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Effect of Fibonacci modulation on superconductivity

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Abstract

We have studied finite-sized single band models with short-range pairing interactions between electrons in the presence of diagonal Fibonacci modulation in one dimension. Two models, namely the attractive Hubbard model and the Penson–Kolb model, have been investigated at half-filling at zero temperature by solving the Bogoliubov–de Gennes equations in real space within a mean-field approximation. The competition between 'disorder' and the pairing interaction leads to a suppression of superconductivity (of usual pairs with zero centre-of-mass momenta) in the strong-coupling limit while an enhancement of the pairing correlation is observed in the weak-coupling regime for both models. However, the dissimilarity of the pairing mechanisms in these two models brings about notable differences in the results. The extent to which the bond-ordered wave and the η -paired (of pairs with centre-of-mass momenta = π) phases of the Penson–Kolb model are affected by the disorder has also been studied in the present calculation. Some finite size effects are also identified.

1. Introduction

The competition between electronic correlation and disorder has remained one of the prime issues of investigation in condensed matter physics during the last few years [1–4]. However, the effect of such disorder is yet to be fully explored in the context of superconductivity. Some earlier experiments observed a lowering of the T_c in disordered weak coupling superconductors, while for some strong coupling materials T_c is nearly insensitive to the strength of disorder [5–7]. Very recent experiments observed [8] the destruction of superconductivity with increasing disorder strength in some low-dimensional superconductors. A lowering of T_c is also well known for some disordered superconducting A-15 materials [9–11]. Anderson [12] showed that weak non-magnetic impurities do not suppress superconductivity appreciably. A very recent work on the negative-U Hubbard model [13] showed that superconductivity is suppressed by bulk impurity. Moreover, it also showed that the diagonal disorder introduces spatial inhomogeneity in pairing correlation. Short-range pairing models, like the negative-U Hubbard model, have been studied extensively in the context of high- T_c and other exotic superconductors [14]. Therefore, the studies of interplay between disorder and superconductivity within the framework of the short-range pairing mechanism would be of great interest. In this work we describe a study on the effect of Fibonacci-modulated disorder on two different models of superconductivity which support short-range pairing.

The models that we have focused on in the present work are the negative-U Hubbard model [14] and the Penson–Kolb (PK) model [15], respectively. These two models have been extensively studied [14–24] in the recent past owing to their tentative relevance in the field of high- T_c cuprates and organic superconductors. However, the pairing mechanism of the two models is of different physical origin. Thus a comparative study of these two models in the presence of 'disorder' is expected to reveal a qualitative difference in the nature of competition between disorder and pairing correlation.

We have chosen a typical one-dimensional model of diagonal aperiodicity, namely, a Fibonacci modulated sequence of the site potentials, for observing the effect of disorder on these superconducting models. This type of quasi-crystalline 'disorder' not only interpolates between the extreme cases of full grown order and random disorder, but also qualifies for the scope of experimental investigations owing to the availability of various quasi-crystalline superlattices in recent times [25]. Thus our main objective, in this paper, is to understand the qualitative manner in which the quasi-crystalline disorder modifies the superconducting correlation in two specific models and how the nature of this competition changes from the weak- to the strong-coupling limit.

Our investigations for both models concentrate on decoupling of the Hamiltonian within a mean-field approximation (MFA) followed by a self-consistent solution of the Bogoliubov–de Gennes (BdG) equations in real space [13] for the decoupled Hamiltonians. The use of a mean-field approach is usually questionable in low dimensions. However, even in a low-dimensional system, such a technique works satisfactorily in a broken-symmetry phase [28]. The two models of short-ranged pairing that we have studied here are known to exhibit several broken-symmetry phases in the ordered limit. Previous mean-field calculations [14, 24] captured these phases satisfactorily in low dimensions and were found to compare well with the results obtained by other methods [19, 21, 22].

