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Topological *d*-wave superconductor

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Hypothetical topologically nontrivial superconducting state of two-dimensional electron system is discussed in connection with the problem of high-temperature superconductivity of cuprates. Direct numerical solution of the self-consistency equation exhibits two nearly degenerate order parameters which can be formally referred to $d_{x^2-y^2}$ and d_{xy} orbital symmetry. Spontaneous breaking of the time-reversal symmetry can mix these states and form fully gapped chiral $d+id$ superconducting state.

In recent years, condensed matter physics has significantly focused on studies of peculiar states of matter, such as two-dimensional ($2D$) topological insulators and superconductors [1]. Both time-reversal (TR) invariant and TR breaking topological superconductors have attracted a lot of interest, in particular, because of their potential applications. TR breaking superconductors are classified by an integer topological invariants [2] similar to those used for classification of quantum Hall states [3]. The simplest chiral topological triplet superconductor with $p_x + ip_y$ orbital symmetry was considered by Read and Green [4] and predicted to exist in Sr_2RuO_4 by Mackenzie and Maeno [5].

Degeneration of the $d_{x^2-y^2}$ and d_{xy} ordered states inherent in doped graphene monolayer has recently considered by Nandkishore et al. [6] as possible origin of a rise of a singlet chiral superconducting (SC) state with $d+id$ orbital symmetry. Such complex order parameter was suggested by Laughlin [7] to connect the TR broken symmetry and the low-temperature phase transition observed in $Bi_2Sr_2CaCu_2O_8$ in external magnetic field [8]. In such a case, the d_{xy} component of the SC order parameter turns out to be field-induced. Similar phase transition was observed in Ni-doped $Bi_2Sr_2CaCu_2O_8$ in zero external magnetic field [9]. Balatsky [10] pointed out that, in the presence of magnetic impurities, the $d_{x^2-y^2}$ superconductor can exhibit a transition exactly into the $d+id$ state due to a coupling between impurity magnetization and the d_{xy} component of the order parameter.

In this communication, we report a possibility of a rise of $d+id$ chiral state in high-temperature SC cuprates.

Recently introduced concept of SC pairing with large pair momentum under screened Coulomb repulsion [11] offers an explanation of principal features of cuprate superconductors: 1) a checkerboard real-space ordering observable in the SC state [12] can be directly related to the pair momentum, comparable with reciprocal lattice spacing [13]; 2) pseudogap (PG) state [14] with a broad region of SC fluctuations above the transition temperature T_c can be explained by a rise of quasi-stationary states of pairs with large momentum due to real-space oscillations of the screened Coulomb potential [15]; 3) high-energy effects observable in optical experiments [16] can be related to the electron-hole asymmetry that becomes apparent in the SC state of the cuprates.

The order parameter originating from SC pairing with large momentum is nonvanishing in the interior of a part of the Brillouin zone (domain of kinematic constraint) due to the fact that, at $T=0$, the momenta of both particles composing a pair should be either inside or outside the Fermi contour (FC). This order parameter turns out to be appreciably nonzero inside vicinities of nested segments of the FC [15]. In the case of SC cuprates, such segments correspond to antinodal region of the Brillouin zone [12].

High values of T_c and specific isotope effect manifested in the cuprates [17] show that, together with the repulsive Coulomb pairing interaction, one should take into account the attractive contribution owing to electron-phonon interaction (EPI), including the forward scattering effect [18].

In the antinodal region, phonon assisted Coulomb pairing with large momentum can predominate over conventional phonon-induced pairing with zero momentum that prevails only in the nodal region. Then, superconductivity at low temperatures should exist as a biordered state formed by the condensates of pairs with large and zero momenta in the antinodal and nodal regions of the momentum space, respectively [15]. On the contrary, the SC order just below T_c should be determined by the pairing with large momentum. Therefore, such an order should arise only in the antinodal region.

