Phase Fluctuations in Strongly Coupled \textit{d}-wave Superconductors

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We present a numerically exact solution for the BCS Hamiltonian at any temperature, including the degrees of freedom associated with classical phase, as well as amplitude, fluctuations via a Monte Carlo (MC) integration. This allows for an investigation over the whole range of couplings: from weak attraction, as in the well-known BCS limit, to the mainly unexplored strong-coupling regime of pronounced phase fluctuations. In the latter, for the first time two characteristic temperatures \(T^*\) and \(T_c\), associated with short- and long-range ordering, respectively, can easily be identified in a mean-field-motivated Hamiltonian. \(T^*\) at the same time corresponds to the opening of a gap in the excitation spectrum. Besides introducing a novel procedure to study strongly coupled \textit{d}-wave superconductors, our results indicate that classical phase fluctuations are not sufficient to explain the pseudo-gap features of high-temperature superconductors (HTS).

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One of the most fascinating aspects of the HTS is that a theoretical description in traditional BCS terms – using Cooper pairs – is feasible, yet in many other aspects these materials seem to deviate considerably from the standard BCS behavior. Most notorious in this respect is the curious “pseudogap” (PG) phase in the underdoped regime. The PG has attracted enormous interest in recent years and its effects have been studied using a wide variety of techniques \(\textsuperscript{1,2}\). It is identified as a dip in the density of states \(\omega\) below a temperature \(T^*\), which is higher than the superconducting (SC) critical temperature \(T_c\), and its presence is sometimes attributed to a strong coupling between the charge carriers and accompanying phase fluctuations \(\textsuperscript{3}\). If this is the case, then conventional mean-field (MF) methods should not work in describing the cuprates, since they cannot distinguish between \(T^*\) and \(T_c\). For this reason, more elaborate techniques such as diagrammatic resummations or Quantum Monte Carlo (QMC) approximations have been used to address the many puzzling questions of strongly coupled superconductors. While for the case of superconductivity with \textit{s}-wave symmetry (\textit{sSC}) this effort can be carried out with the attractive Hubbard model \(\textsuperscript{4}\), the direct study of phase fluctuations for \textit{d}-wave superconductors (\textit{dSC}) remains a challenge. To our knowledge, in the vast literature on cuprates there is no available model where the physics of a strongly coupled \textit{dSC} with short coherence lengths and large phase fluctuations can be studied accurately, with nearly exact solutions \(\textsuperscript{5}\). From the theory perspective, this is a conspicuous bottleneck in the HTS arena.

Here, we introduce a novel and simple approach to alleviate this problem. The proposed method allows for an unbiased treatment of phenomena associated with classical (thermal) phase fluctuations and non-coherent pair-binding. It represents an extension of the original solution of the pairing Hamiltonian and has been made possible mostly due to the advance of computational resources in the past decade. The focus is on the more interesting and important case - at least as far as HTS are concerned - of a nearest-neighbor (n.n.) attraction, necessary for \textit{dSC}. With regards to the cuprates, this approach is only meaningful to the extent that the relevant phase fluctuations are thermal rather than quantum mechanical and in fact it has been argued \(\textsuperscript{6}\) that phase fluctuations in cuprates may be assumed as predominantly classical, with quantum (dynamical) fluctuations \(\textsuperscript{6}\) suppressed.

Our approach is built on the insight that Hamiltonians that are quadratic in fermionic operators can be efficiently studied with the help of Monte Carlo techniques, as has been demonstrated in particular for the “double-exchange” model \(\textsuperscript{7}\). This is possible here because the original interacting model has been stripped of quantum fluctuations in the pairing approximation. The Hamiltonian \(H_{\text{SC}}\) describes an effective attraction between fermions on a 2D lattice and is given by

\[
H_{\text{SC}} = -\sum_{\text{i},\delta,\sigma} t \left( c_{\text{i}\sigma}^\dagger c_{\text{i}+\delta\sigma}^+ + V \sum_{\text{i},\delta} |\Delta_\text{i}\rangle^2 - \mu \sum_{\text{i}} n_{\text{i}} \right) - V \sum_{\text{i},\delta} \left( c_{\text{i}+\delta\uparrow}^\dagger c_{\text{i}\downarrow}^+ + c_{\text{i}\uparrow}^\dagger c_{\text{i}+\delta\downarrow}^+ \right) \Delta_\text{i}^A + \text{H.c.} \tag{1}
\]

