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Hartree-Fock interaction in superconducting condensate fractals

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Abstract

It is well-known that the Hartree-Fock (HF) interaction does not alter superconducting observables in conventional superconductors, as its effect is mainly reduced to a chemical potential shift. Deviations from this behavior can only arise in situations of translational symmetry breaking, such as caused by the presence of external fields that induce spatial variations of the order parameter and electron density. We demonstrate that this scenario changes fundamentally in quasicrystalline systems, where the intrinsic lack of translational symmetry leads to a fractal spatial distribution of the superconducting condensate and electron density. By investigating a Fibonacci chain as a prototype quasicrystal, we numerically solve the Bogoliubov-de Gennes (BdG) equations and show that beyond the half-filling, the HF potential significantly enhances the self-similar spatial oscillations of the order parameter while simultaneously reducing its average value and altering its critical exponent. Consequently, the critical temperature is suppressed; for our chosen microscopic parameters, this suppression can reach up to 20%. Therefore, an accurate analysis of condensate distribution and related quantities in quasicrystalline superconductors requires the comparison of results obtained with and without the HF interaction.

Keywords

allenylsilanes; rhodium(II) octanoate-mediated rearrangement; silylketenes; titanium carbenoids; ylide

Introduction

It is well-known, dating back to the classical book by de Gennes [1], that in conventional superconducting materials, the Hartree-Fock interaction merely reduces to a shift of the chemical potential, as the observables are not affected due to translational invariance. Hence, the Hartree-Fock (HF) field is a kind of 'spectator' that defines the single-particle states and chemical potential but does not act on the pair formation and, thus, can be neglected, as in the standard formulation of the BCS model [2,3]. Nevertheless, the HF potential cannot be neglected in the presence of external fields [4], such as impurity potentials [5,6], quantum confinement in nanoscale superconductors [7], potential barriers at interfaces [8], etc. Such external fields break the translational invariance, which is the condition for the HF field to make a contribution to the formation of the superconducting condensate.

This raises an interesting question about systems that exhibit an intrinsic lack of translational invariance even in the absence of any applied field. Among those are quasicrystals, which were first discovered in 1984 [9-11]. Quasicrystals exhibit long-range orientational order - such as the five-fold symmetry in $\text{Al}_{86}\text{Mn}_{14}$ alloys [9,10] - but lack the translational invariance [11]. The superconductivity of quasicrystals was established in 2018 with the discovery of superconducting signatures in an Al-Zn-Mg alloy below a critical temperature of $T_c \sim 0.05$ K [12]. More recently, in 2024 and 2025, much higher critical temperatures of $T_c \sim 1$ K and $T_c \sim 5.47$ K were reported in van der Waals layered dodecagonal quasicrystals $\text{Ta}_{1.6}\text{Te}$ [13] and in a monoclinic approximant to the decagonal quasicrystal $\text{Al}_{13}\text{Os}_4$ [14].

The experimental observations of the superconductivity in quasicrystals ignited a big interest in many open problems related to the superconducting condensate in quasiperiodic systems. Most of the recent results were obtained for a superconducting Fibonacci chain, being a simplified one-

dimensional model for superconducting quasicrystals [15]. Using this model, researchers explored a range of phenomena in quasiperiodic systems, including proximity effects in quasicrystal-metal hybrids [16-18], enhanced superconductivity from staggered hopping amplitudes [19], and the interplay between the Josephson effect and quasiperiodicity [20]. The model has also been used to investigate topological superconductivity [21] and anomalous local critical temperatures (left-end, right-end and at the chain center) in quasiperiodic chains [22]. These investigations demonstrate that the spatial distribution of the superconducting condensate in quasiperiodic chains exhibits a distinct fractal character, with significant oscillations of the order parameter along the system. A similar fractal inhomogeneous distribution of the pair condensate has been calculated for the Penrose and Ammann-Beenker tilings [23], being a well-known representation of two-dimensional quasicrystals.