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Considerable enhancement of T_c, observable in the cuprates, can be qualitatively related to specific phonon induced "symmetrization" of real-space oscillations of the screened Coulomb potential [19]. The SC order parameter $\Delta(\mathbf{k};\mathbf{K})$, where $\mathbf{k}$ and $\mathbf{K}$ are relative motion and center-of-mass momenta of SC pair, respectively, should be obtained as a self-consistent solution to the mean-field gap equation with the momentum representation of such a symmetrized potential $U(\mathbf{k},\mathbf{k}';\mathbf{K})$. The gap equation at $T=0$ can be written as

$$\Delta(\mathbf{k};\mathbf{K}) = -\frac{1}{2}\sum_{\mathbf{k}'}\frac{U(\mathbf{k},\mathbf{k}';\mathbf{K})\,\Delta(\mathbf{k}';\mathbf{K})}{\sqrt{\epsilon_+^2(\mathbf{k}';\mathbf{K})+\Delta^2(\mathbf{k}';\mathbf{K})}}. \qquad (1)$$

Here, $2\epsilon_+(\mathbf{k};\mathbf{K}) = \varepsilon(\mathbf{k}_+) + \varepsilon(\mathbf{k}_-)$ is kinetic energy of a singlet pair composed of the particles with momenta $\mathbf{k}_\pm = \mathbf{K}/2 \pm \mathbf{k}$, the summation is taken over momenta $\mathbf{k}'$ belonging to the domain of kinematic constraint relevant to given pair momentum $\mathbf{K}$.

In the case of pairing with $\mathbf{K} \neq 0$, in common with the well-known Fulde–Ferrel–Larkin–Ovchinnikov (FFLO) problem [20, 21], the order parameter can be represented in the form of either a running wave [20], $\Delta \sim \exp i\mathbf{KR}$, or a standing wave [21], $\Delta \sim \cos(\mathbf{KR})$, that is as a symmetric superposition of running waves with pair momenta $\pm\mathbf{K}$. Here, $\mathbf{R}$ is center-of-mass radius-vector of the pair. It should be noted that, unlike the FFLO state, the SC state with nonzero center-of-mass momentum considered here arises without external magnetic field and, generally speaking, preserves TR symmetry.

One can expect that, along with the symmetric superposition, antisymmetric superposition of the same waves, $\Delta \sim \sin(\mathbf{KR})$, could be a solution to the gap equation as well. Both symmetric and antisymmetric solutions are defined in common domain of kinematic constraint which has to be constructed as the union of the domains for running waves with $\pm\mathbf{K}$.

Because of the crystal symmetry of the system, FFLO order parameter can be defined as a more complicated linear combination of running waves with equivalent momenta [22]. In a similar way, one can define zeroth-order approximation of the order parameter arising as a result of SC pairing with large pair momentum.

In the case of the cuprates, tetragonal symmetry of CuO_2 plane results in four crystal equivalent pair momenta: $\pm\mathbf{K}$ and $\pm\mathbf{K}'$, where $\mathbf{K}'$ is perpendicular to $\pm\mathbf{K}$. It is convenient to form standing waves as symmetric and antisymmetric (with respect to in-plane reflection from a line perpendicular to pair momentum) superpositions for each of two running waves with momenta, $\pm\mathbf{K}$ and $\pm\mathbf{K}'$, respectively. Then, the order parameter in the whole of the Brillouin zone can be written as a linear combination of these standing waves. Coefficients in such linear combinations specifies the orbital symmetry of the order parameter [23].

Coefficients of like signs correspond to extended s-wave symmetry (the order parameter is invariant with respect to rotation by $\pi/2$ about C_4-axis). In the case of coefficients of unlike signs, the order parameter reverses sign under rotation by $\pi/2$ and therefore can be referred to d-wave orbital symmetry.

One can represent the order parameter by any of four linear combinations (two s-wave and two d-wave) directly following from the gap equation. The SC ground state of the system should be expressed by the linear combination which has a lower free energy.

For solving the gap equation, we present interaction energy $U(\mathbf{k},\mathbf{k}';\mathbf{K})$ as a sum of screened Coulomb repulsion, $U_s(\mathbf{k},\mathbf{k}')$, defined in the whole of the domain of kinematic constraint and EPI induced effective attraction which is assumed nonzero inside a narrow region enveloping the FC [15]. Width of this region in the momentum space is of the order of $2\omega_{\mathrm{D}}/v_{\mathrm{F}}$, where ω_{D} and v_{F} are characteristic Debye frequency and Fermi velocity normal to the FC, respectively. We assume that attractive contribution into interaction energy is nonzero if and only if momenta of particles before and after scattering ($\mathbf{k}$ and $\mathbf{k}'$, respectively) both belong to this region. Also, we assume that this contribution is independent of momenta inside the region.