where \(t\) - the energy unit - is the hopping amplitude for electrons \(c_{\text{i}\sigma}\) on n.n. sites. \(\mu\), the chemical potential, controls the particle density \(\langle n \rangle = 1/N \sum n_{\text{i}}\), \(\delta = \pm x, y\) denotes n.n. on an \(N = L \times L\) lattice, and in the standard derivation \(\Delta_\text{i}^A = (c_{\text{i}\uparrow} c_{\text{i}+\delta\downarrow}) \left( \ldots \right)\) signals thermal averaging. In the usual MF approach to Eq. (1) the gap function \(\Delta_\text{i}\) is assumed a real number, but here we retain the degrees of freedom associated with the phases and therefore write \(\Delta_\text{i} = |\Delta_\text{i}| \exp(i\phi_\text{i})\). The amplitudes are regarded as site variables, whereas the phases are treated as

\[
\Delta_\text{i} = |\Delta_\text{i}| \exp(i\phi_\text{i}) = \sum_{\text{i},\delta,\sigma} a_{\text{i},\delta,\sigma}^{\uparrow,\downarrow} \exp(i\phi_{\text{i},\delta,\sigma}^{\uparrow,\downarrow})
\]
link variables. $V(>0)$, the n.n. attraction, is assumed to be constant throughout the lattice, but inhomogeneous generalizations can be implemented in a straightforward manner. To calculate observables one needs to determine the corresponding partition function $Z_{SC}$ at temperature $T=1/\beta$,

$$Z_{SC} = \prod_{i=1}^{2N} \int_0^{2\pi} d\phi_i^x d\phi_i^y Z_c(|\Delta_i|, \{\phi_i^{\phi,y}\})$$

which is calculated via a canonical MC integration over both $|\Delta_i|$ and the phases $\{\phi_i^{\phi,y}\}$. The electronic partition function $Z_{el} = \text{Tr} \{e^{-\beta H_{el}(\Delta_i, \phi_i^{\phi,y})}\}$, $H_{el}$, being the purely fermionic part of $H$, is obtained after exactly diagonalizing $H_{el}$ for a given fixed set of $|\Delta_i|$s and $\{\phi_i^{\phi,y}\}$ and finding the eigenvalues $E_n^\phi$; it is then calculated in a standard fashion as $Z_{el} = \prod_{n=1}^{N} (1 + \exp(-\beta E_n^\phi))$. The classical part of $Z_{SC}$ is $Z_{cl} = e^{-\beta V(\sum_i |\Delta_i|)}$. The most CPU-time consuming task is the diagonalization leading to the eigenvalues $E_n^\phi$ for a given set of classical fields, limiting the lattice size. The results presented here were obtained for lattices up to $N=14 \times 14$, and for temperatures as low as $T = 0.002T_{c}$. Observables such as the spectral function $A(k,\omega)$, $\sum_n\Delta(k,\omega)$ or the optical conductivity $\sigma(\omega)$ can be calculated straightforwardly.

Here, however, we focus on other quantities of particular interest, namely the phase correlation function $S_{n}=(\langle \Delta_{i} \Delta_{j}\rangle^{\phi} e^{i\phi_{i}^{x} \phi_{j}^{y}})/\Delta_{i} \Delta_{j}$, the “mixed” correlation $F_{n}=\sum_{n=1}^{N} (\sum_{n=1}^{N} (\langle \Delta_{i} \Delta_{j}\rangle^{\phi} e^{i\phi_{i}^{x} \phi_{j}^{y}}))$, which is determined by the internal density of the doping electrons as shown below [1], and the gap $\Delta_{MC}\approx 1/4 \sum_{n} |\Delta_{i}|$.

Figure 1(a) shows $S_{n}(x,y)$, $F_{n}(0,0)$ on a $12 \times 12$ lattice, at $\langle n \rangle = 1$ and $T=0.01$. The different regimes emerging as $V$ is increased can easily be identified: (i) a BCS phase extending up to $V \approx 3$, where the correlation between n.n. sites $(i, j)=i+x$ and $(j=i+(L/2,0))$ is virtually identical, (ii) an intermediate region $3.5 \lesssim V \lesssim 6$, and (iii) the strongly coupled regime $V \gtrsim 6$, with short-range (SR) phase correlations only, at least at the lowest temperatures of our simulations. For the BCS state, $F(0)\approx 0.1$, equivalent to $\langle \Delta_{i}\Delta_{j}\rangle \approx \Delta_{i} \Delta_{j}$, clearly exposing the $d_{x^2-y^2}$-character caused by strong scattering for the Fermi surface at $(\pm \pi,0),(0, \pm \pi)$, this regime is characterized by a unique global phase, with only thermal fluctuations (and finite size effects) responsible for the small deviations from a perfect dSC [10]. This is revealed by the phase histograms, which feature two well-defined Gaussian curves centered around $\phi_i^x$ and $\phi_i^y = \phi_i^y + \pi$, respectively. On the other hand, the until now unexplored strong-coupling regime of Eq.(1) is characterized by distributions with multiple peaks and no evident global phase [11]. Such complicated distributions appear irrespective of starting configurations and other details of the MC process. Below, we will work with $H_{SC}$ as well as with a $d$-wave-projected ("id-p") model where $\Delta_{i}^{f} = \Delta_{i}^{t}$ is enforced, a commonly used approximation for dSC.

