Gap inversion in one-dimensional Andreev crystals

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We study a 1D AC formed by a periodic arrangement of magnetic regions in a one-dimensional superconducting wire. Due to the local exchange field, each region supports Andreev bound states that hybridize forming Bloch bands in the subgap spectrum of what we call the Andreev crystal (AC). As an illustration, ACs with ferromagnetic and antiferromagnetic alignment of the magnetic regions are considered.

We relate the spectral asymmetry index of a spin-resolved Hamiltonian to the spin polarization and identify it as the observable that quantifies the closing and reopening of the excitation gap. In particular, antiferromagnetic ACs exhibit a sequence of gapped phases separated by gapless Dirac phase boundaries. Heterojunctions between antiferromagnetic ACs in neighboring phases support spin-polarized bound states at the interface. In a close analogy to the charge fractionalization in Dirac systems with a mass inversion, we find a fractionalization of the interface spin.

Whereas non-magnetic impurities in a superconductor do not modify substantially its spectrum, a magnetic region may lead to bound states localized around the defect. If the magnetic exchange coupling is strong and concentrated at a point-like impurity, two non-degenerate states with opposite energies appear in the superconducting gap, the so-called Yu-Shiba-Rusinov (YSR) states. In contrast, if the exchange energy is small compared to the Fermi energy, μ, a pair of degenerate bound states appears. This latter case is well described semiclassically: high energy Fermi surface electrons do not back-scatter when traversing the magnetic region, but only accumulate a spin-dependent phase, e^iμΦ. Here Φ = ∫ dx vF h(x) for a collinear exchange field, h(x), the Fermi velocity is vF, and σ = ± for spin up/down electrons. Holes accumulate the same phase, but with opposite sign, e^−iμΦ. Despite the absence of a normal back-scattering, a semiclassical defect in superconductors allows for Andreev reflection, which couples the electron- and hole-branches at either kF or −kF. This coupling induces two pairs of degenerate spin-polarized bound states in the superconducting gap with opposite energies, ±μ, known as Andreev bound states.

It is natural to expect that in a one-dimensional (1D) chain of semiclassical magnetic impurities, Andreev bound states hybridize forming Andreev bands, significantly changing the spectral properties, and turning the system into an Andreev crystal (AC). Chains of magnetic atoms have been widely studied in the YSR-limit, but little attention has been paid to semiclassical chains that can be, for example, realized in a mesoscopic superconducting wire connected to a periodic array of ferromagnetic electrodes, as sketched in Fig. 1a.

In this letter we study a 1D AC formed by a periodic chain of magnetic impurities with collinear magnetization and analyze its spectral properties and phases. We first identify the total spin of the system as the observable which reveals the different phases. From a very general perspective we first show that the spin is determined by the asymmetry index of the spin-resolved Hamiltonian, i.e., the difference between the number of states below and above the Fermi energy. In gapped systems this index, and hence the spin, can only change by closing the gap. We then focus on two types of ACs, ferromagnetic and antiferromagnetic chains, and determine the corresponding spectra. By changing the magnetic phase Φ we find gapped and gapless phases. In particular, antiferromagnetic ACs demonstrate a sequence of gapped phases separated, at half-integer values of Φ/π, by gapless phase boundaries with Dirac points. We show that a hybrid system with two seminfinte antiferromagnetic ACs may exhibit spin-polarized bound states at the interface, which are similar to the states found in Dirac systems with a spatial mass inversion.

We consider a 1D s-wave superconductor in the presence of a collinear exchange field, h(x) = σz h(x), such that the spin along the z direction is a conserved quantity (here, σz stands for the third Pauli matrix). The Bogoliubov-de Gennes (BdG) Hamiltonian describing the system is block diagonal in spin with

\[ \tilde{H}_\sigma = \tilde{\tau}_3 \xi + \tilde{\tau}_1 \Delta(x) - \sigma h(x). \]  

Here, \( \tilde{\tau}_{i=1,2,3} \) are the Pauli matrices spanning the Nambu (electron-hole) space, \( \xi \) stands for the quasiparticle energy operator, \( \Delta(x) \) describes the superconducting order parameter, and \( \sigma \) is the spin label. From the corresponding imaginary-frequency Green’s functions, \( \tilde{G}_\sigma^{(\pm)}(\epsilon) = (\epsilon - \tilde{H}_\sigma^{(\pm)}(\epsilon))^{-1} \), one can compute the total spin polarization of the system at zero temperature:

\[ S = \frac{\hbar}{4} \lim_{\tau \to 0} \text{Tr} \int \frac{d\epsilon}{2\pi} \left[ \tilde{G}_\uparrow(\epsilon) - \tilde{G}_\downarrow(\epsilon) \right] e^{i\epsilon \tau}, \]  