Thus, $U(\mathbf{k},\mathbf{k}';\mathbf{K}) = U_s(\mathbf{k},\mathbf{k}') - V$, if both momenta belong to the region, $U(\mathbf{k},\mathbf{k}';\mathbf{K}) = U_s(\mathbf{k},\mathbf{k}')$ when even if one of the momenta $\mathbf{k}$ and $\mathbf{k}'$ belonging to the domain of kinematic constraint does not belong to the region. One can assume that $U(\mathbf{k},\mathbf{k}';\mathbf{K}) = 0$ when even if one of the momenta does not belong to the domain of kinematic constraint.

To solve the gap equation numerically, we approximate the interaction energy by a simple step function of $\kappa = \mathbf{k} - \mathbf{k}'$ [13]. Step length in the direction of $\mathbf{K}$ is limited by the length of the nested segment of the FC. In the direction perpendicular to $\mathbf{K}$, left step at κ_l corresponds to phonon-mediated decrease in energy taking into account the forward scattering effect [18] whereas right step at κ_r reflects the fact that values of the order parameter turn out to be very small at all points distant from the FC. Therefore, the order parameter turns out to be weakly sensitive to κ_r [13].

We use the electron dispersion that conforms to the FC observable in hole doped cuprates,

$$\varepsilon(k_x,k_y) = 2t_0 - 2t(\cos k_x + \cos k_y) - 4t'\cos k_x \cos k_y - {} - 2t''(\cos 2k_x + \cos 2k_y), \qquad (2)$$

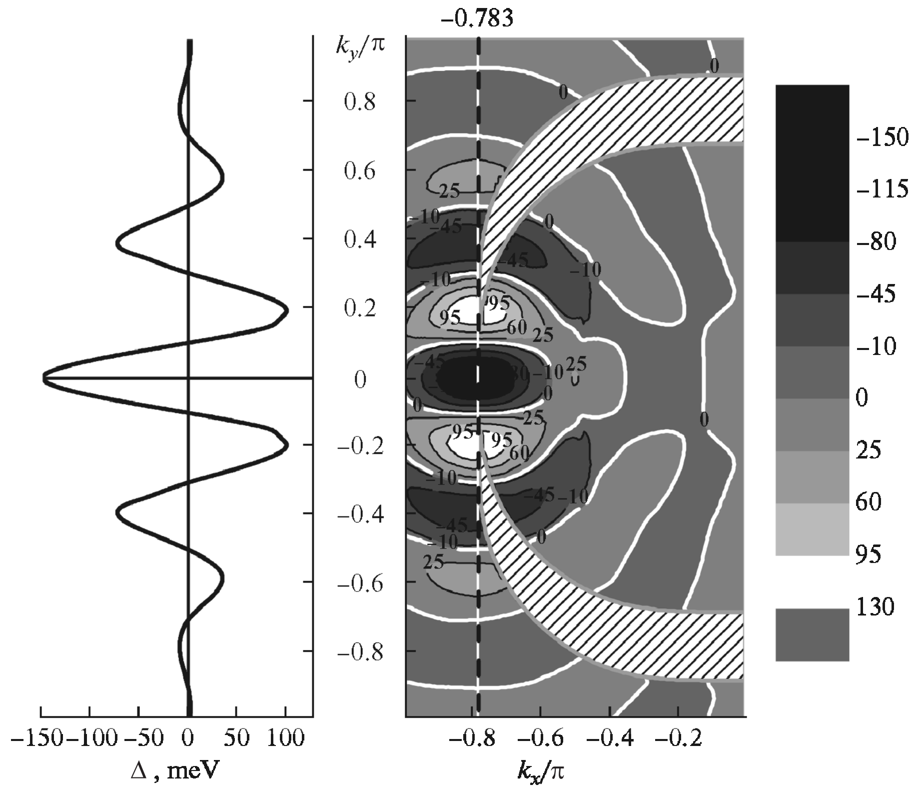

Fig. 1. Symmetric superposition $\Delta_s(\mathbf{k};\mathbf{K})$ of running waves with wave vectors $\pm\mathbf{K}$ directed along k_y-axis. Left panel – dependence of $\Delta_s(\mathbf{k};\mathbf{K})$ on k_y at $k_x = -0.783\pi$ that corresponds to the position of the left vertical nested segment of the FC. Right panel – topology of $\Delta_s(\mathbf{k};\mathbf{K})$; only left half of the Brillouin zone is shown. White lines present the intrinsic zero lines on which $\Delta_s(\mathbf{k};\mathbf{K}) = 0$. White background between the Fermi contours shifted by $\pm\mathbf{K}/2$ with respect to initial position of the FC reflects the kinematic constraint

