Cooper instability and superconductivity of the Penrose lattice

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Bulk superconductivity (SC) has recently been observed in the Al-Zn-Mg quasicrystal (QC). To settle several fundamental issues of the SC on the QC, we use an attractive Hubbard model to perform a systematic study on the Penrose lattice. The first issue is the Cooper instability of the QC, i.e., no Fermi surface under an infinitesimal attractive interaction. Starting from the two-electron problem outside a filled Fermi sea, we analytically prove that an infinitesimal Hubbard attraction can lead to the Cooper instability as long as the density of the state is nonzero at the Fermi level. The findings provide a basis for the SC on the QC. Our numerical results show that the Cooper pairing always takes place between two time-reversal states, satisfying Anderson’s theorem. On this theorem, we perform a mean-field (MF) study at zero and finite temperatures. The MF study shows that an arbitrarily weak attraction can lead to a pairing order, with the resulting pairing state being well described by the Bardeen-Cooper-Schrieffer theory and the thermal dynamic behaviors being well consistent with the experimental results. The second issue is about the superfluid density on the QC without translational symmetry. Our findings clarify that although the normal state of the system locates at the critical point of the metal-insulator transition, the pairing state exhibits a real SC, carrying finite superfluid density that can be verified by the Meissner effect. This finding is consistent with the experimental results. This study also reveals that the properties of the SC on the Penrose lattice are universal for all QCs.

superconductivity, quasicrystal, cooper instability

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1 Introduction

A quasicrystal (QC) represents a regular-type lattice structure that possesses a certain form of long-range order but lacks translational symmetry [1, 2]. One famous QC structure is the one-dimensional Fibonacci chain composed of a long (L) stick and a short (S) one, created by repeating the substitution of \( L \rightarrow LS \) and \( S \rightarrow L \) [2, 3]. For two- or three-dimensional QCs, hundreds of materials have been found in metal alloys, especially in aluminum alloys [2]. These QCs often have an axis with 5-, 8-, 10-, or 12-fold local symmetric axes, which are forbidden in periodic lattices [1]. Various interesting properties have also been revealed...
about the electron states on the QC, including the magnetic order [4-6], quantum-phase transition and criticality [7-9], strong correlation behavior [10-12], and topological phases [13-16]. Here, we focus on the superconductivity (SC) on the QC [17-20], which has recently caught considerable interests [21-27].

Recently, definite experimental evidence for the SC was revealed in the Al-Zn-Mg QC with fivefold symmetric axes [20]. This evidence, together with those in previous ternary QCs [17, 18] and crystalline approximates [19], have attracted a lot of research interests. Sakai et al. [21] studied the extended-to-localized crossover of Cooper pairs on the Penrose lattice. The pairing state for electrons moving in the quasiperiodic potential of the Ammann-Beenker tiling was studied by the Bogoliubov-de Gennes (BdG) approach [24], wherein conventional SC consistent with the Bardeen-Cooper-Schrieffer (BCS) theory was found. In ref. [27], a new numerical skill was developed to treat the BdG equation associated with the SC of the Penrose lattice. However, there are still a few fundamental issues for the SC on the QC that remain to be settled, which are the focus of the present work.

The first issue is the Cooper instability under an infinitesimal attractive interaction. Generally, on a periodic lattice, a pair of electrons with opposite momenta and spins near the Fermi surface (FS) will be induced by an arbitrarily weak attractive interaction to form a bound state, dubbed as the Cooper pair [28]. Such insight provides a solid basis for the succeeding BCS theory for the SC [29]. In comparison with a pair of isolated electrons in free space, the presence of an FS is the key ingredient for the Cooper instability. Here, in the QC without an FS, will the Cooper instability still be universal for any weak attractive interaction? The second issue is about the superfluid density and Meissner effect [30]. Although the mean-field (MF) calculations here yield a nonzero pairing gap, whether the superconducting phase coherence can survive the disorder-like scattering of the nonperiodic lattice is a problem. Intuitively, one might wonder how a supercurrent can freely flow through the nonperiodic QC lattice, where the momentum is no longer a good quantum number. Actually, there is a basic fact about the transport property on the QC: the normal-state conductivity is critical [31]. That is, it decays with the size in power law and converges to zero in the thermodynamic limit. Hence, a macro electronic system on the QC is at the metal-insulator-transition critical point. This knowledge naturally leads to the following problem: will the Cooper pairing obtained on the QC lead to a real SC with a detectable Meissner effect?

In this paper, we examine the Cooper instability and SC in the negative-U Hubbard model on the Penrose lattice. Our main results lie in the following aspects: first, we study a pair of electrons outside a filled Fermi sea and investigate their ground state under the Hubbard attraction U. Consequently, we analytically prove that an infinitesimal U will lead to a Cooper pairing as long as the density of state (DOS) is nonzero at the Fermi level. This result generalizes the Cooper instability from periodic lattices to QCs, providing the SC basis of QCs. Second, we perform an MF study for the model at zero and finite temperatures. Our MF result at the zero temperature is consistent with that of the two-body problem: an infinitesimal attraction can lead to a nonzero pairing order parameter, as analytically proven. The MF result at the finite temperature suggests that the thermodynamic properties of the pairing state can be well described by the BCS theory and are well consistent with the recent experimental results in the Al-Zn-Mg QC superconductor [20]. Finally, we obtain a nonzero value for the superfluid density of the pairing state, which leads to the real SC with a measurable Meissner effect, also consistent with the experimental results [20].