2. The models

2.1. The negative-U Hubbard model

The negative-U (attractive) Hubbard Hamiltonian with Fibonacci modulation in the site potentials is given by

$$\mathcal{H}_{-U} = \sum_{i} (\epsilon_{i} - \mu) n_{i} - \left(t \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i+1\sigma} + \text{h.c.} \right) + U \sum_{i} c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}, \quad (1)$$

where $c_{i\sigma}^{\dagger}(c_{i\sigma})$ creates (destroys) an electron of spin σ ($\sigma = \uparrow, \downarrow$) on the *i*th site. $n_{i\sigma} = c_{i\sigma}^{\dagger}c_{i\sigma}$ and $n_i = n_{i\uparrow} + n_{i\downarrow}$. ϵ_i is the site energy at the *i*th site; it takes on the value ϵ_A or ϵ_B according to the Fibonacci sequence: ABAABABAABAABAABAABAABA...; μ is the chemical potential and *t* is the single-particle hopping integral. The last term is the on-site Hubbard interaction. We will take negative values of *U* in our calculations for the attractive Hubbard model.

The attractive Hubbard model without any modulation in site potential ($\epsilon_i = 0$) has been extensively studied [14, 16–18, 26]. In this limit ($\epsilon_i = 0$), there is a competition between the single-particle hopping (t) and the Hubbard correlation (U < 0). The on-site Hubbard

correlation favours the formation of localized singlet pairs of electrons while the hopping term tends to break the pairs. Due to the local pairing mechanism the superconducting (SC) state and charge density wave (CDW) phases become degenerate in the ground state for a half-filled band at zero temperature [19]. This model has been extensively used in describing high- T_c and other related SC systems [14]. The effect of random diagonal disorder on the attractive Hubbard interaction has already been studied [13, 27]. It is interesting to observe how the Fibonacci modulation alters its SC properties.

2.2. The Penson-Kolb model

The PK model with Fibonacci-modulated site potentials is written below:

$$\mathcal{H}_{\mathrm{PK}} = \sum_{i} (\epsilon_{i} - \mu) n_{i} - \left(t \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i+1\sigma} + \mathrm{h.c.} \right) - V \left(\sum_{i} c_{i+1\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{i\downarrow} c_{i\uparrow} + \mathrm{h.c.} \right).$$
(2)

The first two terms have similar implications as in the Hubbard Hamiltonian (1). The third term is the pair-hopping term which is responsible for transfer of a singlet pair of electrons $(\uparrow\downarrow)$ between neighbouring sites. V is the nearest-neighbour pair-hopping amplitude. The PK model with $\epsilon_i = 0$ favours the formation of singlet pairs in real space due to this short-range pair hopping, and therefore shows a non-local pairing mechanism. In this sense the study of this model is complementary to the study of the on-site pairing model, namely the negative-UHubbard model. The PK model ($\epsilon_i = 0$) and its various generalizations have been widely studied over the years [20–24]. For V > 0, this model shows SC instability which corresponds to usual pairing with pairs of zero centre-of-mass momenta. However, for V < 0, in the strong coupling limit (beyond some value of V, say V_c), this model is shown to exhibit *n*-pairing with centre-of-mass momentum $q = \pi$ [21, 23, 24]. There is a phase which does not support SC ordering for $V_c < V < 0$. A real-space RG calculation showed the existence of a CDW phase in this regime [21] and did not consider the possibility of the existence of antiferromagnetic bondorder wave (BOW) which was later shown to coexist with the CDW within a Bosonization calculation [22]. A mean-field study, however, showed only the antiferro-BOW state in this region [24]. It seems rather interesting how these properties are modified in the presence of disorder.

3. The calculation within the MFA and the BdG equations

3.1. For the negative-U Hubbard model with Fibonacci modulation

We solve the negative-*U* Hubbard model first by decoupling the Hamiltonian in favour of superconductivity and then by solving the BdG equations of motion in real space in a self-consistent manner. The decoupled Hamiltonian looks like

$$\mathcal{H}_{-U} = \sum_{i} (\epsilon_{i} - \mu) n_{i} - \left(t \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i+1\sigma} + \text{h.c.} \right) + U \sum_{i\sigma} \langle n_{i\sigma} \rangle c_{i,-\sigma}^{\dagger} c_{i,-\sigma} - U \sum_{i\sigma} \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + U \sum_{i\sigma} \langle c_{i\sigma}^{\dagger} c_{i,-\sigma}^{\dagger} \rangle c_{i,-\sigma} c_{i\sigma} - U \sum_{i} \langle c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} \rangle \langle c_{i\downarrow} c_{i\uparrow} \rangle.$$
(3)