Here, \( \tilde{\tau}_{i=1,2,3} \) are the Pauli matrices spanning the Nambu (electron-hole) space, %z stands for the quasiparticle energy operator, %(x) describes the superconducting order parameter, and % is the spin label. From the corresponding imaginary-frequency Green’s functions, %^Nambu^{(pm)}(x) = [(x - H^{(pm)}(x))^{-1}_Nambu^{(pm)}(x) for a collinear exchange field, h(x) = z h(x), such that the spin along the z direction is a conserved quantity (here, z stands for the third Pauli matrix). The Bogoliubov-de Gennes (BdG) Hamiltonian describing the system is block diagonal in spin with

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where the trace runs over the coordinate ⊗ Nambu space. Because $H_1 = -\tilde{\tau}_2 H_1 \tilde{\tau}_2$, then $G_1(\epsilon) = -\tilde{\tau}_2 G_1(-\epsilon) \tilde{\tau}_2$. Substituting this relation into Eq. (3) and using the cyclic property of the trace we obtain:

$$\frac{2S}{\hbar} = -\frac{1}{2} \lim_{\tau \to 0} \sum_n \text{sgn}(E_{n\uparrow}) e^{-|E_{n\uparrow}|\tau}, \quad (3)$$

where $E_{n\uparrow}$ stands for the energy of the $n$-the eigenstate of the spin-up Hamiltonian. This expression corresponds to the difference between the number of states below and above the Fermi energy for a given spin projection, and it is known as the spectral asymmetry index, widely used in the context of quantum field theory and condensed matter physics. In a gapped system, an adiabatic deformation of the Hamiltonian can only change the value of this index by closing and reopening the gap. This precisely occurs in ACs, as we discuss next.

We define an AC as a periodic arrangement of semiclassical magnetic regions in a superconductor. In the following we consider a collinear 1D structure of magnetic regions located at the points $X_n = an$, see Fig. 1, and assume that the width of each region is much smaller than the superconducting coherence length. The latter allows to treat the magnetic regions in the semiclassical limit as point-like impurities with the strength proportional to the corresponding magnetic phase $\Theta_n$, such that the BdG equations for a spin projection $\sigma$ read

$$\left[ -i\hbar v_F \tilde{\tau}_2 \partial_x + \tilde{\tau}_1 \Delta - \sigma i\hbar v_F \sum_n \Phi_n (x-na) \right] \Psi_{\nu\sigma}(x) = \epsilon_{\nu\sigma} \Psi_{\nu\sigma}(x), \quad (4)$$

where $\nu = \pm$ describes two Fermi valleys at $\pm k_F$. In absence of back-scattering, these two valleys are decoupled and can be treated separately, so that we drop the $\nu$ index for brevity. The general solution to Eq. (4) in the region between two neighboring impurities, $X_n < x < X_{n+1}$, is

$$\Psi_{\sigma}(x) \equiv \begin{cases} B_{\sigma_{n+1}} e^{-\frac{x-X_{n+1}}{\xi}} |+\rangle + B_{\sigma_{n}} e^{-\frac{x-X_n}{\xi}} |-\rangle, & \text{if } \sigma = \uparrow, \\ B_{\sigma_{n+1}}^{-1} e^{\frac{x-X_{n+1}}{\xi}} |+\rangle + B_{\sigma_{n}}^{-1} e^{\frac{x-X_n}{\xi}} |-\rangle, & \text{if } \sigma = \downarrow, \end{cases} \quad (5)$$

Here $\xi \equiv \frac{\hbar v_F}{\Delta}$ is the superconducting coherence length, $B_{\sigma_{n}}^{-1}$ is the amplitude of the contribution from the spinor that decays from the $n$-th magnetic region to the left (right), and

$$|\pm\rangle \equiv \frac{e^{\pm i\theta/2}}{\sqrt{2\cos \theta}} \left( \begin{array}{c} 1 \\ \pm i e^{\mp i\theta} \end{array} \right), \quad (6)$$

where $e^{\pm i\theta} \equiv \sqrt{\Delta^2 + e^2} \pm ie$ is the Andreev factor.

