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# Density of bound states in a vortex core

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The local density of states as derived from Kramer and Pesch's theory of bound states in a vortex core is compared with recent scanning-tunneling experiments. Effects of impurities and finite flux-line distance are approximately taken into account. In the isolated vortex regime one finds qualitative, but not quantitative, agreement with all experimental data reported so far. The results depend sensitively on impurity content. A nonmonotonic behavior of the density of states as a function of the distance from the flux-line center is predicted. The unexpected properties of the density of states are discussed in terms of the direction-dependent single-particle excitations bound to the core.

Recent progress in low-temperature scanning-tunneling microscope (STM) technique has offered a possibility to study the local density of states in spatially inhomogeneous superconductors. In these experiments the tunneling conductance $\sigma(V,\mathbf{r})=dI/dV$ can be measured with high spatial resolution. At sufficiently low temperatures this quantity directly reflects the behavior of the density of states $N(E,\mathbf{r})$. The most prominent inhomogeneous system is, of course, the vortex state of type-II superconductors, which has been dealt with in two experimental studies reported recently.[1,2] The measurements[1,2] have been performed on the material $NbSe_2$ which is an anisotropic, weak-coupling, extreme type-II superconductor. The main result reported in the first paper of Hess *et al.*[1] was a pronounced peak of $\sigma(V,r)$ at $V=0$ with the STM tip positioned at the flux-line center $r=0$. In its spatial dependence $\sigma(V,r)$ showed a peak at $r=0$ if $dI/dV$ was taken at constant voltage $V=0$. In the second paper by Hess *et al.*,[2] new data on the voltage and position dependence of $\sigma(V,r)$ were presented. In the isolated vortex regime essentially two new effects were reported, a nonmonotonic behavior of $\sigma(V,r)$ as a function of $V$ (flat maximum at $V\sim0.4$ mV) for a radial distance $r=90$ Å, and a broadening of the peak at $r=0$ with increasing voltage $V$.

If such effects are assumed to lie within the realm of standard BCS theory, then they can only occur in superconductors of sufficient purity[3] (they will sensitively depend on impurity degree) and will be connected with the low-lying bound states localized inside the vortex core.[4,5] In fact, numerically solving the Bogoliubov equations for the bound states, Shore *et al.*[6] were able to qualitatively reproduce the observed peak of $\sigma$ at zero bias. These authors[6] also predicted a nonmonotonic behavior of $N(E,r)$ which has probably been observed experimentally in Ref. 2 (the first of the two new effects mentioned above). The zero-bias peak has also been inferred from phenomenological considerations[7] and from the behavior of the single-particle excitations[8] of the quasiclassical theory.

In this Rapid Communication a study of bound-state effects based on Kramer and Pesch's solution[5,9] of the quasiclassical equations is presented. The influence of impurities and of a finite vortex distance is approximately taken into account. We find that all (isolated vortex) effects reported by Hess *et al.*[1,2] can be reproduced with rather low numerical effort. In particular, it turns out that the observed broadening of the peak of $\sigma$ at $r=0$ with increasing voltage should actually be interpreted as a shift of the peak to a distance $r>0$. On the other hand, there are considerable quantitative differences between theory and experiment. We discuss some of the possible reasons for this disagreement.

As is well known, the quasiclassical theory and the Bogoliubov equations are physically equivalent except for extremely low temperatures $T/T_c<T_c/E_F$. In the quasiclassical (Green's functions) method the quasiparticle states may be labeled by two parameters, say $\theta$ and $\phi$, characterizing the direction of the wave vector $\mathbf{k}_F$. These parameters are defined as follows. If the vortex axis lies parallel to the $z$ direction, then $\pi/2-\theta$ is the angle between $\mathbf{k}_F$ and the $z$ axis and $\phi$ is the azimuth angle (for an isolated vortex the $\phi$ dependence is in a sense spurious since states belonging to different $\phi$ are related to each other by a rotation).

Kramer and Pesch's[5,9] bound-state solution of the quasiclassical equations makes use of the assumptions[10,11] $E/\Delta_{BCS}\ll1$ and $r_\perp/\xi_{BCS}\ll\cos\theta$, where $r_\perp$ is the shortest distance of the (straight) quasiparticle path[8] from the vortex axis. Recently, the steps leading to the final equations of Kramer and Pesch have been reviewed[8] in detail. Analytical results for the direction-dependent density of states $N(E,\theta,\phi,\mathbf{r})$ have been worked out[8] using the model order parameter

$$\Delta=\begin{cases}\Delta_{BCS}r/\xi_1, & r<\xi_1\\ \Delta_{BCS}, & r>\xi_1\end{cases},$$

and assuming negligible vector potential $\mathbf{a}\sim0$. In the considered version of the Kramer-Pesch theory,[9] weak interactions between (almost isolated) flux lines are taken into account. To study the effect of impurities in a rough approximation a small imaginary number $-i\delta$ has to be added[12,13] to the energy $E$. In the present system of units,[8] where energies are measured in units of $\pi k_BT_c$, this imaginary part is just given by the impurity parameter $\delta=0.882\xi_{BCS}/l$.