The remaining part of this work is organized as follows. In sect. 2, we introduce the attractive-U Hubbard model on the Penrose lattice. In sect. 3, we study the two-electron problem outside the Fermi sea to show that an infinitesimal attractive interaction can lead to the Cooper instability. In sect. 4, we provide our MF results at zero and finite temperatures to show that the SC of the QC can be well described by the BCS theory. In sect. 5, the superfluid density is studied, where we show that the pairing state obtained is a real SC with a finite superfluid density. Lastly, in sect. 6, a brief conclusion is summarized with some discussion.

### 2 Model

The Penrose lattice represents a two-dimensional QC (see Figure 1(a)), whose original point is the center of the five-fold rotational symmetry. The parameter R gives the radius of the considered region. There are two types of rhombic tilings in the lattice, as shown in Figure 1(b): the fat one with an interior angle of 72° and the slender one with an interior angle of 36°. They have the same side length a. As R increases, the number N of the sites enclosed in the circular region with a radius R is roughly proportional to the square of R, i.e., \( N \approx (\sqrt{5} - 1) \pi R^2 / a^2 \). In this work, three cases, i.e., \( R/a = 40, 60, \) and 80, are adopted to show the size dependence, whose site numbers are \( N = 6171, 13926, \) and 24751, respectively.

Here, we consider the following TB model:

\[
H_{TB} = - \sum_{i,j,\sigma} t_{ij} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} - \mu \sum_{i,\sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma},
\]

where \( \hat{c}^\dagger_{i\sigma} (\hat{c}_{i\sigma}) \) is the creation (annihilation) operator of the
electron with spin $\sigma$ on the $i$-th site and $\mu_k$ is the chemical potential. The hopping integral $t_{ij}$ between the $i$-th and $j$-th sites reads

$$t_{ij} = e^{-|r_i - r_j|/a} - \delta_{ij}, \quad (2)$$

which implies a zero on-site energy, i.e., $t_{ii} = 0$. Note that the shortest distance between any two sites on this lattice is equal to $(\sqrt{5} - 1)/2 \approx 0.618a$ (see Figure 1(b)). Through a direct diagonalization, $H_{TB}$ in eq. (1) can be rewritten as:

$$H_{TB} = \sum_{m,\sigma} E_m \hat{e}_{m\sigma}^{\dagger} \hat{e}_{m\sigma}, \quad (3)$$

where $E_m \equiv E_m - \mu_k$ represents the energy of the state $|m\sigma\rangle$ relative to the chemical potential $\mu_k$. The creation operator of $\hat{c}_{m\sigma}^{\dagger}$ is defined as:

$$\hat{c}_{m\sigma}^{\dagger} = \sum_{\sigma'} \xi_{m\sigma'} \hat{c}_{m\sigma'}, \quad (4)$$

where $\xi_{m\sigma} \in R$ provides the spatial part of the wave function of the state $|m\sigma\rangle$, satisfying

$$\sum_{\sigma} \xi_{m\sigma}^2 = \sum_{m} \xi_{m\sigma}^2 = 1. \quad (5)$$

As shown in the inset of Figure 1(c), the DOS in the low-filling-fraction region is small and possesses self-similarity, while it sharply increases with the enhancement of the filling fraction. This character is also observed from the integrated DOS, i.e., the red solid line in Figure 1(c). Such a doping dependence of the DOS suggests that the SC is more favored in the high-filling region than in the low-filling region. As examples, we take three chemical potentials of $\mu_k = 0.19$, 0.45, and 0.50 without loss of generality in the following study. Their filling fractions are $\delta \approx 0.3$, 0.5, and 0.6 with the corresponding DOSs to be $\rho \approx 0.45$, 1.40, and 2.53, respectively.

To study the SC on the Penrose lattice, the following attractive Hubbard interaction is adopted:

$$H_{int} = -U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \quad (6)$$

where $\hat{n}_{i\sigma} \equiv \hat{c}_{i\sigma}^{\dagger} \hat{c}_{i\sigma}$. This Hamiltonian can be transformed to the eigen-basis representation of $H_{TB}$ as:

$$H_{int} = -U \sum_{mn,\sigma \sigma'} f_{mn,\sigma \sigma'} \xi_{m \sigma}^\dagger \xi_{n \sigma'}^\dagger \xi_{m \sigma} \xi_{n \sigma'}, \quad (7)$$

where

$$f_{mn,\sigma \sigma'} \equiv \sum_{\sigma''} \xi_{mn,\sigma''}^\dagger \xi_{mn,\sigma''}. \quad (8)$$

The total Hamiltonian of the system reads

$$H = H_{TB} + H_{int}, \quad (9)$$

which sets our start point.

### 3 Cooper instability

The Cooper instability [28] is the basis of the BCS theory [29] on periodic lattices. This instability describes the fate of two electrons with arbitrarily weak attractive interactions on the background of a filled Fermi sea. That is, their ground state is a bound state with the total momenta and spin as zero and with an energy lower than zero (relative to the Fermi level) by a finite gap. Such a bound state is called the Cooper pair. The condensation of Cooper pairs leads to the SC [29].

In comparison with the case of two electrons in free space, the presence of an FS as a boundary of the filled Fermi sea is the key ingredient for the Cooper instability on a periodic lattice. However, for the Penrose lattice where the momentum is no longer a good quantum number, the Cooper instability

![Figure 1](image.png)

*Figure 1* (Color online) (a) Penrose lattice and (b) its ingredients: fat and slimmer rhombuses with interior angles of 72° and 36°, respectively. They have the same side length $a$. The original point $O$ in (a) is the center of the fivefold rotational symmetry and $R$ denotes the radius of the considered region. (c) DOS (left axis) and corresponding integrated DOS (right axis). The inset presents the details of the DOS in the low-filling region.
under an infinitesimal attractive interaction is still an issue to be investigated, which is the focus of this section.