Recent studies confirm that the superconducting condensate in quasiperiodic systems possesses a highly nontrivial spatial structure. This finding naturally raises the question of how sensitive the theoretical predictions for quasicrystalline superconductors are to the inclusion of the HF potential in the fundamental microscopic equations. Our work addresses this open problem through an investigation of the superconducting Fibonacci chain, a standard prototype for quasiperiodic systems.

Bogoliubov-de Gennes equations for superconducting Fibonacci chains

To investigate the superconducting properties of a Fibonacci chain, we use an attractive Hubbard model with the grand-canonical Hamiltonian (absorbing the chemical potential μ) given by [4-6,8, 19,22]

$$\hat{H} = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \sum_{i\sigma} \mu \hat{n}_{i\sigma} - g \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \quad (1)$$

where $c_{i\sigma}$ and $c_{i\sigma}^\dagger$ are the annihilation and creation operators of an electron with the spin projection $\sigma = (\uparrow, \downarrow)$ at sites $i = 1, \dots, N$, t_{ij} is the hopping amplitude, $\hat{n}_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and $g > 0$ is the on-site attractive electron-electron interaction.

Within the mean-field approximation, the Hamiltonian (1) is reduced [4] to the effective BCS-Bogoliubov Hamiltonian in the form (for the s-wave pairing)

$$\hat{H}_{\text{eff}} = \sum_{ij\sigma} h_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i [\Delta(i) c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \Delta^*(i) c_{i\downarrow} c_{i\uparrow}], \quad (2)$$

where

$$h_{ij} = -t_{ij} - \delta_{ij} [\mu - U_{\text{HF}}(i)], \quad (3)$$

with δ_{ij} the Kronecker delta, and $\Delta(i)$ and $U_{\text{HF}}(i)$ are the superconducting order parameter and the HF interaction potential, respectively. The latter obey the self-consistency relations

$$\Delta(i) = g \langle c_{i\uparrow} c_{i\downarrow} \rangle, \quad U_{\text{HF}}(i) = -g \langle \hat{n}_{i\uparrow} \rangle = -g \langle \hat{n}_{i\downarrow} \rangle, \quad (4)$$

here we exclude spin-imbalanced regimes when $\langle \hat{n}_{i\uparrow} \rangle \neq \langle \hat{n}_{i\downarrow} \rangle$.

It is well-known that the effective Hamiltonian is diagonalized by applying the Bogoliubov-Valatin transformation [4]

$$\begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow}^\dagger \end{pmatrix} = \sum_\nu \begin{pmatrix} u_\nu(i) & -v_\nu^*(i) \\ v_\nu(i) & u_\nu^*(i) \end{pmatrix} \begin{pmatrix} \gamma_{\nu\uparrow} \\ \gamma_{\nu\downarrow}^\dagger \end{pmatrix}, \quad (5)$$

where $u_\nu(i)$ and $v_\nu(i)$ are the particle-like and hole-like quasiparticle (bogolon) wavefunctions, and $\gamma_{\nu\sigma}$ and $\gamma_{\nu\sigma}^\dagger$ are the annihilation and creation operators for bogolon state ν, σ . The quasiparticle

90 wave functions obey the Bogoliubov-de Gennes equations

$$91 \quad \sum_j h_{ij} u_\nu(j) + \Delta(i) v_\nu(i) = \epsilon_\nu u_\nu(i), \quad (6a)$$

$$92 \quad \Delta^*(i) u_\nu(i) - \sum_j h_{ij}^* v_\nu(j) = \epsilon_\nu v_\nu(i), \quad (6b)$$

93 where ϵ_ν is the quasiparticle energy. As a result of the diagonalization, one obtains

$$94 \quad \langle \gamma_{\nu\uparrow}^\dagger \gamma_{\nu\uparrow} \rangle = \langle \gamma_{\nu\downarrow}^\dagger \gamma_{\nu\downarrow} \rangle = f_\nu, \quad \langle \gamma_{\nu\uparrow} \gamma_{\nu\downarrow} \rangle = 0, \quad (7)$$

