

## Low-Energy Quasiparticle States near Extended Scatterers in $d$ -Wave Superconductors and Their Connection with SUSY Quantum Mechanics

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Low-energy quasiparticle states, arising from scattering by single-particle potentials in  $d$ -wave superconductors, are addressed. Via a natural extension of the Andreev approximation, the idea that sign variations in the superconducting pair potential lead to such states is extended beyond its original setting of boundary scattering to the broader context of scattering by general single-particle potentials, such as those due to impurities. The index-theoretic origin of these states is exhibited via a simple connection with Witten's supersymmetric quantum-mechanical model.

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In the present Letter we shall explore the low-energy quasiparticle states available in  $d$ -wave superconductors due to the presence of an extended scatterer such as a boundary or an impurity more than a few Fermi wavelengths across. In the context of boundary scattering, such states represent an important signature of sign variations of the superconducting order parameter, as they have been shown to originate in the possibility of scattering between momentum orientations that are subject to superconducting pair potentials of differing sign. The main aims of our work are to extend the idea that sign variations in the superconducting pair potential lead to low-energy quasiparticle states to the context of scattering by general single-particle potentials, such as those due to impurities (i.e., beyond scattering by boundaries), and to explore the robustness of this effect.

The theoretical framework that we shall adopt is the semiclassical approach to the quantum-mechanical problem of scattering from the single-particle potential, via which the eigenvalue problem at hand reduces to a family of effectively one-dimensional problems for the particle-hole dynamics in the presence of the superconducting pair potential. Through this approach, we shall be able to see that the density of low-energy quasiparticle states (DOS) is determined solely by the *classical scattering properties* of the single-particle potential and, furthermore, that this DOS is insensitive to any suppression of the pair potential that the impurity might cause. This approach also provides us with a framework for classifying and calculating corrections to the DOS at low energies, such as those due to diffraction during scattering from the single-particle potential itself, or due to any pair-potential modifications beyond mere suppression (such as the induction of any out-of-phase components of the pair potential).

Along the way, we shall discuss the fact that the emerging one-dimensional eigenproblem is a realization of Witten's supersymmetric quantum-mechanical model [1,2] which, via the Witten index [1,2], provides a natural setting in which to explore zero-energy states [3,4]. Through this identification with Witten's model we shall

see that the conditions under which zero-energy states exist are indeed those mentioned above, viz., propagation between pair potentials of differing signs. In addition, we shall examine the role played by the semiclassical approximation to the scattering problem vis-à-vis the existence of zero-energy states, and thus see how it is that going beyond this semiclassical approximation introduces transition amplitudes between classical scattering trajectories, causing the dispersion of the formerly zero-energy states, e.g., into one or more low-energy peaks in the DOS.

We stress at the outset that the issue of the origin of the low-energy states, viz., sign changes in the pair potential, has already been soundly understood and extensively developed theoretically in several contexts: notable examples include the works of Buchholtz and Zwicknagl [6] on  $p$ -wave superconductors near surfaces, and of Hu [8], Buchholtz *et al.* [7], and Fogelström *et al.* [9] on  $d$ -wave superconductors near flat surfaces. Low-energy states have also received extensive experimental attention in the context of boundary scattering in high-temperature superconductors. In particular, measurements of the (macroscopic) tunneling conductance [10] reveal a zero-bias anomaly indicating the existence of low-energy states near boundaries.

Apart from the effects of flat boundaries, theoretical research on low-energy quasiparticle resonances in  $d$ -wave materials has mostly been concerned with the effects of *pointlike impurities* (i.e., impurities for which the size of the impurity is not much larger than the Fermi wavelength  $\lambda_F$ ). Of particular interest has been the effect of the impurity strength on the energies and wave functions of the resonances [11,12]. More recently, attention has been paid to the effects on these resonances of impurity-induced suppression of the superconducting order parameter [13,14]. Emerging from this body of work is a picture in which each strong, pointlike impurity gives rise to a low-energy resonance. This resonance, which would show up in the tunneling DOS as a pair of peaks symmetrically located around zero energy, transforms (in the particle-hole symmetric case) into a single, marginal,

bound state at zero energy in the unitary scattering limit. As the impurity strength is reduced, the energy of this resonance moves towards the gap maximum. Moreover, the quantitative details of the band structure and/or order parameter can play important roles [15]. In particular, in particle-hole asymmetric systems the energies of the resonances no longer tend to zero in the unitary limit.