where $t_0 = 1\,\text{eV}$, $t = 0.5\,\text{eV}$, $t'/t = -0.3$, $t''/t = 0.14$, and dimensionless components of momentum k_i ($i = x, y$) vary within $-\pi < k_i \leq \pi$.

Recently obtained numerical solution to the gap equation [13] corresponding to a symmetric superposition of two running waves is presented in Fig. 1 (only left half of the Brillouin zone is shown) in which the momenta of the running waves $\pm\mathbf{K}$ are chosen as directed along k_y-axis. The order parameter $\Delta_s(\mathbf{k};\mathbf{K})$ is characterized by intrinsic system of zero lines intersecting the FC. One can see that $\Delta_s(\mathbf{k};\mathbf{K})$ possesses distinct values only in a vicinity of nested segments of the FC. Similarly, one can obtain the symmetric superposition $\Delta_s(\mathbf{k};\mathbf{K}')$ corresponding to the running waves with $\pm\mathbf{K}'$.

The symmetric superposition $\Delta_s(\mathbf{k};\mathbf{K})$ can describe a stripe structure of the SC state [13], in particular, an emergence of the SC order parameter appearing in the PG state of the cuprates [12]. Recently, Berg et al. [24] discussed similar striped SC state as a unidirectional pair-density wave (PDW) phase with periodic real-space dependence of the order parameter on the center-of-mass position. The coupling between such a PDW and other ordered states was also considered in the framework of Ginzburg–Landau theory [24].

To obtain the order parameter in the whole of the Brillouin zone, one should compose either s- or d-wave linear combination of obtained symmetric superpositions [11],

$$\Delta_s^{(\pm)}(\mathbf{k}) \sim \Delta_s(\mathbf{k};\mathbf{K}) \pm \Delta_s(\mathbf{k};\mathbf{K}'). \qquad (3)$$

The first of them ($\Delta_s^{(+)}$), corresponding to extended s-wave orbital symmetry, displays the intrinsic zero lines only, whereas the second one ($\Delta_s^{(-)}$), corresponding to $d_{x^2-y^2}$ orbital symmetry, besides the intrinsic zero lines, displays four straight zero lines (nodal lines) along the diagonals of the Brillouin zone.

In the cuprates, it seems that such orbital d-wave nodal lines are consistent with available experimental facts including angle-resolved photoemission spectroscopy (ARPES) data [25]. In particular, it is very likely that SC gap near the diagonals takes small values and can even vanish. On the contrary, intrinsic zero lines, situated close to the FC, hardly ever can be detected directly from ARPES measurements but they un-