To further explore the validity of the MC integration we have also performed calculations in the low-density limit, $(\langle n \rangle) \approx 0.18$, with results for $S(1)$, $F(1)$ presented in Fig. 1(b). Here, $F(0,0)\approx 1$ emerges naturally (T small), and therefore the expected $d_{x^2-y^2}$-symmetry $(\equiv s^\ast, \cos k_x + \cos k_y)$ is realized. Again, it is possible to differentiate between weak- and strong-coupling regimes, based on the same arguments as in (a).

$\Delta_{MC}(T=0.01, \langle n \rangle = 1)$ is shown in the table below for both $H_{SC}$ and the d-p model $(\equiv \Delta_{MC,dp})$. For small $V$, $\Delta_{MC}$ barely deviates from its MF (dSC) value $\Delta_{MF}$, but it is definitely larger than $\Delta_{MF}$ in the strongly fluctuating regime [12]. This, together with the results shown in Fig 1(a), where $F(0,0)$ is very different from -1, signals the gradual transition from a dSC into what should be a $s^\ast + id$-SC [13]. The SC properties for large $V$ are not so much dictated by the FS topology (and band-filling) any more; instead the interaction $V$ forces all electronic states to take part in the pairing and not just the “preferred” ones near the FS, driving the system away from the $d$-wave state. Such a transition, desired to appear for any non-sSC, can easily be overlooked in studies biased towards dSC. For $V \gtrsim 1$, $\Delta_{MC}$ is slightly smaller than the MF gap for the simple s-wave state, $\Delta_{MF}$; thus, in this regime both the $d$- and the $s^\ast$-wave gap will have almost the same amplitude $\Delta_{s}\approx \Delta_{d}$ and it may resemble a disordered sSC. Because of its $s$-wave component, the resulting state has a nodeless FS, i.e. no gapless excitations, and thus

![FIG. 1: (a) The phase correlation functions $S(V)$, $F(V)$ at the shortest and maximum (linear) lattice distance at low $T$ and $(n)=1$. (b) Same functions as in (a), now for $(n)=0.18$, leading to (extended) $s$-wave behavior. The symbols stand for $S(1.0)$ (filled squares), $S(5.0)$ (open triangles) and $F(0.0)$ (filled triangles). The statistical error is much smaller than the symbols for $V < 4$, and roughly the symbol size for $V \lesssim 5$. (b) Correlation length $\xi(T)$ for $V=5.8$ at $(n)=1$ from the $H_{SC}$ model. From the Kosterlitz-Thouless fit (broken line) we obtain $T_{c} \approx 0.08$. Also shown are results for the d-p model at $V=4.8$, that lead to $T_{c} \approx 0.17$.](image-url)
TABLE I: Comparison of $\Delta_{MC}$ ($\Delta_{MC,dp}$) with the MF gap function, for both d- and conventional s-wave.

| V  | $\Delta_{MF}^{10^{-10}}$ | $\Delta_{MC,dp}^{10^{-10}}$ | $\Delta_{MC}^{10^{-10}}$ | $\Delta_{MC,dp}^{10^{-10}}$ |
|----|--------------------------|-----------------------------|---------------------------|-----------------------------|
| 1.2| 0.322                    | 0.241                       | 0.32±0.02                 | 0.32±0.02                   |
| 2.0| 0.627                    | 0.666                       | 0.62±0.02                 | 0.62±0.03                   |
| 4.0| 1.420                    | 1.747                       | 1.42±0.03                 | 1.63±0.18                   |
| 4.8| 1.743                    | 2.213                       | 1.90±0.20                 | 2.05±0.18                   |
| 5.6| 2.066                    | 2.636                       | 2.50±0.20                 | 2.50±0.20                   |

is strikingly different from the weak-coupling state.