In contrast, the present work suggests that an extended (rather than pointlike) impurity induces a zero-energy peak in the DOS with a weight of order the linear size of the impurity (measured in units of the Fermi wavelength). Moreover, the resulting low-energy DOS is much less sensitive to details such as the precise form of the band structure and any in-phase order parameter variations, i.e., the peak at zero energy is inert. In this respect, extended impurities behave more like flat boundaries than like pointlike impurities.

The theoretical distinctions between pointlike and extended impurities raised here have, to some extent, been addressed experimentally via scanning tunneling spectroscopy on  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  surfaces [16,17]. Work on native defects [16,17], which often appear to be essentially pointlike in STM imaging, yield weak signatures in the (smeared, local) DOS near each defect. Such signatures can each be interpreted as being induced by a pointlike impurity that yields a resonance of unit weight. In contrast, the artificially induced defects described in Ref. [16], which appear to be more extended in STM imaging, show much stronger signatures in the DOS. This is consistent with the idea that extended impurities produce many states, as the present work indicates.

*Bogoliubov–de Gennes eigenproblem.*—We regard the single-quasiparticle excitations as being described by the Bogoliubov–de Gennes (BdG) eigenproblem [18,19]

$$\begin{pmatrix} \hat{h} & \hat{\Delta} \\ \hat{\Delta}^\dagger & -\hat{h} \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}, \quad (1)$$

where the components  $u(\mathbf{x})$  and  $v(\mathbf{x})$  of the energy eigenstate, respectively, give the amplitudes for finding an electron and a hole at the position  $\mathbf{x}$ ,  $E$  is the energy eigenvalue, and  $\hat{h} = -\nabla^2 - k_F^2 + V(\mathbf{x})$  is the one-particle Hamiltonian, in which  $k_F^2$  is the chemical potential [i.e.,  $k_F \equiv 2\pi/\lambda_F$  is the Fermi wave vector] and  $V$  is the single-particle potential. We have adopted units in which  $\hbar^2/2m = 1$ , where  $m$  is the (effective) mass of the electrons and holes. The operator  $\hat{\Delta}$  (which should ultimately be determined self-consistently) is the pair-potential (integral) operator, whose action on the wave functions is specified by the (nonlocal) kernel  $\Delta(\mathbf{x}, \mathbf{x}')$  via  $[\hat{\Delta}v](\mathbf{x}) = \int d\mathbf{x}' \Delta(\mathbf{x}, \mathbf{x}')v(\mathbf{x}')$ . We assume that sufficiently far from the scatterer  $\Delta$  returns to the value

that characterizes the bulk superconductor (e.g.,  $s$ -wave,  $d$ -wave, mixed, etc.). As we shall see below, our computation of the low-energy DOS is insensitive to the precise form of any suppression of the superconducting order induced by the single-particle potential, and therefore continues to hold when  $\Delta$  is replaced by its self-consistent value. However, as we shall also see below, induced modifications of the superconducting order parameter that go beyond simple suppression in a manner that causes local supercurrents (i.e., via the addition of any intrinsically out-of-phase component to  $\Delta$ ) spoil this robustness.