The BdG equations of motion for the operators $c_{i\uparrow}$ and $c_{i\downarrow}^{\uparrow}$ are

$$i\dot{c}_{i\uparrow}^{\dagger} = [c_{i\uparrow}^{\dagger}, \mathcal{H}_{-U}] = tc_{i-1\uparrow}^{\dagger} + tc_{i+1\uparrow}^{\dagger} - U\Delta_{i}^{\dagger}c_{i\downarrow} - U\langle n_{i\downarrow}\rangle c_{i\uparrow}^{\dagger} - (\epsilon_{i} - \mu)c_{i\uparrow}^{\dagger}$$

$$\tag{4}$$

$$i\dot{c}_{i\downarrow} = [c_{i\downarrow}, \mathcal{H}_{-U}] = -tc_{i+1\downarrow}^{\dagger} - tc_{i-1\downarrow}^{\dagger} - U\Delta_i c_{i\uparrow}^{\dagger} + U\langle n_{i\uparrow}\rangle c_{i\downarrow} + (\epsilon_i - \mu)c_{i\downarrow}$$
(5)

where $\dot{c}_{i\sigma} = \frac{dc_{i\sigma}}{dt}$ and $\Delta_i^{\dagger} = \langle c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} \rangle$. We study the Fourier transform of the SC gap parameter, $\Delta_q = (1/N) \sum_{i\sigma} e^{iq \cdot r_i} \Delta_i$, where r_i is the position of the *i*th site.



Figure 1. Plots of Δ_q , the Fourier transform of the SC gap parameter, as a function of q for different 'disorder' strengths (ϵ_B) in the Fibonacci-modulated attractive Hubbard model (for U = -2.8) for N = 144. The scale of energy in this figure as well as in all subsequent ones is given by t = 1.0. (The inset shows the corresponding case for N = 34.)

3.2. For the Penson-Kolb model with Fibonacci modulation

The decoupled PK Hamiltonian is given below:

$$\mathcal{H}_{PK} = \sum_{i} (\epsilon_{i} - \mu) n_{i} - \left[\sum_{i\sigma} (t + V p_{i,-\sigma}^{\dagger}) c_{i\sigma}^{\dagger} c_{i+1,\sigma} + \text{h.c.} \right] - V \left(\sum_{i} \Delta_{i} c_{i+1\uparrow}^{\dagger} c_{i+1\downarrow}^{\dagger} + \text{h.c.} \right) - V \left(\sum_{i} \Delta_{i+1} c_{i\uparrow\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} + \text{h.c.} \right) + (V \Delta_{i}^{\dagger} \Delta_{i+1} + \text{c.c.}) + (V p_{i\downarrow}^{\dagger} p_{i\uparrow}^{\dagger} + \text{c.c.})$$
(6)

where $\Delta_i^{\dagger} = \langle c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} \rangle$ and $p_{i\sigma}^{\dagger} = \langle c_{i+1\sigma}^{\dagger} c_{i\sigma} \rangle$.

The BdG equations corresponding to the PK Hamiltonian for the operators $c_{i\uparrow}$ and $c_{i\downarrow}^{\dagger}$ in real space are given below:

$$i\dot{c}_{i\uparrow}^{\dagger} = (t + Vp_{i\downarrow}^{\dagger})c_{i-1\uparrow}^{\dagger} + (t + Vp_{i\downarrow})c_{i+1\uparrow}^{\dagger} + V\Delta_{i-1}^{\dagger}c_{i\downarrow} + V\Delta_{i+1}^{\dagger}c_{i\downarrow} - (\epsilon_{i} - \mu)c_{i\uparrow}^{\dagger}$$
(7)

$$i\dot{c}_{i\downarrow} = -(t + Vp_{i\uparrow}^{\dagger})c_{i+1\downarrow}^{\dagger} - (t + Vp_{i-1\uparrow})c_{i-1\downarrow}^{\dagger} + V\Delta_{i+1}c_{i\uparrow}^{\dagger} + V\Delta_{i-1}c_{i\uparrow}^{\dagger} + (\epsilon_{i} - \mu)c_{i\downarrow}.$$
(8)

We solve the BdG equations self-consistently to determine the Fourier transform of the SC gap, Δ_q , together with the bond-order parameter (in *q*-space), $B_q = (1/2N) \sum_{i\sigma} \sigma e^{iq \cdot r_i} p_{i\sigma}$.