95 where f_ν is the Fermi-Dirac distribution of bogolons with the quasiparticle energy ϵ_ν . The quan-
 96 tum number ν enumerates the quasiparticle states in the ascending energy order. In our study, we
 97 employ the open boundary conditions [5,8,22] for the quasiparticle wavefunctions $u_\nu(i)$ and $v_\nu(i)$,
 98 which corresponds to the physical scenario of electrons being quantum-confined within the chain.
 99 When using Eqs. (5) and (7), the self-consistency relations given by Eq. (4) are represented in the
 100 form

$$101 \quad \Delta(i) = g \sum_\nu u_\nu(i) v_\nu^*(i) [1 - 2f_\nu], \quad U_{\text{HF}}(i) = -g \sum_\nu [|u_\nu(i)|^2 f_\nu + |v_\nu(i)|^2 (1 - f_\nu)]. \quad (8)$$

102 In addition, the averaged occupation number of electrons is given by

$$103 \quad n_e = \frac{1}{N} \sum_{i\sigma} \langle \hat{n}_{i\sigma} \rangle = 2 \sum_{i\nu} [f_\nu |u_\nu(i)|^2 + (1 - f_\nu) |v_\nu(i)|^2], \quad (9)$$

104 which defines the chemical potential μ . The summation in Eqs. (8) and (9) is over the quasiparticle
 105 species with the positive energies. In addition, the summation in $\Delta(i)$ is limited to the states in the
 106 Debye window around the Fermi level, i.e. $0 \leq \epsilon_\nu \leq \hbar\omega_D$. However, in the current study, we
 107 assume $\hbar\omega_D$ is much larger than the half-bandwidth. This assumption renders the Debye energy
 108 constraint ineffective, as all solutions of the BdG equations with positive quasiparticle energies
 109 consequently fall within the Debye window.

110 The self-consistent calculation procedure follows the same protocol as for the periodic Hubbard
 111 model. First, we solve the BdG equations (6) using an initial guess for μ , $\Delta(i)$, and $U_{\text{HF}}(i)$. Sec-
 112 ond, using the resulting quasiparticle energies and wave functions, we compute new values for $\Delta(i)$
 113 and $U_{\text{HF}}(i)$ from Eq. (8). Third, we adjust μ to achieve the desired average occupation number n_e
 114 from Eq. (9). The new values of μ , $\Delta(i)$, and $U_{\text{HF}}(i)$ are then reinserted into the BdG equations,
 115 and the entire procedure is repeated until convergence is achieved. The calculation is considered
 116 converged when the relative changes in the order parameter and the HF field are below 10^{-7} .
 117 To model quasicrystal superconducting properties, as the first step, we consider a finite Fibonacci
 118 sequence (Fibonacci approximant) S_n , with n being the characteristic sequence number [15]. This
 119 is a sequence of symbols A and B , which is the concatenation of sequences S_{n-1} and S_{n-2} , i.e.,
 120 $S_n = [S_{n-1}, S_{n-2}]$, where $S_1 = [B]$ and $S_2 = [A]$ include the only symbol, see [15]. Based on
 121 this Fibonacci rule, we have $S_3 = [AB]$, $S_4 = [ABA]$, $S_5 = [ABAAB]$, $S_6 = [ABAABABA]$ etc.
 122 The number of symbols in S_n is F_n , and $\{F_1, F_2, F_3, F_4, F_5, \dots\} = \{1, 1, 2, 3, 5, \dots\}$, which are
 123 the Fibonacci numbers. We then map this sequence onto a physical lattice using the off-diagonal
 124 model. Each symbol A or B in the sequence defines the hopping parameter t_A or t_B , respectively,
 125 between adjacent lattice sites. This results in a one-dimensional chain with a total of $N = F_n + 1$
 126 sites, following the well-established off-diagonal formulation of the Fibonacci model [15,19,24,25].
 127 All energy-related quantities – $\Delta(i)$, $U_{\text{HF}}(i)$, μ , T , t_A , and g – are expressed in units of the hopping
 128 parameter t_B . We set $g = 2$ and consider two different values of the Fibonacci sequence index, $n =$
 129 12 and 13, for a more detailed illustration. Furthermore, we investigate two variants of the hopping
 130 amplitudes: $t_A = 0.5$ and $t_A = 1.5$ (in units of t_B). Our calculations are performed away from
 131 half-filling, as this regime was shown to produce a uniform electronic distribution in Fibonacci
 132 chains [22], where the HF potential does not alter superconducting properties. Here, we adopt an
 133 electron density of $n_e = 0.5$. Our conclusions are robust and not sensitive to the specific choice of
 134 these model parameters.