Let us consider two electrons with opposite spins in the background of a filled Fermi sea. The Pauli exclusion principle requires that the single-particle energy of each electron should be higher than the Fermi energy. As a result, the candidate ground-state wave function of this two-electron problem should take the following formula:

$$\langle \Psi_A \rangle = \sum_{m, n} a_{mn} \langle \hat{\mathbf{r}}_m \hat{\mathbf{r}}_n \rangle |\mathbf{FS}\rangle,$$

(10)

where $|\mathbf{FS}\rangle$ represents the filled Fermi-sea state, and the set of real coefficients $(a_{mn})$ satisfies the normalized condition:

$$\sum_{m, n} a_{mn}^2 = 1.$$

(11)

The sum condition $\hat{\epsilon}_{m, n} > 0$ denotes that $\hat{\epsilon}_m$ and $\hat{\epsilon}_n$ are both larger than zero. The problem now is the minimization of the expectation value of the Hamiltonian $(9)$ under the trial state in eq. (10), where the normalized $(a_{mn})$ are the variational parameters.

In the following, we consider a special case of the wave function (10) that satisfies the condition $a_{mn} = a_{mn} \hat{\epsilon}_{mn}$, i.e.,

$$\langle \Psi_C \rangle = \sum_m a_m \langle \hat{\mathbf{r}}_m \rangle |\mathbf{FS}\rangle,$$

(12)

with the constraint

$$\sum_m a_m^2 = 1.$$

(13)

We provide analytical proof that for any weak $U > 0$, one can always find a two-electron state described by eq. (12) with the constraint (13). Its energy is below zero by a finite gap in the thermodynamic limit as long as the DOS at the Fermi level is nonzero, suggesting the formation of a two-electron bound state. This two-electron bound state, each up-spin single-electron state labeled by $|m\rangle$ can only be paired with its TR partner, i.e., the down-spin state labeled by $|m\rangle$. Such a pairing satisfies Anderson’s theorem [32]. If the minimized energy among this special class of states in eq. (12) is already lower than zero, then that among the more general class in eq. (10) should not be higher.

The variational energy, i.e., the expectation value of the Hamiltonian $(9)$ in the two-electron trial state (see eq. (12)), can be written as:

$$E_C = 2 \sum_m \frac{\hat{\epsilon}_m}{N} \hat{\epsilon}_m - U \sum_{m, n} \frac{\hat{\epsilon}_{mn} a_m a_n}{\langle \hat{\mathbf{r}}_{n} \rangle}.$$

(14)

with

$$f_{mn} \equiv N \sum_i \frac{\hat{\epsilon}_{i, mn}}{\langle \hat{\mathbf{r}}_{i} \rangle} = f_{nm}.$$

(15)

Minimizing $E_C$ under the constraint (13) leads to the following self-consistent equation for $(a_m)$:

$$\frac{\partial}{\partial a_m} \left( \frac{\hat{\epsilon}_m}{N} \sum_n f_{mn} a_n a_n - U \sum_{m, n} \frac{\hat{\epsilon}_{mn} a_m a_n}{\langle \hat{\mathbf{r}}_{n} \rangle} \right) = 0,$$

(16)

that is,

$$2a_m \hat{\epsilon}_m - \frac{\hat{\epsilon}_m}{N} \sum_n f_{mn} a_n = \lambda a_m.$$

(17)

The Lagrangian multiplier $\lambda$ is just equal to $E_C$ when eq. (16) or (17) is satisfied because

$$\lambda = \lambda \sum_m a_m^2 = \sum_m 2a_m^2 \hat{\epsilon}_m - \frac{\hat{\epsilon}_m}{N} \sum_n f_{mn} a_n a_n = E_C.$$

(18)

In the following, we prove that for an arbitrarily weak $U > 0$, there always exists a nonzero solution $(a_m)$ satisfying eq. (17) with finite $\lambda = E_C < 0$ in the thermodynamic limit as long as the DOS at the Fermi level is nonzero. This condition suggests the formation of a bound state with a finite energy gap, i.e., the Cooper pair. For this purpose, we rewrite eq. (17) into the following form:

$$A_m = U \sum_n F_{mn}^c A_n,$$

(19)

where

$$A_m \equiv a_m \sqrt{2 \hat{\epsilon}_m - \lambda},$$

(20)

$$F_{mn}^c \equiv \frac{1}{N} \frac{f_{mn}}{\sqrt{(2 \hat{\epsilon}_n - \lambda)(2 \hat{\epsilon}_m - \lambda)}}.$$  

(21)

Here, only the possible candidate states with $\lambda = E_C < 0$ are considered. The equation (19) takes the form of the eigenvalue problem of the Hermitian matrix $F^c$, whose elements are $F_{mn}^c$. The largest eigenvalue of $F^c$ attains $\lambda$, and the corresponding eigenvector $\lambda$ determines $(a_m)$ through eq. (20). Below, we prove that the largest positive eigenvalue of $F^c$ diverges in the limit of $\lambda \rightarrow 0^-$. Therefore, by properly tuning $\lambda$ to a finite negative value, the largest positive eigenvalue of $F^c$ can certainly attain $1/2$ for any weak $U$, suggesting the formation of a Cooper pair.