4. Results

4.1. For the Fibonacci-modulated negative-U Hubbard model

The negative-U Hubbard model has been studied at half-filling on a one-dimensional chain for system sizes N = 34 and 144. We have chosen $\epsilon_A = 0$ always. The plot of Δ_q in figure 1 reveals a maximum at q = 0. This bears a signature of a normal SC phase with singlet pairs having zero centre-of-mass momentum. The nature of competition between the disorder and correlation strongly depends on the value of U (figure 2). It is observed that for lower values of |U|, the value of $\Delta_0(\Delta_q \text{ at } q = 0)$ is enhanced due to Fibonacci modulation. This is due to the formation of double occupancies at the sites of lower energy. A crossover takes place



Figure 2. Plots of the SC gap parameter Δ_0 (for pairs with zero centre-of-mass momentum) versus U in the Fibonacci-modulated attractive Hubbard model for N = 144 for different 'disorder' strengths. (Inset: N = 34.)



Figure 3. Plots of the local pairing amplitude Δ_i versus site index *i* for the attractive Hubbard model with different strengths of Fibonacci modulation. The plot clearly reveals an underlying Fibonacci pattern which is strengthened for larger values of ϵ_B .

at intermediate values of |U|. After that Δ_0 decreases with increasing Fibonacci modulation. This happens due to increased backscattering in the presence of Fibonacci 'disorder'. The value of |U| where the crossover takes place becomes lower with increasing system size; this is a reflection of the stronger effect of electronic correlation in larger system sizes. Figure 3 shows the plot of Δ_i against *i* at U = -2.8 (a value of |U| below which the crossover has taken place) for N = 34. This plot clearly depicts the spatial inhomogeneity in pairing brought about by the Fibonacci modulation. Such results are in agreement with [13]. Competition between disorder and correlation is further revealed in figure 4, showing the plot of Δ_0 as a function of ϵ_B . It is interesting to observe that for low values of |U| (U = -1.0), Δ_0 increases with Fibonacci disorder, while for strong |U| (U = -4.0) Δ_0 sensibly decreases with increasing disorder. This is precisely what we have observed in figure 2. However, the variation of Δ_i alone is not sufficient to determine the superconductor–insulator transition occurring at high values of ϵ_B (not considered in the present work) which has been studied quantitatively in earlier quantum Monte Carlo studies of the attractive Hubbard model with random disorder [30].



Figure 4. Plots of Δ_0 versus ϵ_B in the Fibonacci-modulated attractive Hubbard model for different values of U.



Figure 5. Plots of Δ_q versus q in the Fibonacci-modulated PK model for the positive V vector for N = 144 for different strengths of 'disorder'. (Inset: N = 34.)

4.2. For the Fibonacci-modulated Penson-Kolb model

The one-dimensional PK model also has been studied for half-filling and for the same system sizes. Let us first discuss the case of V > 0. Figure 5 shows the plots of Δ_q for V = 1.0. The peaks of Δ_q at q = 0 for V > 0 reveal that the system is in a normal SC phase. The effect of Fibonacci disorder for the high and low values of V can be seen from figure 6. For low values of V, Δ_0 increases with ϵ_B , while the opposite phenomenon occurs at larger values of V. However, the fall in Δ_0 with ϵ_B for V = 2.0 is extremely slow compared to the notable variation of Δ_0 for V = 1.0. Thus, even a very strong disorder does not seriously affect the SC properties of the system at high values of V. This is in sharp contrast to the case of large |U|. This can be qualitatively understood in the following way. A closer look at equations (4) and (5) reveals that the Hubbard interaction directly renormalizes the 'effective' site potentials for the electrons of opposite spins to different extents. Thus for the larger values of |U| the site potential seen by an up-spin electron at a particular site differs considerably from that seen by a down-spin electron. Therefore, the possibility of formation of singlet pairs is reduced due to the competition between strong correlation and disorder. But this should not be so drastic in the case of the PK model as suggested by equations (7) and (8). Figure 7 shows that Δ_0 , as a function of V, remains very small until a value of V, say V_0 , is reached. The value of V_0 decreases with system size. The reason behind this is that the finite size gap in the energy