Results and Discussion

Figure 1 shows results of numerically solving the BdG equations in a self-consistent manner for $n = 12$ and $t_A = 1.5$. In this case, $F_{n=12} = 233$ and, so, the number of atomic sites in the chain is $N = 234$. In panel (a), one can see the spatial profile of the order parameter $\Delta(i)$ calculated at zero temperature by taking into account the HF interaction. The order parameter exhibits significant oscillations due to the quasiperiodic character of the system. These oscillations in the Fibonacci approximant with $n = 12$ are connected with the fractal distribution of the condensate in the infinite Fibonacci chain. In agreement with the previous investigation [22], there are three spatial regions with clearly different averages of the order parameter: the left-end domain, the center of the chain, and the right-end region. The order parameter is enhanced up to 0.43 near the left end, while it is reduced to 0.16 near the right end. The average value of $\Delta(i)$ near the chain center (averaging in the interval from $i = 70$ to 170) is 0.28. This feature is related to the presence of the three critical temperatures - the left-end, the right-end, and the center (bulk) superconducting temperature, as reported in paper [22].

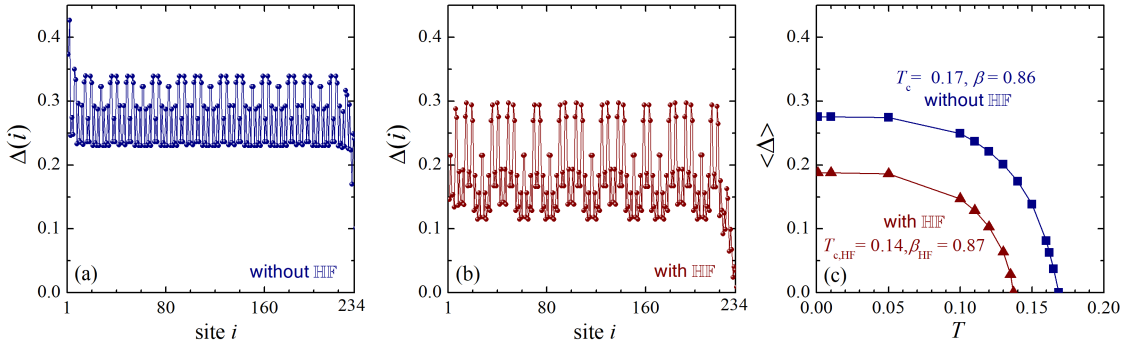


Figure 1: The spatial distribution of the order parameter in the Fibonacci chain with $n = 12$ and $t_A = 1.5$, taking into account the HF potential (a) and neglecting it (b). Panel (c) represents the temperature dependence of the average order parameter in the chain center with (triangles) and without (squares) the HF interaction. The critical temperatures with and without the HF interaction are $T_{c, HF} = 0.14$ and $T_c = 0.17$; the corresponding critical exponents of the averaged order parameter $\beta_{HF} = 0.87$ (with HF) and $\beta = 0.86$ (without HF).