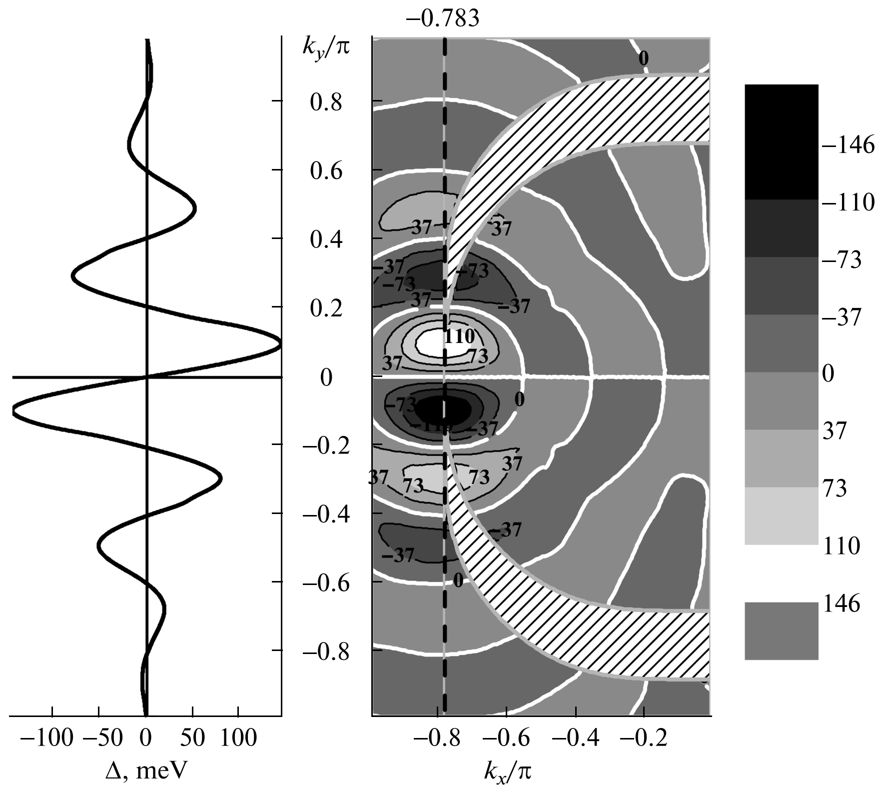

Fig. 2. Antisymmetric superposition $\Delta_a(\mathbf{k};\mathbf{K})$ of running waves with wave vectors $\pm\mathbf{K}$ directed along k_y-axis. Left panel dependence of $\Delta_a(\mathbf{k};\mathbf{K})$ on k_y at $k_x = -0.783\pi$ that corresponds to the position of the left vertical nested segment of the FC. Right panel – topology of $\Delta_a(\mathbf{k};\mathbf{K})$; only left half of the Brillouin zone is shown. White lines present the intrinsic zero lines on which $\Delta_a(\mathbf{k};\mathbf{K}) = 0$. White background between the Fermi contours shifted by $\pm\mathbf{K}/2$ with respect to initial position of the FC reflects the kinematic constraint

doubtedly should become apparent in thermodynamical properties.

In Fig. 2, we present new numerical solution to the gap equation, namely, the order parameter in the form of antisymmetric superposition of two running waves with opposite momenta, $\Delta_a(\mathbf{k};\mathbf{K})$.

This solution, just as symmetric superposition $\Delta_s(\mathbf{k};\mathbf{K})$, has its own system of intrinsic zero lines. As one can see from Fig. 2, one of such lines turns out to be parallel to one of the coordinate axes.

Extreme values of both $\Delta_s(\mathbf{k};\mathbf{K})$ and $\Delta_a(\mathbf{k};\mathbf{K})$ are concentrated in the antinodal regions near nested segments of the FC. It should be noted especially that, as results from direct numerical solution to the gap equation, both symmetric and antisymmetric superpositions exhibit comparable extreme values.

The order parameter in the whole of the Brillouin zone should be presented as either s- or d-wave linear combination of antisymmetric superpositions,

$$\Delta_a^{(\pm)}(\mathbf{k}) \sim \Delta_a(\mathbf{k};\mathbf{K}) \pm \Delta_a(\mathbf{k};\mathbf{K}'). \qquad (4)$$

The s-wave combination corresponding to plus sign in Eq. (4), besides some closed intrinsic zero lines, displays eight straight zero lines parallel both sides and diagonals of the Brillouin zone. Formally, such an order parameter can be referred to the so-called g-wave orbital symmetry discussed by Zhao [26].

The d-wave combination corresponding to minus sign in Eq. (4), besides some closed intrinsic zero lines, displays four intrinsic straight zero lines directed along the sides of the Brillouin zone. These lines can be formally considered as the nodes of the order parameter with d_{xy} orbital symmetry.

It is the pairing interaction that makes the choice in favor of a certain set of coefficients in Eqs. (3) and (4). For example, near a spin-density-wave instability typical of the cuprate superconductors, antiferromagnetic fluctuation-induced interaction component of the pairing interaction, sensitive to band structure and band filling, gives rise to singlet d-wave pairing with zero center-of-mass momentum. Such an interaction favors (suppresses) $d_{x^2-y^2}$ (d_{xy}) channel [27, 28].