The investigation of the temperature dependence of $S(I)$ for both $H_{SC}$ and the d-p model allows us to introduce for the first time in a BCS-like Hamiltonian two characteristic temperatures $T^*$ and $T_c$ in the case of strong coupling, in contrast to the BCS regime, where this distinction does not exist. We associate $T^*$ with the temperature where SR phase correlations develop (defined here as $S(1,0)\geq0.1$, but other cutoffs lead to quite similar qualitative conclusions). On the other hand, $T_c$ is commonly identified with the onset of long-range phase coherence (here we use the criterion $S(L/2,0)\geq0.1$). $T^*$ and $T_c$ are essentially identical for $V$ not too large (Fig.2(a)), and they are only clearly different for $V\geq3$, with $T^*$ larger than $T_c$ by a factor of 3-4 for $V>5$ (Fig.2(a)) [16]. Based on such MC results, a phase diagram, presenting $T_c$ and $T^*$ as a function of the pairing attraction, is displayed in Figs.2(b), (c). Remarkably, the values of $T_c$ reach a maximum $T_c^{max}\approx0.2$ for $V_{max}\approx3$ (similar to other such reported values), whereas $T^*$ increases steadily with $V$ [17]. For the “rigid” projected model (Fig.2(c)), $T_c^{max}\approx0.3$, accompanied by a more prominent regime of SR correlations. The regime of a d-wave PG (dPG) is indicated, and although it is sizeable for the d-p model, it is a rather small window for the more realistic $H_{SC}$. For the latter model, the state with a large difference between $T^*$ and $T_c$ (typical for HTS) is only found for values of $V$ that do not lead to a dSC at low $T$, nowadays widely accepted for HTS, owing to strong experimental evidence. For $(n)<1$, the dPG should be even less prominent than shown in Fig.2(b). This disagreement between theory and experiment puts the thermal phase-fluctuation scenario for HTS into serious doubt. $T_c$ itself is a continuous function (Fig.2(b),(c)), smoothly connecting the limits $V\rightarrow0$, as predicted in an early work [17]. Although the existence of $T_c^{max}$ has long been known, this is - to our knowledge - the first time it has been directly established in the framework of $H_{SC}$, since self-consistent methods are tracking $T^*$ rather than $T_c$ [18]. Yet, as demonstrated in Fig.2 they work very well for $V$ not excessively large.

For $V\geq V_{max}$ one presumably enters the realm of pronounced Kosterlitz-Thouless (KT) physics [19], whence $T_c$ is dictated by vortex binding rather than Cooper pairing. The critical temperature $T_{KT}\approx T_c$ in such models is proportional to $1/V$, following a perturbative analysis, similar to what is found in Fig.2(b),(c). It is certainly non-trivial to establish whether or not KT-behavior is found for $H_{SC}$, which, unlike the standard XY model, couples fermions to classical fields. For this purpose, we extract a correlation length $\xi$ by fitting $S(I)$ with an exponential, $S(r_x)\propto\exp(-r_x/\xi)$, and explore its temperature dependence, which should behave as $\xi(T)\propto\exp[A/\sqrt{T-T_c}]$. In the case of $V=5.6$, such a KT analysis (for $0.10\leq T\leq0.35$) produces a very good fit for $\xi(T)$ (see Fig.1(c)) and yields $T_c=0.08\pm0.01$, remarkably close to what has been established with our alternative definition of $T_c$ above. In addition, the exponential fit is not possible for $T\leq0.08$ - signalling that $H_{SC}$ is entering a state with different scaling behavior. In a similar fashion, $T_c$ is found to be 0.17(±0.02) for the d-p model at $V=4.8$, only slightly lower than its estimate from $S(I)$. Although the precise values cited above - having been obtained on relatively small lattices - need to be cautiously considered, our results are compatible with KT physics governing the region between $T_c$ and $T^*$, even in the presence of fermions.

As the PG scenario would suggest, the effect of $T^*$ is clearly visible in $N(\omega)$, which is shown for $V=1.20$ and $V=4.0$ in Fig.3. In the BCS limit (a), a gap appears for temperatures $T^*\approx T_c=0.09$ (compare to Fig.2(b)), whereas $N(\omega)$ shows non-correlated behavior and a van-Hove peak just above $T_c$. The remaining small peak at $\omega=0$ ($T<T_c$) is a finite size effect. At $V=4.0$ (Fig.3(b)), however, there is a wide region below $T^*\approx0.30$ (coinciding with the onset of SR fluctuations (Fig.2(b)) where a
characteristic temperatures $T^\ast$ and $T_c$, and an associated non-trivial phase diagram, has been numerically demonstrated. Our results for $H_{SC}$ seem to indicate that the observed PG features of HTS cannot be reconciled with a (classical) phase-fluctuation-dominated dSC. The integration method presented here can easily be extended to study disordered systems as well as to simultaneously investigate the competition of several fluctuation channels, such as dSC, antiferromagnetism and charge order [21], in an unbiased fashion. As such, this method (maybe best dubbed “mean-field Monte Carlo”) should be an invaluable tool in unlocking the secrets of the cuprates and possibly other systems with strong-coupling aspects such as Bose-Einstein condensates in cold fermions.

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