We now examine the zero-temperature order parameter for the system with the HF potential, as shown in Fig. 1(b). The oscillations of the order parameter are immediately apparent and are significantly more pronounced than in the system without the HF potential. In Fig. 1(a), the total

range of the oscillations (from their minimum to their maximum in a given region) is approximately 30% of the average order parameter value, whereas in Fig. 1(b), this reaches nearly 100%. Furthermore, including the HF interaction qualitatively alters the spatial distribution of the condensate near the chain edges. Specifically, the enhancement of the order parameter near the left end, which is clearly present without the HF potential, is suppressed when the HF interaction is included, as seen in Fig. 1(b). Concurrently, the suppression of the order parameter near the left chain end becomes even more pronounced in the system with the HF interaction.

To further analyze the system, Fig. 1(c) shows the temperature dependence of the order parameter averaged over the center of the chain, $\langle \Delta \rangle$ (in the interval from $i = 80$ to 160). The inclusion of the HF interaction results in a significant decrease of both the order parameter in the chain center and the corresponding critical temperature. When the HF potential is included, the zero-temperature order parameter is $\langle \Delta \rangle_{T=0, \text{HF}} = 0.19$, compared to a value of approximately 0.28 without it. The critical temperatures are $T_c = 0.17$ and $T_{c, \text{HF}} = 0.14$, respectively. The ratio $\langle \Delta \rangle_{T=0, \text{HF}} / T_{c, \text{HF}} = 1.36$ is notably smaller than the corresponding ratio without the HF field, $\langle \Delta \rangle_{T=0} / T_c = 1.64$. Furthermore, both values are smaller than the universal BCS prediction of $\Delta(0) / T_c = 1.76$.

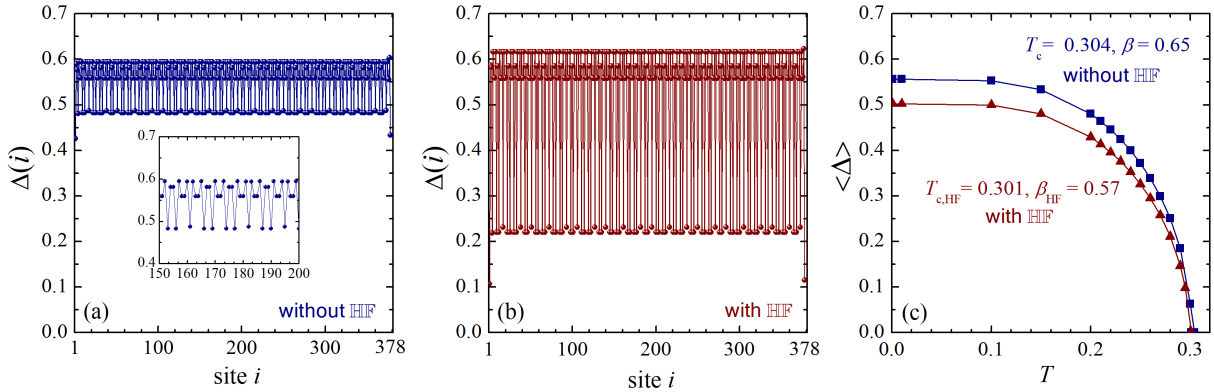


Figure 2: The same as in Figure 1 but for the Fibonacci chain with $n = 13$ and $t_A = 0.5$. Here, the critical temperatures of the systems with and without the HF interaction are only slightly different: $T_c = 0.304$ and $T_{c, \text{HF}} = 0.301$. However, the order-parameter critical exponent for the case with the HF potential, $\beta_{\text{HF}} = 0.57$, is notably smaller than the value of $\beta = 0.65$ for the chain without the HF interaction.