The present results for the local density of states

 

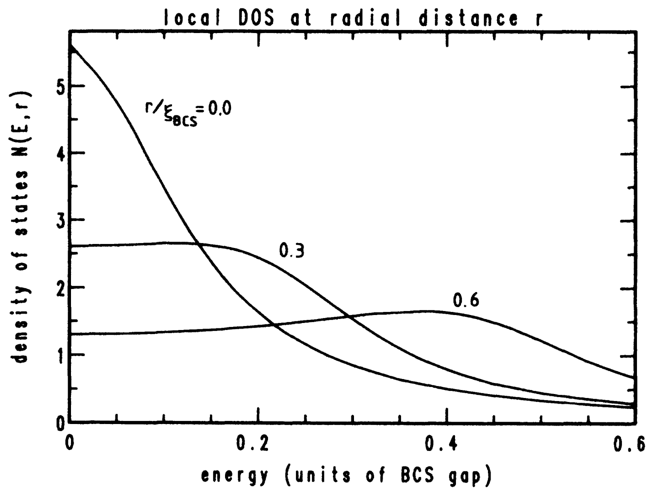


FIG. 1. Energy dependence of the local density of states at three different distances $r$ from the center of an isolated vortex. Parameters corresponding approximately to $NbSe_2$ have been chosen (see text), in particular $\delta=0.07$.

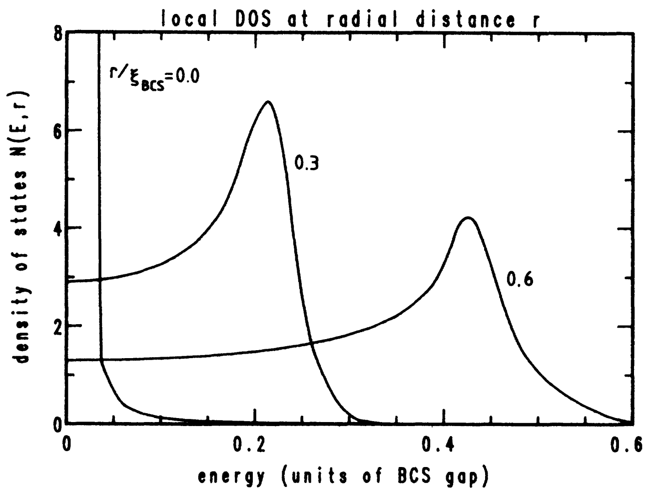


FIG. 2. Density of states at three different distances $r$ as in Fig. 1. The same set of parameters as in Fig. 1 has been chosen, except for $\delta=0.001$.

$N(E,r)$ have been obtained by integrating the quantity $N(E,\theta,\phi,r)$ with respect to $\theta$ and $\phi$. Then, the local tunneling conductance $\sigma(V,r)$, which is defined as the convolution of $N(E,r)$ and the derivative of the Fermi distribution function,[14] could be computed. Both $N(E,r)$ and $\sigma(V,r)$ have been normalized with respect to their normal-state values. The following parameters appropriate for $NbSe_2$ have been chosen: $\delta=0.07$ (which brings the thermally broadened Meissner state density of states in agreement with experimental data[2] and is consistent with previous estimates[15] in the literature) and $\xi_1=\xi_{BCS}$ [$\sim 100$ Å according to Ref. 16, this choice is rather arbitrary in view of the fact that the actual vortex structure will differ noticeably from the ideal (bulk) one]. The anisotropy of the material will be neglected as was done in Ref. 6; $\xi_{BCS}$ denotes the coherence length parallel to the layers of $NbSe_2$

We now proceed to a discussion of the numerical results. Only the positive-energy part of $N(E,r)$, which is a symmetric function of $E$, will be displayed in the following figures [a similar remark applies to $\sigma(V,r)$]. Figure 1 shows $N(E,r)$ for three different radial distances $r$. For $r=0$ we recover the zero energy peak and for $r>0$ the structure (maximum at $E>0$) predicted in Ref. 6. [Of course, in the present quasiclassical approach the rapid, irrelevant oscillations of $N(E)$ on a scale $\Delta^2_{BCS}/E_F$, visible in Fig. 3 of Ref. 6, are absent.] In contrast to Ref. 6 the maxima of $N(E)$ at $E>0$ are rather flat. This is a consequence of increased impurity content in the present calculations; the value of $\delta$ used in Fig. 1 ($\delta=0.07$) is large enough to yield a considerable suppression of the maxima of $N(E)$ although it still corresponds to a very clean superconductor. To illustrate the sensitivity of the results on impurity content, corresponding data for an extremely pure ($\delta=0.001$) superconductor are shown in Fig. 2.