*Andreev’s approximation for a strong single-particle potential.*—To analyze the BdG eigenproblem we first apply a semiclassical approximation, which reduces the full problem to a family of first-order differential eigenproblems labeled by the classical trajectories of a particle at the Fermi energy in the presence of the full single-particle potential. This amounts to extending the Andreev approximation to situations in which there is a single-particle potential whose energy scale  $V_0$  is not negligible compared with the Fermi energy. In technical terms, we are making an asymptotic approximation valid when  $k_F^2 \gg (\Delta_0, E)$ ,  $V_0 \sim k_F^2$ , and  $V(\mathbf{x})$  is slowly varying relative to  $\lambda_F$ . To implement this approximation we consider the semiclassical solution of

$$[-\nabla^2 - k_F^2 + V(\mathbf{x})][\mathcal{A}(\mathbf{x})e^{ik_F S(\mathbf{x})}] = 0, \quad (2)$$

i.e., the “large” part of the BdG eigenproblem, where both  $\mathcal{A}(\mathbf{x})$  and  $S(\mathbf{x})$  are taken to be slowly varying (with respect to  $\lambda_F$ ) [20]. By retaining the first and second powers in  $k_F$  we obtain, from Eq. (2), the Hamilton-Jacobi equation  $|\nabla S(\mathbf{x})|^2 = 1 - k_F^{-2}V(\mathbf{x})$  and the conservation condition  $\nabla \cdot [\mathcal{A}(\mathbf{x})^2 \nabla S(\mathbf{x})] = 0$ . We then use the resulting semiclassical solution, which is specified in terms of the incoming momentum orientation  $\mathbf{n}$  via the asymptotic behavior  $S(\mathbf{x}; \mathbf{n}) \sim \mathbf{n} \cdot \mathbf{x}$  [21] (for  $\mathbf{x}$  far from the scattering center) and includes all of the fast (i.e., order of  $\lambda_F$ ) variations of the exact BdG eigenfunctions, to perform a generalized separation of rapidly and slowly varying components by writing  $(u(\mathbf{x}), v(\mathbf{x}))$  as  $\mathcal{A}(\mathbf{x})e^{ik_F S(\mathbf{x}; \mathbf{n})}(\bar{u}(\mathbf{x}), \bar{v}(\mathbf{x}))$ , where  $\bar{u}$  and  $\bar{v}$  are assumed to be slowly varying relative to  $\lambda_F$ . Then, by inserting this form into Eq. (1) we obtain  $[\hat{h}(\mathcal{A}e^{ik_F S}\bar{u})](\mathbf{x}) \sim -2ik_F \mathcal{A}(\mathbf{x})e^{ik_F S(\mathbf{x}; \mathbf{n})}(\nabla S) \cdot (\nabla \bar{u})$ .

We now turn to the “small” part of the BdG eigenproblem, which involves the off-diagonal integral operator  $\hat{\Delta}$ . It is convenient to transform to relative and center-of-mass coordinates,  $\mathbf{r}$  and  $\mathbf{R}$ :  $\bar{\Delta}(\mathbf{r}, \mathbf{R}) \equiv \Delta(\mathbf{x}, \mathbf{x}')$ ,  $\mathbf{r} \equiv \mathbf{x} - \mathbf{x}'$ , and  $2\mathbf{R} \equiv \mathbf{x} + \mathbf{x}'$ . Then the action of  $\hat{\Delta}$  can be asymptotically approximated (for  $k_F^2 \gg \Delta_0$ ) as

$$[\hat{\Delta}(\mathcal{A}e^{ik_F S}\bar{u})](\mathbf{x}) = \int d\mathbf{r} \bar{\Delta}(\mathbf{r}, \mathbf{x} - \mathbf{r}/2)\bar{u}(\mathbf{x} - \mathbf{r}/2)\mathcal{A}(\mathbf{x} - \mathbf{r}/2)e^{ik_F S(\mathbf{x} - \mathbf{r}/2; \mathbf{n})} \approx [\mathcal{A}(\mathbf{x})e^{ik_F S(\mathbf{x}; \mathbf{n})}]\bar{u}(\mathbf{x})\Delta_{\text{eff}}(\mathbf{x}; \mathbf{n}), \quad (3a)$$

$$\Delta_{\text{eff}}(\mathbf{x}; \mathbf{n}) \equiv \int d\mathbf{r} \bar{\Delta}(\mathbf{r}, \mathbf{x} - \mathbf{r}/2)\mathcal{A}(\mathbf{x})^{-1}\mathcal{A}(\mathbf{x} - \mathbf{r}/2)\exp[ik_F S(\mathbf{x} - \mathbf{r}; \mathbf{n}) - ik_F S(\mathbf{x}; \mathbf{n})], \quad (3b)$$