Let us consider the following column vector:

$$\psi = \frac{1}{\sqrt{Z_\psi}} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{2 \hat{\epsilon}_m - \lambda}} \\ \frac{1}{\sqrt{2 \hat{\epsilon}_n - \lambda}} \end{pmatrix}^T,$$

(22)

with

$$Z_\psi = \sum_m \frac{1}{2 \hat{\epsilon}_m - \lambda}.$$  

(23)
Taking $\psi$ as a quantum state $|\psi\rangle$ and $\hat{F}^C$ as an operator $\hat{F}^C$, we calculate the expectation value of $\hat{F}^C$ in the state $|\psi\rangle$. The expectation value $\langle \hat{F}^C \rangle$ is given by

$$\langle \hat{F}^C \rangle = \frac{1}{N\bar{z}_\psi} \sum_{mn} \frac{f_{mn}}{(2E_m - \lambda)(2E_n - \lambda)}.$$  \hspace{1cm} (24)

Substituting eq. (15) into the above formula, we get

$$\langle \hat{F}^C \rangle = \frac{1}{N\bar{z}_\psi} \sum_{m} \frac{N\sum_i \xi_{im}^2 \xi_{im}^2}{(2E_m - \lambda)}$$  

$$= \frac{1}{N\bar{z}_\psi} \sum_{m} \frac{(\sum_i \xi_{im}^2 \xi_{im}^2)}{2E_m - \lambda} = \frac{1}{N\bar{z}_\psi} \sum_{m} \frac{1}{2E_m - \lambda} \sum_{i} \xi_{im}^2 \xi_{im}^2.$$  

$$\geq \frac{1}{N\bar{z}_\psi} \left( \sum_{m} \frac{1}{2E_m - \lambda} \right)^2 = \frac{1}{N\bar{z}_\psi} \left( \sum_{m} \frac{1}{2E_m - \lambda} \right)^2,$$  \hspace{1cm} (25)

where the Cauchy’s inequality is used. Substituting eqs. (5) and (23) into the above formula, we have

$$\langle \hat{F}^C \rangle \geq \frac{e(0)}{2E - \lambda} \int_0^\infty \frac{1}{2E - \lambda} \, d\varepsilon.$$  \hspace{1cm} (26)

Here, $\varepsilon$ represents the DOS. In the limit of $\lambda \to 0^-$, we have

$$\langle \hat{F}^C \rangle \geq \frac{e(0)}{2E - \lambda} \rightarrow +\infty,$$  \hspace{1cm} (27)

as long as the DOS at the Fermi level, $e(0)$, is nonzero.

Because the expectation value $\langle \hat{F}^C \rangle$ of the Hermitian operator $\hat{F}^C$ in the constructed state $|\psi\rangle$ diverges in the limit of $\lambda \to 0^-$, the largest positive eigenvalue of $\hat{F}^C$, which should be no less than $\langle \hat{F}^C \rangle$, must also diverge in this limit. Therefore, for weak $U$, there always exists a finite negative $\lambda$ dictating that the largest eigenvalue of $\hat{F}^C$ attains $\frac{1}{\bar{z}_\psi}$, satisfying eq. (19). The parameter $\lambda = E_C < 0$ is the minimized energy among the special variational class of states described by eq. (12). Thus, the minimized energy among the more general variational class of states described by eq. (10), which should be no higher than $\lambda$, is also negative. The single-particle state $|m, n\rangle$ on the Penrose lattice is critical [33], instead of localized. Hence, to make the energy of the state (10) negative, it should be a two-electron bound state, i.e., a Cooper pair. To this point, we have proven that an infinitesimal attractive Hubbard interaction can lead to the Cooper instability on the QC once the DOS at the Fermi level is finite.

The DOS of the electron states on a QC exhibits a fractal character [33]. Concretely, the DOS curve is singular smooth: on the one hand, it contains a singular part manifested as sharp infinite-height peaks here and there. On the other hand, the integrated DOS curve is smooth, suggesting that the energy-level points for the sharp DOS peaks form no measure. Such a fractal character of the DOS leads to pseudogaps and sharp peaks here and there in the DOS curve. In addition, the DOS curve can contain a smooth part superposed on the singular part [33], which leads to a finite DOS background. Therefore, the pseudogaps at most places in the DOS curve are not real gaps, and the DOS there is nonzero. Due to the singular part in the DOS curve, the DOS is not mathematically rigorously defined. However, on the above proof, we only require that the averaged DOS in an infinitesimal energy shell near the Fermi level is larger than zero, as embodied in eq. (27), which is satisfied at most places in the DOS spectrum. Of course, under such a singular energy dependence of the DOS spectrum, the properties of the SC, including the $T_c$, pairing gap, and superfluid density, will exhibit very sensitive dependence on the filling fraction. However, in real materials, the presence of weak randomness can largely smear out the singular part of the DOS spectrum [34]. This condition leads to a much smoother filling-fraction dependence of the superconducting properties of the system. In the experiment on the Al-Zn-Mg QC [20], the linear dependence of the specific heat with low temperatures suggests a finite DOS at the Fermi level, which thus satisfies the condition required here for the Cooper instability.

To obtain the optimized Cooper-pair wave function, we consider the general variational state in eq. (10). The expectation value of the Hamiltonian (9) in this state reads,

$$E_A = \sum_{mn} a_{mn}^2 (\varepsilon_m + \varepsilon_n) - \frac{U}{N} \sum_{m,n} f_{mn,n'0} a_{mn} a_{mn,n'0}. \hspace{1cm} (28)$$