Finally, using the temperature-dependent data from Fig. 1(c), we calculate the critical exponent β

168 of the order parameter near the critical temperature:

$$169 \quad \langle \Delta \rangle \propto \tau^\beta, \quad (10)$$

170 where $\tau = 1 - T/T_c$ (or $T_{c,\text{HF}}$ for the chain with the HF interaction). Our analysis shows that
171 $\beta = 0.86$ without the HF field, while $\beta_{\text{HF}} = 0.87$ with it. These values are only slightly differ-
172 ent. However, both of them are significantly larger than the BCS order-parameter critical exponent
173 of 0.5. This observation agrees with previous expectations [26,27] of power-law scaling with non-
174 standard exponents for thermodynamic properties of superconducting quasicrystals near T_c . Here
175 we note an early investigation of another quasiperiodic one-dimensional quantum system, namely,
176 the Ising model on a transverse applied field, that study the phase transition occurring in its cou-
177 pling parameter and related critical indexes. [28].

178 For a further illustration, we consider a numerical solution of the BdG equations for a different
179 parametric set, i.e., for $n = 13$ and $t_A = 0.5$ (other microscopic parameters are the same). In
180 this case $F_{n=13} = 377$ and $N = 378$. The corresponding results are shown in Fig. 2. Panels (a)
181 and (b) of this figure demonstrate the order-parameter spatial distribution without (a) and with the
182 HF interaction (b), as calculated for zero temperature. Similarly to the previous case, one observes
183 significant oscillations of the order parameter, and these oscillations are notably enhanced when in-
184 cluding the HF interaction. The maximal difference between the order-parameter minima and max-
185 ima in Fig. 2(a) is about 20% of the spatially averaged order parameter. In Fig. 2(b) this becomes
186 about 60%.

187 However, despite a significant enhancement of the spatial oscillations of the order parameter in the
188 presence of the HF interaction, its spatially averaged value (in the interval from $i = 140$ to 240)
189 does not exhibit a significant drop, reducing by less than 10%. Even a smaller difference is ob-
190 served between the two critical temperatures, $T_c = 0.304$ and $T_{c,\text{HF}} = 0.301$. In addition, for the
191 present case, we have $\langle \Delta \rangle_{T=0,\text{HF}}/T_{c,\text{HF}} = 1.82$, which is larger than the corresponding ratio without
192 the HF field, $\langle \Delta \rangle_{T=0}/T_c = 1.67$. In this case, the BCS value of the ratio of the zero-temperature
193 order parameter to the critical temperature 1.76 is between the two values calculated for the Fi-

194 bonacci approximant. Finally, the critical order-parameter exponents for the system with the HF
195 interaction $\beta_{\text{HF}} = 0.57$ and without $\beta = 0.65$ are still larger than the corresponding BCS value 0.5,
196 yet this difference is less pronounced than for the previous parametric choice.

197 **Conclusions**

198 Based on a numerical solution of the BdG equations for superconducting Fibonacci chains, we
199 demonstrate that including the HF interaction significantly enhances the spatial oscillations of the
200 order parameter when the averaged electron density is beyond the half-filling regime. These os-
201 cillations are a direct consequence of the system's quasiperiodicity, reflecting a general feature of
202 superconducting quasicrystals. The enhancement of these oscillations leads to a reduction of the
203 critical temperature, which can be pronounced depending on the model's microscopic parameters.
204 We also find that the critical exponent β of the order parameter differs significantly from that of a
205 uniform BCS condensate. Moreover, the value of β changes when the HF interaction is included.
206 Finally, the ratio of the zero-temperature order parameter to the critical temperature is also sensi-
207 tive to the HF potential and deviates notably from the universal BCS value. Consequently, a rig-
208 orous analysis of the condensate distribution in quasicrystalline superconductors requires a direct
209 comparison of results with and without the HF interaction.
210 Finally, we remark that our results are obtained in the regime beyond the half-filling. The half-
211 filling is the special regime with uniform density of electrons so that the HF field appears to be just
212 a shift of the chemical potential, not altering other thermodynamic quantities, see the discussion in
213 paper [22].

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217 **References**

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