The spinors at the right ($X_{n\uparrow}$) and left ($X_{n\downarrow}$) side of the $n$-th magnetic region are related via a phase factor, $\Psi_{\sigma}(X_{n\uparrow}) = e^{i\sigma \tau_3 \Theta_n/2} \Psi_{\sigma}(X_{n\downarrow})$. Here, $\sigma$ and $\tau_3$ reflect the fact that the sign of the accumulated phase is different for spin up/down quasiparticles and for electrons/holes, respectively. From this relation we obtain the equations for the $B$ coefficients in Eq. (5), which can be recast into an effective tight binding model by keeping terms up to first order in $e^{-a/\xi}$. We find that $B_{\sigma_n} \approx \sigma i\frac{\Delta \sin \Phi_n}{\sqrt{\Delta^2 - e^2}} B_{\sigma_n}$ and

$$(\sigma \omega_\sigma - \omega_0 \sigma) b_{\sigma_n} = t_n b_{\sigma_{n+1}} + t_n b_{\sigma_{n-1}}, \quad (7)$$

where $b_{\sigma_n} \equiv \sin \Phi_n B_{\sigma_n}^+$, $\omega_\sigma = \frac{\omega}{\sqrt{\Delta^2 - e^2}}$, $\omega_0 = \frac{\cos \Phi_n}{\sin \Phi_n}$ is the value of $\omega_\sigma$ at the energy $\epsilon_0 = \frac{\Delta \sin \Phi_n}{\tan \Phi_n}$, and $t_n \equiv -\frac{e^{-a/\xi}}{\sin \Phi_n}$ is the hopping amplitude. The expression in Eq. (7) is valid for any AC with arbitrary distribution of collinear magnetization. Here we focus on two cases that show rather different qualitative results: the ferromagnetic and antiferromagnetic ACs described by constant, $\Phi_n = \Phi$, and alternating, $\Phi_n = (-1)^n \Phi$, magnetic phases, respectively.

In the ferromagnetic case the unit cell contains a single magnetic region and the solution of Eq. (7) simply reads $b_{\sigma_n} = e^{i\kappa n a}$ and $\omega_\sigma(k) = \sigma (\omega_0 + 2t \cos ka)$, where $k$ is the Bloch momentum. Hence, the physical Andreev energy bands are

$$\epsilon_{\sigma}(k) = \frac{\omega_0 + 2t \cos ka}{\sqrt{1 + (\omega_0 + 2t \cos ka)^2}}, \quad (8)$$

where $t$ has to be evaluated at the energy of the single impurity level $\epsilon_0$. In Fig. 1b we show the resulting energy spectrum within the Brillouin zone, $-\pi/a < k < \pi/a$, for different values of $\Phi$. It consists of two symmetric Andreev bands, one for each spin projection $\sigma$, centered at $\sigma \epsilon_0$, with a bandwidth $2t$. With increase of $\Phi$ the
two bands overlap, but remain independent as they correspond to different spin projections. As long as there is a gap between the bands, variations of \( \Phi \) do not modify the spectral asymmetry and, hence, the spin polarization per unit cell remains unchanged [cf. Eq. (3)]. When the bands overlap the spin continuously changes with the further shift of \( \Phi \) until the bands pass through each other and the gap reopens. After reopening the total spin change is \( h/2 \) per Fermi valley (i.e., by \( h \) in total).

Antiferromagnetic ACs are more interesting. In this case the unit cell contains two anti-aligned impurities (see the inset sketch in Fig. 1) and it is convenient to rewrite Eq. (7) as follows:

\[
(\sigma \omega - \hat{\Omega}_0)C_{\sigma m} = \hat{T}C_{\sigma m-1} + \hat{T}^\dagger C_{\sigma m+1},
\]

where \( C_{\sigma m} = [b_{\sigma 2m \ b_{\sigma 2m+1}}]^T \), and the matrices

\[
\hat{\Omega}_0 = \begin{pmatrix} \omega_0 & t \\ t & -\omega_0 \end{pmatrix}, \quad \hat{T} = \begin{pmatrix} 0 & -t \\ 0 & 0 \end{pmatrix},
\]