The sum condition $\varepsilon_{m,n,n',0} > 0$ denotes $\varepsilon_m$, $\varepsilon_n$, $\varepsilon_{n'}$, and $\varepsilon_{0'}$, are all larger than zero. By minimizing $E_A$ under the constraint (11),

$$\frac{\partial}{\partial a_{mn}} \left( \sum_{mn} a_{mn}^2 (\varepsilon_m + \varepsilon_n) - \frac{U}{N} \sum_{m,n} f_{mn,n'0} a_{mn} a_{mn,n'0} \right) = 0,$$  \hspace{1cm} (29)

leads to the following self-consistent equation for the set of $(a_{mn})$,

$$(\varepsilon_m + \varepsilon_n) a_{mn} - \frac{U}{N} \sum_{n',n'0} f_{mn,n'0} a_{mn,n'} = \lambda a_{mn}.$$  \hspace{1cm} (30)
Here, again, the Lagrange multiplier $\lambda$ is equal to $E_{\alpha}$ when the self-consistent equation is satisfied. Equation (30) takes the form of the eigenvalue problem of the Hermitian matrix $F_{\alpha,m,n,m',n'}$:

$$\sum_{m,n} F_{\alpha,m,n;m',n'} a_{m,n} = \lambda a_{m,n}$$

(31)

with

$$F_{\alpha,m,n;m',n'} = (E_m + E_n) \delta_{m,n} - \frac{U}{N} \delta_{m,n;m',n'}$$

(32)

which can be solved numerically.

Considering 100 states above the Fermi level, the numerical solution of eq. (31) is obtained. For each doping and $U$, the ground state of the two-body system is a bound state, whose wave function is plotted in Figure 2(a)-(c) for the three doping levels with $\mu = 0.19, 0.45,$ and 0.5, where the $x$ and $y$ axes represent $m$ and $n$ and the color represents $a_{m,n}$. From Figure 2(a)-(c), for each $m$, we have $|a_{m,n}| > |a_{n,m}|$. Such a solution makes the general wave function (10) decay to the special one (12), which satisfies Anderson’s theorem. In a small energy scale, the fractal structure of the DOS, together with some finite-size effect, is responsible for the nonmonotonic dependence of the pairing amplitudes on the index of levels or energy (levels are arranged in the ascending order of energy). When the energy scale is large enough, the pairing magnitudes decay with the index of levels in a whole (see Figure 2(a)-(c)), suggesting that the Cooper pairing is mainly contributed by the states near the Fermi level. This is also reflected in the increase in the length of the red line-shape region from Figure 2(a)-(c). This result is attributed to the energy range that covers the considered 100 states, which decreases for increasing DOS. These results suggest that the Cooper pairing only takes place between the two TR states near the Fermi level, satisfying Anderson’s theorem [32].

We further investigate the binding energy $E_B \equiv |E_A| = |E_C|$ of the Cooper pair, i.e., the bound-state gap, which reflects the strength of the pairing. Figure 2(d)-(f) show $E_B$ as a function of $U$, where the vertical axis adopts the logarithmic coordinate for $E_B$ while the horizontal one adopts the reciprocal coordinate for $-U$. From Figure 2(d)-(f), $E_B$ reasonably enhances with the enhancement of $U$. We focus on the regimes framed in the blue parallelogram in Figure 2(d)-(f). Here, on the one hand, the binding energy is much larger than the finite-size level spacing, so the thermodynamic-limit behavior is shown. On the other hand, the Hubbard-$U$ is not so strong. Consequently, in this regime, $\ln(E_B)$ linearly depends on $-\frac{1}{U}$, suggesting that

$$E_B \propto \exp \left[ \frac{1}{\alpha U} \right].$$

(33)

This result is consistent with the BCS theory for the periodic lattice [28,29]. In the latter case, we further have $\alpha \propto \rho(0)$. This relation is qualitatively consistent with our results here. The slope of the linear-dependence relation between $\ln(E_B)$ and $-\frac{1}{U}$ shown in Figure 2(d)-(f) decreases with the doping and hence $\rho(0)$. However, due to the finite size adopted in our calculations, we cannot quantitatively check this relation.

4 MF results

On the above, we prove that an infinitesimal Hubbard interaction on the Penrose lattice would lead to the Cooper instability, which provides the basis of the SC in the system. In this section, we perform an MF study for the system at zero and finite temperatures. Our zero-temperature MF study further confirms the above results: an infinitesimal Hubbard attraction would lead to a pairing order. Our finite-temperature results reveal that the thermal dynamic behavior of the superconducting state on the QC can be well described by the BCS theory.

4.1 Zero-temperature results

The last section shows that the Cooper pairing formed by the
two electrons outside the Fermi sea obeys Anderson’s theorem. That is, the single-particle state $|m\uparrow\rangle$ can only be paired with its TR partner $|m\downarrow\rangle$. Accordingly, the MF state with the order parameter $\langle c_{m\uparrow}^c c_{m\downarrow}^c \rangle$ naturally emerges as the result of the condensation of the Cooper pairs. The MF decomposition of the Hamiltonian (9) in this channel leads to the following BdG Hamiltonian:

$$H_{BdG} = \sum_{m} \tilde{e}_m c_{m\uparrow}^c c_{m\downarrow} - \sum_{m} \langle \Delta_m c_{m\uparrow}^c c_{m\downarrow}^c + \text{h.c.} \rangle + \text{const}. \quad (34)$$

where the pairing order parameters of $\langle \Delta_m \rangle$ are defined as:

$$\Delta_m = \frac{U}{N} \sum_{n} f_{mn} \langle \hat{c}_{m\uparrow} \hat{c}_{n\uparrow} \rangle. \quad (35)$$