As follows from Figs. 1 and 2, the amplitudes of two superpositions, $\Delta_s(\mathbf{k};\mathbf{K})$ and $\Delta_a(\mathbf{k};\mathbf{K})$, are comparable. Therefore, under certain conditions, the order parameter with spontaneously broken TR symmetry,

$$\Delta^{(c)}(\mathbf{k}) \sim \Delta_s^{(-)}(\mathbf{k}) + i\Delta_a^{(-)}(\mathbf{k}), \qquad (5)$$

can be expected as a chiral fully gapped ground state of the system. The components of $\Delta^{(c)}(\mathbf{k})$, phased by $\pi/2$ with respect to each other, should be formally referred to d-wave orbital symmetry, $d_{x^2-y^2}$ and d_{xy}, respectively.

It should be noted that, in the problem of triplet pairing with large center-of-mass momentum, superpositions $\Delta_a(\mathbf{k};\mathbf{K}')$ and $\Delta_a(\mathbf{k};\mathbf{K})$ themselves, can be considered as the p-wave order parameters corresponding to p_x and p_y symmetry, respectively. These superpositions can be used to form chiral triplet SC state with $p_x + ip_y$ orbital symmetry.

Values of the d_{xy} component, $\Delta_a^{(-)}(\mathbf{k})$, should be nonzero for momenta belonging to the nodal region because of the proximity effect in the momentum space and a contribution of SC pairing with zero momentum into biordered SC state [15] (both ignored in Figs. 1 and 2). As a result, a finite SC gap should appear at the points that correspond to the nodes of the pure $d_{x^2-y^2}$ state.

Both symmetric and antisymmetric superpositions, Δ_s and Δ_a, that describe superconducting condensates of pairs with large total momenta, are doubly degenerate owing to crystal equivalence of $\mathbf{K}$ and $\mathbf{K}'$. These superpositions are found numerically as the solutions to the self-consistency equation defined inside the domains of kinematic constraint corresponding to $\mathbf{K}$ and $\mathbf{K}'$. To obtain these solutions, we used a model potential describing screened Coulomb repulsion and phonon-induced effective attraction between electrons.

The interactions which are not taken into account by this computational procedure remove degeneration and result in a rise of linear combinations $\Delta_s^{(\pm)}$ and $\Delta_a^{(\pm)}$ corresponding to s-wave ($\Delta_s^{(+)}$ and $\Delta_a^{(+)}$) and d-wave ($\Delta_s^{(-)}$ and $\Delta_a^{(-)}$) symmetries, respectively.

We believe that antiferromagnetic fluctuation-induced interaction [27, 28] plays crucial role in a rise of d-wave ordering in the cuprates, especially in the underdoped region of the phase diagram. Such paramagnon-exchange-induced interaction results in π-shifted phase of the order parameter under rotation by $\pi/2$ in the momentum space. Therefore, one can think it is the paramagnon exchange that selects one of the d-wave combinations ($\Delta_s^{(-)}$), as the ground state of hole-doped cuprate compounds.

It should be emphasized that antiferromagnetic fluctuation-induced interaction leads to phase shift π in both cases of $d_{x^2-y^2}$ and d_{xy} symmetries. Therefore, such an interaction should result in topologically stable state $\Delta^{(c)}$ with $d + id$ ordering, Eq. (5).

The d_{xy} order parameter is often accepted in a simple form, $\sin k_x \sin k_y$, that reveals maxima just on the diagonals. On the contrary, $d + id$ order (5) turns out be concentrated in antinodal vicinities of the nested segments of the FC (see Fig. 2). Therefore, the smallness of the d_{xy} component of Ex. (5) in the nodal region can make it difficult to detect such a gap (for example, using ARPES technique). It should be noted, however, that recent ARPES data [29] can be considered as an unambiguous evidence in favor to $d_{x^2-y^2}$-wave-like SC gap in optimally doped $YBa_2Cu_3O_{7-\delta}$ that exhibits a nonzero minimum of about 12 meV along the nodal direction.

Chiral SC ground state with the order parameter (5) turns out to be topologically nontrivial. Indeed, by continuous deformation of the parameters of the mean-field Hamiltonian without opening a gap, this state can be transformed into that considered by Volovik [30]: both states are topologically equivalent and should be characterized by the topological invariant $\mathcal{N} = \pm 2$.

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