(10)
correspond to the unit-cell Hamiltonian and the inter-cell hopping, respectively. Equation (9) describes a chain with diatomic unit cell and a dispersion relation that equals \( \omega_r = \pm \sqrt{\omega_0^2 + 4t^2 \sin^2 \frac{k}{a}} \). This translates to the following Andreev bands:

\[
\epsilon_{\sigma}(k) = \pm \sqrt{\omega_0^2 + 4t^2 \sin^2 \frac{k}{a}} - \omega_0 \cos \Phi = \pm \sqrt{\omega_0^2 + 4t^2 \sin^2 \frac{k}{a}} - \omega_0 \cos \Phi = \omega_{\sigma},
\]

shown in Fig. 1. Because the period is doubled with respect to the ferromagnetic case, the number of bands is also doubled. There are two bands per spin specie which are fully symmetric with respect to the Fermi energy and, therefore, according to Eq. (3), the spin polarization is zero. The spectrum shows a gap equal to \( 2\omega_0 = \frac{2\cos \Phi}{\sin \Phi} \). The gap is finite for all \( \Phi \), except for half-integer values of \( \Phi/\pi \), when it closes and the spectrum exhibits a Dirac point at \( k_D = 0 \). In the vicinity of the critical values, \( \Phi = \pi(l+\frac{1}{2}) \), where \( l \) is an integer, the eigenvalue problem of Eq. 9 linearized around the Dirac point in the \( k \)-space reads:

\[
\begin{pmatrix} \sigma \omega - \omega_0 & -2itka \\ 2itka & \sigma \omega + \omega_0 \end{pmatrix} C_{\sigma}(k) = 0.
\]

(12)

It has the form of a 1D Dirac equation with \( \omega_0 \) playing the role of the mass. The closing and reopening of the gap is associated with a sign change of the mass term (gap inversion). Interestingly, the gap can also get inverted without closing: at values of \( \Phi = l\pi \) the Andreev bands merge into the continuum of the spectrum and reenter in the superconducting gap in inverted order.

Various realizations of an inhomogeneous Dirac model with the mass inversion have been widely studied in quantum field theory and condensed matter physics[14,17,26,31,42]. The most striking features of this model are the presence of bound states at the interface where the mass-inversion takes place, and fractionalization of the interface charge. As we discuss next, a junction between two antiferromagnetic ACs with inverted gap is another example of such systems, but with a fractionalized interface spin, instead of charge.

To establish the analogy, we consider a junction between two semi-infinite 1D antiferromagnetic ACs, where the separation between impurities, \( a \), remains constant all along the structure and the magnetic region in the left and right crystal are described by a magnetic phase equal to \( \Phi_L \) and \( \Phi_R \), respectively (see the sketch in Fig. 2). Such a system is described by the tight-binding equations, Eq. (9), at each side of the junction, namely

\[
(\sigma \omega - \hat{\Omega}_0)C_{\sigma m} = \hat{T}_m C_{\sigma m-1} + \hat{T}_{m+1} C_{\sigma m+1},
\]

(13)
at the left chain \( (m < 0) \) and

\[
(\sigma \omega - \hat{\Omega}_0)C_{\sigma m} = \hat{T}_m C_{\sigma m-1} + \hat{T}_{m+1} C_{\sigma m+1},
\]

(14)
at the right chain \( (m \geq 0) \). Here, \( \hat{\Omega}_0 \) (\( \hat{\Omega}_0 \)) stands for the expression of \( \hat{\Omega}_0 \) in Eq. (10) with \( \Phi = \Phi_L \) (\( \Phi = \Phi_R \)). We look for bound states, i.e. a solution that decays as \( C_{\sigma m} = C_{\sigma L}^m e^{\kappa_{\sigma L} m} \) into the left crystal and as \( C_{\sigma m} = C_{\sigma R}^m e^{\kappa_{\sigma R} m} \) into the right one, where the decay is determined by the positive-real-part complex number, \( \kappa_{\sigma L}^m(R) \). From Eqs. (13) and (14) we find that

\[
\sinh \frac{\kappa_{\sigma L} L(R)}{2} = \frac{\sqrt{\omega_0^2 L(R) - \omega_\sigma^2}}{2|l_{L(R)}|},
\]

(15)
where \( t_{m<0} = t_L \) and \( t_{m\geq0} = t_R \), and the bound state exists only when the following equation

\[
\frac{\sigma \omega_{\sigma} - \omega_0 L}{\sqrt{\omega_0^2 L - \omega_\sigma^2}} e^{-\kappa_{\sigma L} L} = -\frac{\sigma \omega_{\sigma} - \omega_0 R}{\sqrt{\omega_0^2 R - \omega_\sigma^2}} e^{-\kappa_{\sigma R} R},
\]