Using the Bogoliubov transformation,

$$\hat{c}_{m\uparrow} = u_m \hat{\gamma}_{m\uparrow} + v_m \hat{\gamma}_{m\downarrow}, \quad (36a)$$

$$\hat{c}_{m\downarrow} = u_m \hat{\gamma}_{m\downarrow} - v_m \hat{\gamma}_{m\uparrow}. \quad (36b)$$

the BdG Hamiltonian can be diagonalized with the Bogoliubov pairing coherence factors:

$$u_m = \sqrt{\frac{1}{2} \left( 1 + \frac{\tilde{e}_m}{E_m} \right)}, \quad v_m = \text{sgn}(\Delta_m) \sqrt{\frac{1}{2} \left( 1 - \frac{\tilde{e}_m}{E_m} \right)},$$

with

$$E_m = \sqrt{\tilde{e}_m^2 + \Delta_m^2}. \quad (38)$$

Substituting eq. (36) into eq. (35), we have

$$\Delta_m = \frac{U}{N} \sum_{n} f_{mn} u_m v_n \left( 1 - \langle \hat{\gamma}_{m\uparrow} \hat{\gamma}_{m\downarrow} \rangle - \langle \hat{\gamma}_{m\downarrow} \hat{\gamma}_{m\uparrow} \rangle \right). \quad (39)$$

At zero temperature, the above equation turns into the following self-consistent one for $\langle \Delta_m \rangle$:

$$\Delta_m = \frac{U}{N} \sum_{n} f_{mn} \frac{\Delta_n}{2 \sqrt{E_n^2 + |\Delta_n|^2}}. \quad (40)$$

With the same approach adopted in the last section, we can prove that an arbitrarily weak $U$ can lead to finite values of $\langle \Delta_m \rangle$ as long as the DOS at the Fermi level is nonzero. To show this, we first transform eq. (40) into

$$\hat{\Delta}_m = U \sum_{n} F_{mn} \Delta_n, \quad (41)$$

with

$$F_{mn} = \frac{\Delta_m}{\left( \tilde{e}_m^2 + |\Delta_m|^2 \right)^{1/2}}, \quad (42)$$

$$F_{mn} = \frac{f_{mn}}{2N \left( \tilde{e}_n^2 + |\Delta_n|^2 \right)^{1/2}}. \quad (43)$$

Again, eq. (41) takes the form of the eigenvalue problem of the Hermitian matrix $F^M$, wherein the largest eigenvalue of $F^M$ attains $\frac{1}{\Delta M}$. For $U \rightarrow 0$, we have $\Delta_m \rightarrow 0$. In this limit, the matrix $F^M$ is just equal to the $F^C$ defined in eq. (21) in the limit of $\Lambda \rightarrow 0$, whose largest eigenvalue has been proven in the last section to diverge. Hence, for any weak $U$, we can always find a group of weak but finite $\langle \Delta_m \rangle$, such that the largest eigenvalue of $F^M$ attains $\frac{1}{\Delta M}$, satisfying eq. (41). Therefore, we have proven here that an infinitesimal Hubbard attraction will lead to the pairing order on the Penrose lattice as long as the DOS at the Fermi level is nonzero.

For a general $U > 0$, the self-consistent gap eq. (40) or equally (41) can be solved numerically using the iterative method. Figure 3(a) shows the maximum SC gap among $\langle \Delta_m \rangle$, i.e., $\Delta_{Max}$, as a function of $U$ at zero temperature for three different system sizes. Similarly, with the results for the two-electron problem provided in Figure 2(d)-(f), the framed regime in Figure 3(a) suggests that for a weak $U$ in the thermal dynamic limit, we have

$$\Delta_{Max} \propto \exp \left[ -\frac{1}{\sigma U} \right]. \quad (44)$$

consistent with the BCS theory [29]. Physically, we should have $\sigma \propto \rho(0)$, which could be tested by large lattices. Because $\Delta_m$ in eq. (35) is a sum of the $\langle \hat{c}_{m\uparrow} \hat{c}_{m\downarrow} \rangle$ for all levels, rather than just $\langle \hat{c}_{m\uparrow} \hat{c}_{m\downarrow} \rangle$, the maximum gap $\Delta_{Max}$ and the

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**Figure 3** (Color online) (a) Maximum pairing gap $\Delta_{Max}$ as a function of $U$. The horizontal and vertical axes are reciprocal for $-U$ and logarithmic for $\Delta_{Max}$, respectively. (b) Real-space distribution of the pairing gap $\Delta_{s}$, (c), (d) Tunneled spectra $|D(\omega)|$ in the superconducting ground state for two different $U$. All the adopted parameters are shown in each panel.
minimum one $\Delta_{\text{Min}}$ are in the same order of magnitude (see Figure 4(a) and (b)). In Figure 3(b), the real-space distribution of the pairing gap function $\Delta_i$ is shown, which reads as:

$$\Delta_i = \sum_{m} \Delta_m e^{i \phi_{m}}. \quad (45)$$

The fivefold symmetric pattern illustrated in Figure 3(b) is consistent with the $\pi$-wave pairing symmetry.

The SC gap can be measured using the tunneling spectrum, provided as:

$$D(\omega) \equiv -\text{Im} \sum_{m} \left( \frac{\alpha^2}{\omega - E_m + i0^+} + \frac{\nu^2}{\omega + E_m + i0^+} \right). \quad (46)$$

The $D(\omega)$ for $U = 0.1$ and $U = 0.05$ are plotted in Figure 3(c) and (d), respectively. The clear U-shape curves reflect the full-gap character of the pairing state.