provided we assume that  $(\bar{u}(\mathbf{x}), \bar{v}(\mathbf{x}))$  varies much more slowly than  $\lambda_F$ . Thus the task of solving the full BdG eigenproblem (1) is reduced to the task of solving the (classical) Hamilton-Jacobi equation, along with the (2 × 2) first-order partial differential eigenproblem

$$\begin{pmatrix} -2ik_F \nabla S \cdot \nabla & \Delta_{\text{eff}}(\mathbf{x}; \mathbf{n}) \\ \Delta_{\text{eff}}^*(\mathbf{x}; \mathbf{n}) & 2ik_F \nabla S \cdot \nabla \end{pmatrix} \begin{pmatrix} \bar{u} \\ \bar{v} \end{pmatrix} = E \begin{pmatrix} \bar{u} \\ \bar{v} \end{pmatrix}. \quad (4)$$

In fact, the eigenproblem is an *ordinary* rather than a *partial* one. To see this, recall the element of the Hamilton-Jacobi theory in which one establishes that the solution  $S$  of the Hamilton-Jacobi equation (at least for classically allowed regions) is indeed the action computed along the classical trajectory  $\mathbf{x}_c(\cdot)$  that solves Newton's equation  $k_F^2 \partial_s^2 \mathbf{x}_c(s) = -\nabla V(\mathbf{x}_c)$  subject to the condition  $|\partial_s \mathbf{x}_c(s)| \rightarrow 1$  as  $s \rightarrow \pm\infty$  (so that the classical motion is at the Fermi energy). Owing to this connection between  $\nabla S$  and  $\dot{\mathbf{x}}_c$ , Eq. (4) can be rewritten as [20]

$$\hat{H} \begin{pmatrix} \bar{u} \\ \bar{v} \end{pmatrix} = E \begin{pmatrix} \bar{u} \\ \bar{v} \end{pmatrix}, \quad \hat{H} \equiv \begin{pmatrix} -2ik_F \partial_s & \Delta_{\text{eff}}(s) \\ \Delta_{\text{eff}}^*(s) & 2ik_F \partial_s \end{pmatrix},$$

where  $\Delta_{\text{eff}}(s)$  is defined to be  $\Delta_{\text{eff}}(\mathbf{x}_c(s); \mathbf{n})$ . This family of first-order ordinary differential eigenproblems is parametrized by  $\mathbf{n}$  and the impact parameter  $b$ , which uniquely specify the classical trajectory  $\mathbf{x}_c(\cdot)$  from among those having energy  $k_F^2$ .

*Zero-energy states.*—To search for zero-energy states it is useful to reduce the eigenproblem via the following sequence of steps. We apply the unitary transformation (in electron-hole space)  $\hat{U} \equiv (1/\sqrt{2}) \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$ , under which

$$\hat{H} \rightarrow \hat{H}' \equiv \hat{U}^\dagger \hat{H} \hat{U} = \begin{pmatrix} 0 & \hat{A} \\ \hat{A}^\dagger & 0 \end{pmatrix}, \quad (5a)$$

$$\hat{A} \equiv -2ik_F \partial_s - i\Delta_{\text{eff}}(s),$$

$$\hat{A}^\dagger \equiv -2ik_F \partial_s + i\Delta_{\text{eff}}(s). \quad (5b)$$

