amounts to a saddle-point approximation of the integral, here $\Delta_i$ are auxiliary fields. Except at zero temperature, where our approach coincides with the BdG solution, the fields $\Delta_i$ are generally different from the local superconducting order parameter $\langle C_i^\dagger C_i \rangle$.

Using the scaling relation [Eq. (2)], we determine $T_c$ as a function of the Hubbard $U$ for a range of values. This technique, as well as others, was previously employed to find the $T_c$ of the Hubbard model. The resulting $T_c(U)$ is schematically plotted in Fig. 1(b) and reveals a dome-like shape. For very large values of the Hubbard coupling $U \gg t$, the kinetic term $t$ can be treated as a perturbation, and a leading-order expansion (away from half-filling) gives an effective XY model with $J \propto U$. The proportionality factor depends on the electron density through the chemical potential $\mu_0$ and is fixed so that the $T_c$ of the effective XY model matches the Hubbard one, with $J \approx (U - V) n (2 - n) \frac{1}{\text{hvF}}$. (The last factor is due to the difference between the classical and the quantum models.)

Note that here $J$ is temperature independent, as is the case in the familiar XY model. The value for $T_c$ for the XY model is plotted as a dashed line, which agrees with the Hubbard critical temperature for $U \gg 12$. Indeed, in the following section, we explicitly show that in the large-$U$ limit, amplitude fluctuations are suppressed due to the high energy cost associated with breaking a Cooper pair. Thus, in the large-$U$ limit, the fermionic degrees of freedom in the Hubbard model become effectively frozen and the model becomes one of interacting bosons on a lattice, i.e., an XY model, with only the phases free to fluctuate.

III. RESULTS

Having established the shape of the Hubbard dome, we see that a given $T_c$, below the maximal possible $T_c$, corresponds to two systems with different values of Hubbard $U$. This nontrivial situation leads us to the main question we wish to address in this paper, namely, What is the difference between the low-$U$ and the high-$U$ Hubbard models that share the same $T_c$?

We chose to concentrate on two values of $U$, $U = 2$ and $U = 15$, both leading to $T_c \approx 0.058$, shown in Fig. 1(b) as the dotted horizontal line (for readability, let us refer to them as weak and strong coupling). The advantage of the choice of these values of $U$ is twofold: the strong-coupling side is well approximated by the equivalent XY model; the weak-coupling side still maintains a (relatively) small superconducting coherence length, $\xi \approx \frac{\hbar v_F}{U} \approx 5$ lattice sites. The coherence length measures the effective size of an amplitude excitation. Therefore a large coherence length necessitates simulation of a larger lattice. We find that for the parameters we chose and temperatures $T < T_c$, finite-size
effects are negligible. To demonstrate this important point we have simulated two system sizes (12 × 12 and 20 × 20), which indeed behave very similarly for $T < T_c$. In what follows, we present results for both system sizes and compare them to the results of the XY model. Above the critical temperature $T_c$, vortex and amplitude fluctuations proliferate, necessitating much larger system sizes. Therefore, to avoid finite-size effects, we limit our investigation to the $T < T_c$ temperature range.

To characterize a given system, we calculate the distribution $P(\theta)$ of the phase difference $\theta = \theta_i - \theta_j$ between two neighboring sites, $i$ and $j$. In the absence of an external magnetic field, the probability of a phase difference, must be symmetric about $\theta = 0$, with $\theta \in [-\pi, \pi]$. Since the system is invariant under translations (we use periodic boundary conditions), the distribution is identical for any nearest-neighbor pair, and we thus average it over all the pairs in the lattice. The filled circles in Fig. 2 show the numerical results for $P(\theta)$ for a $U = 2$ Hubbard model on a $20 \times 20$ lattice for a range of temperatures. Interestingly, we find that the distribution function can be fit quite accurately by that of a single, isolated link (or Josephson junction), with an effective, temperature-dependent coupling $J_{\text{eff}}(T)$ (solid lines in Fig. 2). In other words, we find

$$P(\theta) = \frac{1}{Z} e^{\beta J_{\text{eff}}(T) \cos(\theta)}, \quad Z = 2\pi I_0(\beta J_{\text{eff}}),$$  

with $Z$ the partition function, $\beta = \frac{1}{kT}$ the inverse temperature, and $I_0$ the zeroth Bessel function. The procedure of singling out two spins, $i$ and $j$, and integrating out all the other spins in the lattice makes the effective coupling $J_{\text{eff}}(T)$ explicitly temperature dependent. Such an explicit temperature dependence resulting from partial integration was investigated long ago. Before proceeding we wish to clarify the following:

1. As the temperature is increased, coherence between $i$ and $j$ gets decreasing contributions from other lattice sites. Indeed, at temperatures well above $T_c$ the lattice contribution to $J_{\text{eff}}$ vanishes, leaving $J_{\text{eff}}$ with only the bare near-neighbor coupling. Therefore, at high temperatures in the strong-coupling Hubbard model, $J_{\text{eff}} \to J \propto \frac{1}{T}$. Naturally, this result also applies for the XY model.

(2) Amplitude fluctuations occupy a length scale of approximately $\xi$. Therefore, to measure their effect, it is advisable to examine the coherence of near neighbors.

(3) We have made vigorous tests, all showing that the above distribution also holds for spin pairs arbitrarily far apart. Moreover, the fitting function is robust for both the XY model and the Hubbard model at arbitrary $U$.

(4) The procedure we employ, integrating out part of the system, is identical to the procedure used to calculate entanglement entropy. Thus we are in a position to calculate the entanglement entropy of one pair with the rest of the lattice. The result can be analytically approximated, $S = -\int d\theta P(\theta) \ln P(\theta) \approx -\beta J_{\text{eff}} I_1(\beta J_{\text{eff}}) + \ln 2\pi I_0(\beta J_{\text{eff}})$. We do not include further discussion of the entanglement entropy in this work.

Using this fit one can extract $J_{\text{eff}}$, which is plotted, as a function of temperature, in Fig. 3. Together, Figs. 2 and 3 constitute the main numerical result of this paper. Figure 3 shows results for both the weak- and the strong-coupling Hubbard models in two lattice sizes, along with the XY model with the same $T_c$. Our main observation is that $J_{\text{eff}}$ for the weak-coupling Hubbard is large at low temperatures but decreases rapidly with temperature, showing a dramatic effect of amplitude fluctuations. In contrast, the strong-coupling Hubbard shows only a modest suppression of $J_{\text{eff}}$ for temperatures $T \lesssim T_c$, similarly to the XY model. We note that different lattice sizes produce nearly the same results, demonstrating that indeed our results are insensitive to finite-size effects.) These results underscore the equivalence of the strong-coupling model to the XY model, in contrast to the weak-coupling model, where amplitude fluctuations are significant.

Moreover, the weak- and strong-coupling curves cross at $T_c$, where both systems measure the same $J_{\text{eff}}$. This agrees with an intuitive percolative description of $T_c$ as the temperature which overcomes near-neighbor coupling, thus destroying
FIG. 4. (Color online) (a) The bare coupling $J_{\text{bare},U}$ of the XY model that gives rise to the same correlations as that of the respective Hubbard model [scaled by $J$ of the XY model with the same $T_c$; see Eq. (7)], as a function of $T$. $J_{\text{bare},U=2}$ shows a stronger temperature dependence, reflecting the effect of amplitude fluctuations. Dashed (black) lines, low-temperature estimate using Eq. (9). (b) Relative amplitude fluctuations $\delta \Delta$ [see Eq. (10)] for $U = 2 \ldots 12$. The weak-coupling values show significant amplitude fluctuations which diminish as coupling is increased.

Thus the reverse-engineering process we have suggested is consistent with its expected low-temperature limit.

So far we have discussed the effect of amplitude fluctuations without providing explicit evidence of their existence. Taking $C_{\uparrow i}$ as the (up) electron destruction operator at site $i$, we define the relative root-mean-square (RMS) amplitude fluctuations $\delta \Delta$,

$$\delta \Delta(T, U) = \frac{1}{N} \sum_i \left( |C_{\uparrow i} C_{\uparrow i}|^2 - \langle |C_{\uparrow i} C_{\uparrow i}|^2 \rangle \right) \left( |C_{\downarrow i} C_{\downarrow i}|^2 - \langle |C_{\downarrow i} C_{\downarrow i}|^2 \rangle \right)$$

with $\langle \ldots \rangle$ the MC (ensemble) average, $N$ the total number of lattice sites, and $\sum$ the sum over all lattice sites.