4.2 Finite temperature

At the finite temperature $T$, by substituting

$$\langle \hat{\gamma}_{m\uparrow}^\dagger \hat{\gamma}_{m\downarrow} \rangle = \langle \hat{\gamma}_{m\downarrow}^\dagger \hat{\gamma}_{m\uparrow} \rangle = \frac{1}{\cosh \frac{E_m}{k_B T} + 1} \quad (47)$$

into eq. (39), we obtain the self-consistent equations for $\Delta_m$ as follows:

$$\Delta_m = \frac{U}{N} \sum_n f_{mn} \frac{\Delta_n}{2 \sqrt{E_n^2 + \Delta_n^2}} \times \tanh \left( \frac{1}{2} \frac{E_n}{k_B T} \right). \quad (48)$$

Here, $k_B$ is the Boltzmann constant. This set of equations are solved numerically using the iteration approach. The maximum gap $\Delta_{\text{Max}}$ and minimum one $\Delta_{\text{Min}}$ as the function of $T$ for three different lattice sizes with $R = 40$, 60, and 80 are shown in Figure 4(a) and (b) for $U = 0.1$ and 0.05, respectively. $\Delta_{\text{Max}}$ and $\Delta_{\text{Min}}$ decrease with $T$ until at a superconducting critical temperature $T_c$, at which both drop to zero. For the case of $U = 0.05$ shown in Figure 4(b), $T_c$ exhibits an obvious size dependence, as the small pairing gap in this case is not far from the finite-size level spacing. The temperature dependence of $\Delta_{\text{Max}}$ and $\Delta_{\text{Min}}$ near $T = 0$ and $T = T_c$ is consistent with the BCS theory for periodic lattices [29]. Particularly, our detailed analysis suggests that $\Delta_{\text{Max}}$ and $\Delta_{\text{Min}}$ scale with $(T_c - T)^{\frac{1}{2}}$ for $T$ slightly lower than $T_c$. Such a temperature-dependent behavior of the pairing gap will lead to an upper critical field $H \propto (T_c - T)$ being well consistent with the experiment of the Al-Zn-Mg QC superconductor [29].

The $U$ dependence of $k_B T_c$ is plotted in Figure 4(c), which also satisfies the similar relation as eqs. (33) and (44).

$$k_B T_c \propto \exp \left[ \frac{-1}{\alpha U} \right]. \quad (49)$$

Varying $U$, the relation between $\Delta_{\text{Max}}$ and $k_B T_c$ is shown in from which we find that $k_B T_c \propto \Delta_{\text{Min}}$ for weak $U$. The situation is similar for $\Delta_{\text{Max}}$. All the temperature-dependent behaviors obtained here are well consistent with those in the BCS theory [29].

To study the thermal dynamic property of the system, especially that of the superconducting phase transition, we calculated the entropy $S$ and specific heat $C_V$, which are formulated as [29]:

$$S = -k_B \frac{2}{N} \sum_{m} \left[ (1 - f_m) \ln(1 - f_m) + f_m \ln f_m \right], \quad (50)$$

$$C_V = (k_B T) \frac{\partial}{\partial (k_B T)} S, \quad (51)$$

where $f_m = \left( 1 + e^{E_m/k_B T} \right)^{-1}$. The temperature dependences of $S$ and $C_V$ for $U = 0.1$ and 0.05 for the three different lattice sizes are shown in Figure 5(a)-(d). From Figure 5(a) and (b), the entropy is continuous at $T_c$, whereas its first-order derivative is discontinuous, which leads to a jump for the corresponding specific heat shown in Figure 5(c) and (d). Such a temperature-dependent behavior of the specific heat is well consistent with the experiment on the Al-Zn-Mg QC superconductor [20]. Figure 5 suggests that the SC transition on the Penrose lattice here is a second-order phase transition, consistent with the BCS theory for periodic lattices [29].

![Figure 4](image-url) (Color online) Maximum gap $\Delta_{\text{Max}}$ and minimum one $\Delta_{\text{Min}}$ as the function of $T$ for three different lattice sizes with $R = 40$, 60, and 80 for (a) $U = 0.1$ and (b) $U = 0.05$. The $U$ dependence of $k_B T_c$ (c) and the relation between $\Delta_{\text{Max}}$ and $k_B T_c$ (d). All the used parameters are shown in each panel.
as the superfluid density, will lead to a real SC with a measurable Meissner effect. Theoretically, the superfluid density reflects the phase rigidity of SC. Assuming a weak uniform $A$, the site-averaged current operator $\hat{j}$ is defined as

$$\hat{j} = -\frac{1}{N} \frac{\partial}{\partial A} H_{\text{TB}}(A),$$

(52)

where $H_{\text{TB}}(A)$ has the form of

$$H_{\text{TB}}(A) = -\sum_{ij,\sigma} t_{ij} e^{i\phi_{ij}} A_{ij} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right).$$

(53)

The vector potential $A$ influences the system by revising the hopping integrals of the tight-binding Hamiltonian. The site-averaged current operator $\hat{j}$ can be separated into

$$\hat{j} = \hat{j}^p - \hat{j}^d$$

(54)

with the site-averaged paramagnetic current operator and diamagnetic one defined as follows:

$$\hat{j}^p = \frac{i}{2N} \sum_{ij,\sigma} t_{ij} r_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.},$$

(55)

$$\hat{j}^d = \frac{1}{2N} \sum_{ij,\sigma} t_{ij} r_{ij} (r_{ij} + A_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}.$$  

(56)

Here, $r_{ij} \equiv r_j - r_i$ denotes the vector pointing from the site $i$ to the site $j$. In a general possibly anisotropic 2D system, the superfluid density $\rho$ should be a $2 \times 2$ tensor. However, due to the $D_5$-point group, it can be proven that $\rho$ is simply a number [35]. Therefore, we are allowed to orientate the vector potential $A$ along the $x$ axis and calculate the $x$-component of the corresponding current $j_x \equiv \langle j_x \rangle$.