Figure 6. Plots of Δ_0 versus ϵ_B in the Fibonacci-modulated PK model for different values of V > 0. The effect of 'disorder' is found to be distinctly different for low and high values of V.



Figure 7. Plots of Δ_0 versus *V* (positive *V* sector) in the Fibonacci-modulated PK model N = 144 for different strengths of disorder. (Inset: N = 34.)

spectrum is larger than the gap in the spectrum due to V, for $V < V_0$. So the system is unable to realize the effect of V in this region and hence Δ_0 remains almost zero. For N = 144 the finite size gap reduces; consequently the value of V_0 goes down. In fact V_0 would go to zero in the thermodynamic limit [31]. For $V > V_0$, Δ_0 increases smoothly and sharply with V. It is interesting to note in figure 7 that Δ_0 has higher values for $\epsilon_B \neq 0$ (compared to the case of $\epsilon_B = 0$) in the regime of small V. In this region the effect of pair hopping is rather weak to form a large number of singlet pairs. However, the Fibonacci modulation generates sites of lower energy which favour the formation of 'doublons'. As a result, a higher value of Δ_0 is observed for $\epsilon_B \neq 0$ than for $\epsilon_B = 0$. A crossover takes place at a certain V, after which the entire process reverses. For large values of V, the pair hopping process can generate a large number of pairs. But the pairing becomes suppressed in the presence of the Fibonacci modulation. This is qualitatively similar to the negative-U case. However, the degree of suppression of Δ_0 due to disorder in the PK model is not very high. Consistent with this observation we also find that the spatial inhomogeneity in Δ_i is less pronounced in the case of the PK model (figure 8) as compared to the negative-U model.

Next we consider the case V < 0. We study the SC properties for larger values of |V|. The plots of Δ_q against q show peaks at $q = \pi$ (figure 9), implying an η -paired (with centreof-mass momentum $q = \pi$) SC phase [21, 32]. The peaks are suppressed by Fibonacci



Figure 8. Plots of Δ_i versus *i* for the PK model (V > 0) with different strengths of Fibonacci 'disorder'. The Fibonacci pattern in Δ_i is very much suppressed compared to the case of the negative-*U* Hubbard model (figure 3) even for a reasonably large disorder ($\epsilon_B = 1.5$).



Figure 9. Plots of Δ_q versus q in the Fibonacci-modulated PK model for V < 0 for N = 144 for different values of ϵ_B . (Inset: N = 34.)

aperiodicity. In figure 10 we show the plot of Δ_{π} against V in the regime V < -2. It is found that for V = -2.0, Δ_{π} has higher value in the periodic limit ($\epsilon_B = 0$) than in the cases of $\epsilon_B \neq 0$. It is interesting to note that the suppression of η -pairing due to the disorder becomes less pronounced in larger system size. Consequently the decrease of the η -SC correlation across $|V| \approx 2.0$ is rather gradual with increasing disorder in larger systems.

Next we discuss the intermediate region of -2 < V < 0. In this regime our result shows a bond-order wave (BOW) phase [22, 24] in the periodic limit (for |V| < 1.9), which is evident from the plot of B_q against q (figure 11). The bond-order parameter shows a peak at $q = \pi$ for V = -1.0. The height of the peak (i.e. the BOW) is found to increase with increasing |V| (below a certain $|V_c| \approx 1.9$ above which η -pairing takes place). Figure 12 depicts simultaneous variations of the BOW order parameter and the η -paired SC gap parameter as functions of V in the regime -2 < V < 0. It is observed that in the periodic limit the transition from the BOW phase to the η -paired phase occurs at around $|V_c| \approx 1.9$ for both N = 34 and 144. This value of $|V_c|$ increases with increasing Fibonacci modulation in the case of N = 34. But this does not happen for the case N = 144. This is a result of the fact that the Fibonacci sequence can significantly disrupt and delay the formation of η -paired ordering for smaller system sizes, a fact already observed in figure 10. For smaller system sizes the finite size gaps are large enough to mask the effects of the pair hopping which reduces the BOW in the region -2 < V < 0.