A calculation of the tunneling conductance $\sigma$ (normalized by its normal-state value) at $r=0$ yields, for $T/T_c=0.2$, a zero-bias peak of 2.9, which is higher by a factor of 2.0 than the experimental one.[2] The clean limit result for the same parameters, except $\delta=0$, is 4.7. Thus, $\sigma$ still sensibly depends on impurity degree for $T/T_c=0.2$ (and below). Calculations for various values of $\delta$ and $\xi_1$ have been performed in an attempt to fit the observed[2] peak with respect to both its height and width. However, the theoretical peaks were always too sharp, agreement could only be obtained by using considerably enhanced temperatures ($T/T_c \sim 0.5$). In the clean limit the present zero-bias peak is similar to the one reported by Shore *et al.*[6] On the other hand, Fig. 3 shows theoretical and experimental[2] data on the (nonmonotonic) voltage dependence of $\sigma(V,r)$ for $r=90$ Å. Here, in contrast to the

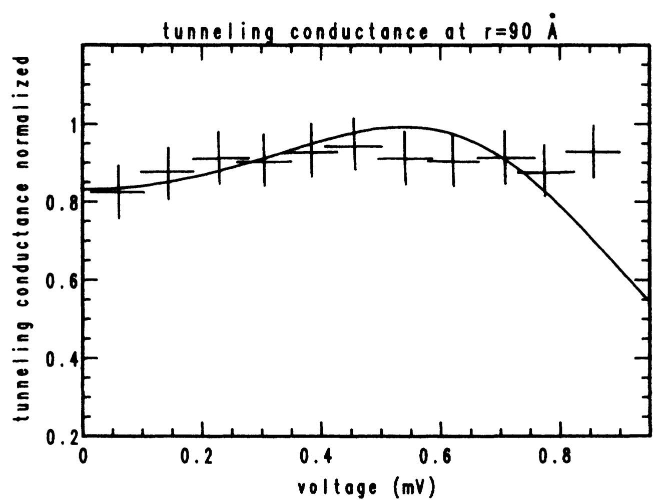


FIG. 3. Theoretical tunneling conductance (solid curve) at a distance of 90 Å from the vortex center. Parameters corresponding approximately to $NbSe_2$ have been used (see text). Also shown are experimental results by Hess *et al.* (Ref. 2). The experimental data had to be scaled by a factor of 1.2 in order to achieve overall agreement.

zero-bias peak, satisfactory agreement has been achieved.

Motivated by the broadening of the $r=0$ peak for nonzero bias reported by Hess *et al.*[2] (the second of the two new effects mentioned above) the space dependence of $N(E,r)$ has been calculated for several fixed energy values. According to the numerical results, shown in Fig. 4, at nonzero energy $E$ the peak position is shifted from $r=0$ to a radial distance $r$ approximately proportional to $E$. Again, decreasing impurity content leads to a more pronounced peak (see the dashed line in Fig. 4). Such a nonmonotonic variation should be visible if the tunneling conductance is measured at sufficiently low temperature. In the experiments by Hess *et al.*[2] this spatial structure has not yet been resolved as a consequence of thermal broadening. On the other hand, it provides a natural explanation for the broadening of the zero-distance peak observed[2] by these authors. (The situation is analogous to the broadening of the zero-bias peak illustrated in Figs. 3 and 4 of Ref. 6).

Recently, the quasiclassical equations have been solved on a hexagonal vortex lattice for real energies.[8] This numerical calculation, which is based on a previous solution[13] for imaginary energies, holds for arbitrary inductions and energies in the clean limit. It yields the local, direction-dependent density of states $N(E,\mathbf{k}_F,\mathbf{r})$, i.e., the local density of states for the single-particle excitations characterized by wave vector $\mathbf{k}_F$ and energy $E$. For small $E$ reasonable agreement with Kramer and Pesch's theory has been found. The properties of these single-particle excitations have already been used[8] to predict some general features (including the zero-bias peak) of $N(E,r)$.