We emphasize that it is not possible to arrive at this structure for values of  $\Delta_{\text{eff}}$  that are intrinsically complex (i.e., cannot be made real by an elementary gauge transformation), as is the case, e.g., for supercurrent-carrying states. The virtue of the structure of Eqs. (5a) and (5b) is that it allows us to recognize that zero-energy eigenfunctions of  $\hat{H}'$  have the form  $\begin{pmatrix} \varphi_+ \\ 0 \end{pmatrix}$  or  $\begin{pmatrix} 0 \\ \varphi_- \end{pmatrix}$ , where the functions  $\varphi_\pm$  obey  $(2k_F \partial_s \mp \Delta_{\text{eff}})\varphi_\pm = 0$ , provided they exist (i.e., are normalizable). Owing to their first-order nature, these (zero-energy) eigenproblems may readily be integrated to give  $\varphi_\pm(s) \propto \exp \pm (2k_F)^{-1} \int^s ds' \Delta_{\text{eff}}(s')$ . However, the ability to normalize  $\varphi_\pm$ , and therefore the existence of zero-energy eigenvalues, depends on the form of  $\Delta_{\text{eff}}$  via the limiting values  $\Delta_\pm \equiv \lim_{s \rightarrow \infty} \Delta_{\text{eff}}(\pm s)$  for a given semiclassical path  $\mathbf{x}_c(\cdot)$  [22]. Specifically, for semiclassical paths for which  $\Delta_+ \Delta_-$  is negative, one or the other (but not both) of  $\varphi_\pm$  is normalizable and, therefore, for such paths provide *precisely one* zero-energy eigenvalue. On the other hand, for semiclassical paths for which  $\Delta_+ \Delta_-$  is positive, neither of  $\varphi_\pm$  is normalizable, and therefore such paths provide no zero-energy eigenvalues.

This diagnostic for when semiclassical paths lead to zero-energy states allows us to assemble the zero-energy

contributions to the DOS. If, for the sake of concreteness, we restrict our attention to two-dimensional systems, then our approximation to the low-energy DOS has the form

$$\rho_{\text{SC}}(E) = \delta(E) \frac{k_F}{2\pi} \int d\mathbf{n} db (1 - \text{sgn} \Delta_+ \text{sgn} \Delta_-). \quad (6)$$

This formula should have corrections, which vanish as  $E$  tends to zero, coming from the nodes in the gap of the homogeneous  $d$ -wave state, as well as suppression of the superconducting state near the impurity.

Let us now highlight some features related to Eq. (6): (i) The evaluation of Eq. (6) requires only knowledge of the classical scattering trajectories for  $V$ . (ii) The DOS peak is located at zero energy. Corrections to this result, owing *inter alia* to particle-hole asymmetry, are of relative order  $\max(1/k_F R, \Delta_0/k_F^2)$  (where  $R$  is the characteristic linear extent of the impurity potential). These corrections lead to the splitting and dispersion of the zero-energy peak. (iii) Only the signs of  $\Delta_{\text{eff}}$  associated with the directions of the momentum asymptotically far from the impurity are featured in Eq. (6); the DOS is unchanged by deformations of the pair potential, provided the asymptotic signs are preserved and no out-of-phase components are induced. (iv) The degeneracy of the zero-energy level, and hence the weight of the zero-bias STM peak, is proportional to the typical impurity scattering cross section (more precisely, of order  $R/\lambda_F$ ), the exact weight depending on the form of  $V$ . (v) For a sparse collection of (extended) scatterers (i.e., scatterers resolvable at the scale  $k_F/\Delta_0$ ) their contributions to the DOS are roughly additive; for a dense collection (i.e., for nearly overlapping impurity potentials) the contribution scales with the linear size of the collection.

*Connection with Witten's model of supersymmetric quantum mechanics and index theory.*—Having seen, within the context of an explicit computation, the emergence (or otherwise) of zero-energy states, we now discuss the structure that underlies this issue, namely, index theory [5]. The relevant aspect of index theory is Witten's index from Witten's model of supersymmetric quantum mechanics (SUSY QM). The specific connection is as follows:  $\hat{H}'^2$  [c.f. our (5a)] is Witten's SUSY Hamiltonian;  $\Delta_{\text{eff}}$  [our (3b)] is Witten's SUSY potential;  $A$  and  $A^\dagger$  [our (5b)] are proportional to Witten's annihilation and creation operators. Indeed, the analysis leading from Eq. (5a) to the conditions for the existence of a zero-energy state mirrors the standard SUSY QM analysis.