The procedure to calculate the expectation value $j_x$ of the current operator $\hat{j}_x$ is as follows: First, we replaced the free-electron term in the BCS-MF Hamiltonian (34) by the $H_{\text{TB}}(A)$ in eq. (53) under a small $A_x$ and keep the pairing term in eq. (34) unchanged. Second, we numerically re-diagonalized the revised Bogoliubov-de Genes MF Hamiltonian to obtain the revised eigenstates and revised Bogoliubov-quasiparticle eigen energies. Finally, we calculated the thermal expectation value $j_x$ of the current operator $\hat{j}_x$ at a given temperature, including those of the diamagnetic and paramagnetic parts provided by eqs. (55) and (56), respectively. The difference between the expectation values of the two parts gives the final value $j_x$.

In Figure 6(a), the responding $-j_x$ toward an imposed weak uniform $A = A_x \epsilon_x$ is shown for two lattices with sizes $R = 40$ and 60 under the open-boundary condition. Here, a linear-response relation is obtained with a positive slope, suggesting that $\rho > 0$. In Figure 6(b), the lattice-size dependence of $\rho$ is shown, which suggests that $\rho$ is saturated to a nonzero value in the thermodynamic limit. Such a nonzero superfluid density leads to a real SC with finite-phase rigidity that can be detected by the Meissner effect. Therefore, a

### 5 Superfluid density

The MF calculations in the last section yield a nonzero pairing gap. However, it is questionable whether a real SC with measurable Meissner effects can be detected. Intuitively, how the supercurrent can freely flow through the nonperiodic QC lattice, where the momentum is no longer a good quantum number, needs to be understood. Generally, the electron transport property on the QC is critical [31]: the normal-state conductivity of the Penrose lattice decays with the size in a power law and converges to zero in the thermodynamic limit. Hence, a macro electronic system on the QC is at the metal-insulator-transition critical point. Therefore, whether such a critical state can be driven to a real SC by attractive electron-electron interactions needs to be clarified. To settle this issue, we should study the superfluid density, whose nonzero value suggests a real SC with a measurable Meissner effect.

The experimental identification of the SC is the Meissner effect. Physically, the Meissner effect is a result of the combination of the universal Maxwell equation and London equation for superconductors [29, 30], i.e., $\langle \hat{j} \rangle = -\rho A$. Here, $A$ represents the weak smooth vector potential imposed on the system, and $\langle \hat{j} \rangle$ represents the expectation value of the current operator $\hat{j}$ as a response of $A$. The nonzero $\rho$, called

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**Figure 5** (Color online) Temperature dependence of the entropy $S(k_a)$ and specific heat $C_v(k_a)$ for $U = 0.1$ (left column) and 0.05 (right column). Three different lattices with sizes $R = 40, 60$, and 80 are studied, and the other parameters are shown on top.
real SC can indeed emerge in the QC system, although the normal state in the QC locates at a metal-insulator-transition critical point. This result is consistent with the experiment of the Al-Zn-Mg superconductor, where the suppression of the SC by the exerted magnetic field just reflects the Meissner effect [20].

The temperature dependences of $\rho_d$, $\rho_p$, and $\rho$ are shown in Figure 6(c) and (d) for $R = 40$ and $R = 60$, respectively. The diamagnetic and paramagnetic superfluid densities are nonzero at a general temperature below $T_c$, and they are unequal. However, when the temperature is above $T_c$, the pairing gap closes, and the obtained diamagnetic and paramagnetic superfluid densities exactly cancel each other to give a zero total superfluid density in the normal state. $\rho_d$ does not obviously change with the temperature, although there is a weak cusp (see the insets) at $T_c$. Instead, $\rho_p$ is obviously enhanced by the temperature. Physically, the enhancement of $\rho_p$ originates from the extra consumption of the superfluid density caused by the Bogoliubov-quasiparticle excitations, which are largely enhanced by the temperature. As a result, the total superfluid density $\rho = \rho_d - \rho_p$ is suppressed by the enhancement of the temperature and vanishes if $T > T_c$, where the SC vanishes too.

6 Discussion and conclusions

The pairing symmetry of the system obtained in this study is a singlet on-site s-wave. Such a pairing symmetry is determined by the on-site attractive character of the interaction part of the negative-$U$ Hubbard model. For a general interaction form, more pairing symmetries are possible, including the singlet or triplet s-wave, $(p_x, p_y)$-wave, $(d_{x^2-y^2}, d_{xy})$-wave, and h-wave pairing symmetries for the Penrose lattice with the $D_5$-point group. The scheme for the classification of the pairing symmetries based on the group theory and the properties of the unconventional pairing states, including the topological pairing states, have been studied in ref. [35].

Essentially, the satisfaction of Anderson’s theorem is crucial for the BCS-like behaviors of the on-site pairing state obtained here. For general pairing states on the QC, such as those driven by repulsive interactions via the Kohn-Luttinger’s mechanism [35], Anderson’s theorem might be broken. As a result, each single-particle state with the state index $m$ can be paired with any other state with index $n$. In such a pairing state, the energy dispersion relation of the Bogoliubov quasiparticles can no longer be described by eq. (38). Generally, no analytical formula is available for the quasiparticle energy. Moreover, the Bogoliubov quasiparticles might, in general, host a gapless spectrum, just like the one in the normal state. The behavior of such a gapless pairing state can be very different from the one presented here. We leave such a topic for future study.

In sum, this systematic study on the attractive Penrose Hubbard model has settled several fundamental issues about the SC on the QC. The first issue is the Cooper instability for infinitesimal attractions on the QC. We provide vigorous proof that an infinitesimal Hubbard attraction can lead to the Cooper pairing between TR partners, satisfying Anderson’s theorem. This result provides a basis for the SC on the QC. Our MF results on the model are well consistent with those of the BCS theory. The second issue is the property of the superfluid density on the QC. Our study clarifies that the pairing state obtained here exhibits the real SC that carries a finite superfluid density in the thermodynamic limit and shows a measurable Meissner effect. The insights acquired here also apply to other QC lattices.

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