(16)
is fulfilled. According to Eq. (15) a bound state exists only if $|\omega_\sigma| < |\omega_{0L(R)}|$, which implies that Eq. (16) has a solution only in inverted junctions with $\text{sign}(\omega_{0R}) = -\text{sign}(\omega_{0L})$. The solution is especially simple for $\omega_{0R} = -\omega_{0L} \equiv \omega_0$, when it reads $\omega_\sigma = \sigma \text{sign}(\omega_0) \left( \sqrt{\omega_0^2 - t^2} - |t| \right)$. This gives the following physical energy of the bound state,

$$
\frac{\epsilon_\sigma}{\Delta} = \sigma \text{sign}(\omega_0) \frac{\sqrt{\omega_0^2 - t^2} - |t|}{\sqrt{1 + \left( \frac{\omega_0^2 - t^2 - |t|}{2} \right)^2}}. 
$$

In Fig. 2b we show the bound states for both spin projections as a function of $\Phi$ for different values of $-t \sin \Phi = e^{-a/\xi}$. Near the inversion point $|\omega_0/t| \to 0$, the bound states are almost degenerate approaching zero energy, $\epsilon_\sigma \to 0$. This is reminiscent of a zero mode in a continuum 1D Dirac model with mass inversion. As the bandwidth gets comparable to $\omega_0$, the states split forming a symmetric pair of levels between the Andreev bands.

To calculate the spin, $S$, induced at the contact between the two semi-infinite antiferromagnetic ACs, we average over all possible terminations of the chains. This is equivalent to the the so-called sliding window average method (see for example section 4.5 of Ref. 12), used to compute the surface charge density by averaging over all possible unit cell choices. The calculation is specially simple in the limit when the single-impurity Andreev states are decoupled from each other, $e^{-a/\xi} \ll 1$. In a previous work, 13 we show the spin polarization of a single semiclassical magnetic impurity of magnetic phase $\Phi$ in a 1D superconducting wire is $2S_0(\Phi)/\hbar = 2 \left[ (\Phi + \pi/2) \mod \pi \right]$, where “mod” stands for the modulo operation and accounts for a jump by two electronic spin units every time the singe-impurity levels cross the Fermi energy. In Fig. 3a, we show the staircase shape of $S_0(\Phi)$ in terms of the magnetic phase for a single impurity. We now consider the junction between the two antiferromagnetic ACs. It has four possible ending configurations: whether both chains have the same number of up and down magnetic impurities, the right (left) Andreev chain has an extra up (down) magnetic region or both chains are unbalanced. Consequently, the total spin polarization of the junction, calculated from the average over the four possible configurations, reads

$$
S = \frac{S_0(\Phi_R) - S_0(\Phi_L)}{2}. 
$$

Starting from the uncoupled impurities, if one adiabatically switches on the coupling, the Andreev bands start widening. However, in the considered configuration the gap never closes and, as we discussed after Eq. (3), the spin cannot change and is hence given by Eq. (18). In Fig. 3b, we show the total spin of the junction in terms of $\Phi_L$ and $\Phi_R$. Interestingly, the spin polarization can now be equal to and odd integer times the electronic unit, in contrast to the always even value of $S_0(\Phi)$. By construction, the half-integer spin (per Fermi valley) is localized at the junction between ACs. In other words, there is a fractionalization of the interface spin. Such fractionalization is a local effect. In a finite system the contribution from the edges will always lead to a total integer spin. Notice that changes of the spin polarization of ACs is determined by the change of the spectral asymmetry index, Eq. (3), and hence Eq. (18) is valid beyond the nearest neighbors tight-binding approximation. This is indeed confirmed by the exact numerical solution of Eq. (18).

In conclusion, we show that the spin polarization of a gapped system with collinear magnetization can only change upon gap closing. This occurs in Andrree crystals for which we present a complete study of their spectral properties for ferromagnetic and antiferromagnetic configurations. The spectrum of antiferromagnetic ACs presents a gap that remains open except for half-integer values of the magnetic phase $\Phi/\pi$, where a Dirac point is formed. We show that junctions between antiferromagnetic ACs with inverted gaps exhibit interface bound states and fractionalization of the surface spin polarization. We propose realization of these structures using, for example, a conventional superconducting wire contacted to ferromagnetic fingers such that a strong periodic exchange field, $h \gg \Delta$, is induced in the superconductor, see Fig. 1. The fingers may be made of ferromagnetic metals like Co or Ni, or ferromagnetic insulators, like EuS or EuO. The spectrum can be measured by a tunneling probe, which in case of being magnetic could also

![Figure 3](image-url)
give the spin-dependent properties of the AC.

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