In SUSY QM, an important tool is the Witten index, i.e., the number of zero-energy states of the form  $\begin{pmatrix} 0 \\ \varphi_- \end{pmatrix}$  minus the number of the form  $\begin{pmatrix} \varphi_+ \\ 0 \end{pmatrix}$ . If the Witten index is nonzero then there certainly are zero-energy states (i.e., SUSY is good; see, e.g., Ref. [2], Sec. 2.1). If the Witten index is zero then there may or may not be zero-energy states, as contributions may cancel. In the present context, we are not *prima facie* concerned with the Witten index and its properties, but rather with ascertaining the number of zero-energy states. However, owing to the fact that there is at most *one* zero-energy state for any semiclassical

trajectory (because the normalizability condition cannot be simultaneously satisfied by both  $\varphi_+$  and  $\varphi_-$ ) the (modulus of the) Witten index does indeed permit the counting of the zero-energy states.

*Discussion and outlook.*—The condition on the existence of zero-energy states, together with Eq. (3b), provides us with a way of calculating the DOS at low energies by a simple counting of the number of classical trajectories that start and end with different signs of the superconducting pair potential [see Eq. (6)]. Thus, the DOS at low energies depends only on the *classical scattering properties of the single-particle potential*.

As we have stressed earlier, this result is valid in the regime in which the single-particle potential is both spatially extended and strong and the pair potential is much smaller than the Fermi energy. Before turning to a discussion (and classification) of the generic corrections to this result for the DOS, which arise upon the relaxation of these conditions, we remark that the foregoing approximation scheme and results also hold for spatially extended single-particle potentials that are *weaker* than the Fermi energy. Moreover, in the regime  $V_0 \lesssim \Delta_0$  our results can be extended to the case of rapidly varying single-particle potentials (such as are due to pointlike impurities). However, as the strength of the single-particle potential is diminished, the classical trajectories tend towards straight lines and, hence, the number of trajectories that “see” different signs of the pair potential is reduced. This results in a corresponding decrease in the degeneracy of the zero-energy level, in accordance with formula (6). Indeed, for  $V_0 \lesssim \Delta_0$  the trajectories are essentially straight lines. Thus, there would be no zero-energy states, but additional resonances (due to the impurity) may arise if the pair potential is suppressed.

By contrast, in the regime  $V_0 \sim k_F^2$  but  $V(\mathbf{x})$  rapidly varying (e.g., for strong, pointlike impurities), the approximation scheme that enabled us to reduce the problem to a family of one-dimensional eigenproblems breaks down, due to the fact that the previously neglected  $\nabla\mathcal{A}$  term becomes comparable to previously retained  $\nabla S$  term. The former term introduces diffraction effects in the (quantum-mechanical) scattering from the single-particle potential, as well as tunneling through the classically forbidden region. These effects can be viewed as consequences of nonzero transition amplitudes between states associated with the classical trajectories, and would result in the dispersion of the previously degenerate zero-energy states.

Let us conclude by remarking that the presence of an extended-impurity induced subdominant component to the pair potential, provided it is *in phase* with the dominant component, would not change the picture presented here: specifically, formula (6) would continue to hold. On the other hand, if an out-of-phase component is induced (i.e., time-reversal symmetry is locally broken, as would be the case, e.g., if the state were locally to become  $d + is$ ), this would cause the zero-energy peak in the DOS to split into two peaks of nonzero width [9,10], symmetrically

located about zero energy, their line shapes depending on the full (rather than solely the asymptotic) details of the pair potential and computable via perturbation theory. If observed (and provided other sources of splitting such as diffraction effects can be ruled out), such a splitting would provide strong evidence for extended-impurity induced local time-reversal symmetry breaking.

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  - [21] To be precise, this asymptotic boundary condition is to be imposed on the branch of the (multivalued) action function  $S$  corresponding to *incoming* trajectories.
  - [22] In fact, the unitary transformation that leads to Eq. (5a) can also be applied to the *full* partial-differential BdG operator, leading to the same off-diagonal structure. At least in simple settings, such as specular reflection from a flat boundary, this structure allows one to demonstrate, again using the criterion of normalizability, that zero-energy states continue to exist beyond the Andreev-type linearization approximation. This provides an example in which zero-energy states arise, despite the absence of particle-hole symmetry.