We plot $\delta \Delta$ in Fig. 4(b) for values of $U$ in $[2, 12]$. Clearly, significant RMS amplitude fluctuations exist only in the weak-coupling case and are, of course, stronger at higher temperatures. Figure 5(a) shows that these curves, for the limited range of $U$ that we have calculated, satisfy a power-law relation, $\delta \Delta(T, U) \sim U^{x(T)}$. The exponent $x(T)$ and its $95\%$ fit confidence values is plotted in Fig. 5(b). Interestingly, $\delta \Delta(T, U)$ drops more rapidly with $U$ as the temperature increases.

IV. SUMMARY AND CONCLUSIONS

Realistic superconducting thin films support both phase and amplitude fluctuations of the order parameter. The simplest model that allows these two degrees of freedom is the attractive two-dimensional Hubbard model. It is known that the critical temperature $T_c(U)$ of the Hubbard model has a dome-like dependence on the coupling $U$. Therefore, there exist two values of $U$, which we call weak ($|U| < 4$) and strong ($|U| > 4$), that satisfy the same $T_c$. In this paper, we have suggested a Josephson approximation that probes the phase coherence near neighbors. The approximation is robust across a wide range of temperatures and is model independent. Using this approximation we were able to extract an effective coupling $J_{\text{eff}}(T)$ which we use as a probe to compare the two sides of the Hubbard dome. We have found a qualitative difference between the two sides of the dome in the temperature dependence of $J_{\text{eff}}(T)$. Specifically, in contrast to the strong-coupling side, which agrees quantitatively with XY model, the weak-coupling model shows a steep decrease
in $J_{\text{eff}}(T)$ as the temperature is increased towards $T_c$. We explain this behavior by the effect of thermal fluctuations on the superconducting amplitude and show evidence to support our explanation. Thus, both processes contribute to the quantitative way in which superconductivity is lost in weak-coupling films, in contrast with the simpler (phase only) mechanism in the strong-coupling regime. In the regime where amplitude fluctuations are important, our approach can be used to generate an effective phase-only action with a temperature-dependent $J(T)$ as shown in Fig. 4(a). The resulting $J(T)$ can be compared with analytical attempts that integrate out the amplitude fluctuations. It can also be used when analyzing heterolayered systems (e.g., Refs. 25 and 26), where different layers can have different couplings and therefore different amplitude fluctuations effects. Specifically, it will be interesting to use our technique to analyze bilayered systems where both layers have the same $T_c$ but one layer is weakly coupled whereas the other is strongly coupled. Experimentally, $J_{\text{eff}}$ could be measured by a two-tip STM experiment, perhaps by coupling the two tips to a SQUID or other sensitive device. Single-tip STM experiments have already been successfully used to probe inhomogeneous thin films.\textsuperscript{27,28}

One advantage of our approach is that it readily generalizes to disordered systems. In fact, our approach is likely to apply to a wide range of systems such as cuprates, heavy fermion and organic superconductors, and magnetic systems, as well as any coherent system where both phase and nonphase degrees of freedom exist.

**ACKNOWLEDGMENTS**

We thank Assa Auerbach for his valuable input. Most calculations were done on the BGU HPC cluster. This work was supported by the ISF. Amir Erez was supported by the Adams Fellowship Program of the Israel Academy of Sciences and Humanities.

\*amir.b.erez@gmail.com

\begin{thebibliography}{99}
\bibitem{8} A. Auerbach, *Interacting Electrons and Quantum Magnetism* (Springer, Berlin, 1994).
\bibitem{22} In directional statistics, the distribution in Eq. (6) is known as the von Mises distribution.\textsuperscript{29} The von Mises distribution is analytically convenient and is widely employed in analyses of interactions in related systems (e.g., liquid helium in porous media\textsuperscript{30} and phase-coupled neural networks),\textsuperscript{31,32} making it a mathematically natural candidate as well as being physically motivated.
\end{thebibliography}