Figure 10. Plots of the SC gap Δ_{π} (for the η pairing with centre-of-mass momentum $= \pi$) versus V in the Fibonacci-modulated PK model (for V < 0) for N = 144 for different strengths of 'disorder'. (Inset: N = 34.)



Figure 11. Plots of B_q , the Fourier transform of BOW order parameter, versus q for N = 144 for the Fibonacci-modulated PK model. (Inset: N = 34.)

Therefore the quasiperiodic disorder makes the value of $|V_c|$ shift in an appreciable manner. For N = 144, the finite size gap becomes much smaller and the effect of the pair hopping dominates. Therefore, $|V_c|$ becomes insensitive to the effect of the disorder.

5. Conclusion

Summarizing, we have studied the negative-U Hubbard model and the Penson-Kolb model with Fibonacci-modulated site potentials at half-filling in one dimension by using a mean-field SC decoupling followed by self-consistent solutions of the corresponding BdG equations in real space. For the negative-U Hubbard model we obtain the normal SC phase corresponding to centre-of-mass momentum q = 0. Here we observe a crossover at intermediate values of |U|. Below this crossover the pairing correlation increases due to Fibonacci disorder while above it the pairing is suppressed by disorder. In the case of the PK model we observe a similar crossover in the positive-V sector. However, the suppression of SC correlation due to 'disorder' is much reduced in the PK model as compared to the negative-U Hubbard model. In case of the negative-U Hubbard model the real space pairing amplitude shows a spatial inhomogeneity which closely follows the underlying quasiperiodic pattern while the feature is less prominent in case of the PK model.



Figure 12. Simultaneous plots of B_{π} and Δ_{π} versus *V* in the negative-*V* sector of the Penson–Kolb model for N = 144. The upper panel shows the case of $\epsilon_B = 0.0$ while the lower one shows the case of $\epsilon_B = 0.4$. (The insets show corresponding plots for N = 34.) The transition point from the BOW to the η -paired phase shifts towards larger values of |V| for an increase of the 'disorder' strength for N = 34 while it is virtually insensitive to the 'disorder' strength for N = 144.

The non-local pairing mechanism in the PK model is already known to give results which are qualitatively different from the negative-U Hubbard model [29, 33]. However, in the present study, the qualitative difference between these two has been further clarified via the mechanism of competition between disorder and the pairing term. In the η -paired phase of the PK model, superconductivity is suppressed by disorder in general. In identifying the bond-ordered phase our calculations match with predictions of previous calculations [22, 24]. It turns out that the transition point from BOW to η -SC phase is not severely affected by the presence of disorder in large systems.

It is interesting to note how the microscopic mechanism of pairing modifies the nature of competition in going from the weak- to the strong-coupling regime. It is to be noted here that these results do not show marked variation in going from N = 34 to 144. On the other hand, the finite size effects that have been identified in the present calculation are essentially controlled (as discussed in section 4) by the finite size gap, which goes roughly as 1/N. Thus no dramatic change in these results is expected to take place beyond N = 144. It may, however, be noted that for obtaining very precise quantitative estimate of quantities, for example, the transition point from the BOW to the η -SC phase in the PK model, a finite size scaling would be necessary. Some future work may proceed in this direction.

For further investigation in this scheme, it would be interesting to include the repulsive Hubbard interaction term in the PK model and see the effect of quasiperiodic modulations in such systems. Also a detailed study of the effect of band filling away from the half-filled case would be very interesting. The possibility of formation of a CDW [21, 22], which is left out in the present calculation, could also be investigated. It would also be significant to study the

case of finite temperatures and higher dimensions. The effect of random diagonal disorder in the PK model also needs some attention.

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