The nonmonotonic behavior of $N(E,r)$ shown in Figs. 2 and 4 may also be understood in terms of these excitations. For a really isolated vortex in a perfectly clean superconductor the spatial region of nonzero $N(E,\mathbf{k}_F,\mathbf{r})$, i.e., the spatial region accessible to a quasiparticle, is given by a straight line of direction $\mathbf{k}_F/k_F$ (its motion is further restricted by Andreev reflection at the order-parameter potential wall). A convenient second parameter to characterize the quasiparticle path is its shortest distance $r_\perp$ from the vortex axis. Theory[5,8] predicts $E=c\,|\psi(r_\perp)|$, where $c$ is $\theta$ dependent but not far from one, and $|\psi(r_\perp)|$ denotes the smallest value of $|\psi|$ along a straight line of direction $\mathbf{k}_F/k_F$ (this direction is characterized by the angles $\theta$, $\phi$ introduced above). Intutitively speaking, a quasiparticle prefers a path where its energy is approximately equal to the minimal "gap" $|\psi(r_\perp)|$ it sees on its way. Along this path the density of states has its maximum at the point nearest to the vortex axis. Summing up all rotationally equivalent contributions, i.e., performing the integration with respect to $\phi$, one obtains a state which must be characterized by its angular momentum (as in Bogoliubov's theory) rather than its linear momentum. Obviously, this $\phi$-integrated density of states $N(E,\theta,r)$ will be zero for $r<r^*$, where $E=c\,|\psi(r^*)|$, and maximal near $r^*$, i.e., it shows precisely the behavior displayed in Fig. 4. Integration with respect to $\theta$ will not lead to qualitative changes because of the weak dependence of the energy levels on $\theta$. The energy dependence of $N(E,r)$, shown in Fig. 1, may be discussed in a similar way.

Finally, we discuss possible reasons for the considerable quantitative disagreement found in our comparison of theory and experiment. In view of a recent, fairly successful, comparison of Kramer and Pesch's theory[5,9] with more extended numerical calculations,[8] it seems unlikely that the approximations entering this theory constitute the main reason for the observed discrepancies.

There are two other possible reasons for this disagreement, besides experimental limitations of a more technical nature, such as uncertainty in the tip temperature. First, a vortex investigated by a STM is modified by surface effects. Where the vortex cuts the surface its core will blow up somehow, which implies a more or less serious modification of its excitation spectrum. Second, the tunneling current is actually not a simple average with respect to all quasiparticle directions but rather a weighted average, where excitations with directions parallel to the vortex axis (perpendicular to the surface) play the most important part.[17] These quasiparticles, with $\theta\sim\pi/2$, are loosely coupled to the bulk order parameter far from the core and should be more similar to normal-conducting excitations than those perpendicular to the vortex axis. For example, for $\theta=\pi/2$ and $r=0$ the (local) solution of the quasiclassical equations yields $N(E,r)=1$ for arbitrary energy $E$, a contribution which tends to broaden the zero-bias peak. It should be pointed out that these states with $\theta$ close to $\pi/2$ have not been properly taken into account in previous theoretical studies including both the Bogoliubov[4] and the quasiclassical[5] formalism. They are also difficult to calculate numerically.[8] Their neglect leads to a very small error in the usual (isotropic averaged) density of states but may be crucial if the tunneling current in the STM experiments is dominated by electrons lying within a cone of very small width. In addition, the question arises whether the isotropic Eilenberger theory used in the present paper is still a good approximation for

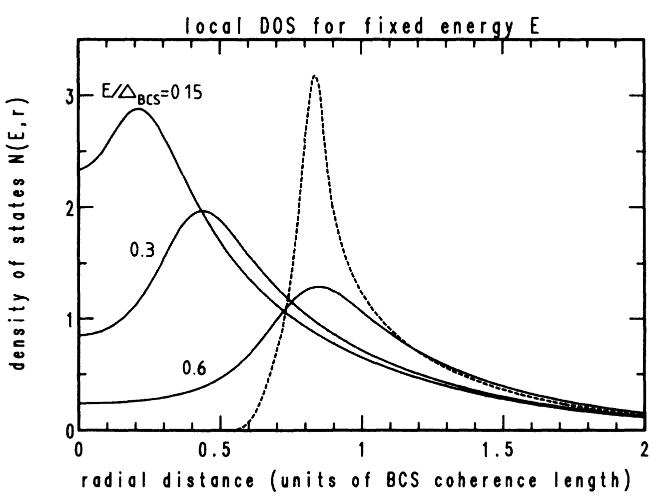


FIG. 4. Local density of states as a function of $r$ for three different values of $E$. The distance where a maximum occurs is approximately given by $1.5E/\Delta_{BCS}$. For the solid curves, parameters corresponding approximately to $NbSe_2$ (see text) have been used. The dashed curve refers to a clean superconductor with $\delta=0.001$ (and $E/\Delta_{BCS}=0.6$).

such a situation. A specification of this cone width as well as further theoretical study is required to settle this point.

If more vortices enter a sample with increasing magnetic field, the sharp energy levels of an isolated vortex become bands of finite width. This broadening of the energy levels (but not the quasiparticle tunneling occurring at higher inductions) can be treated, for large flux-line distance, by means of the present theory.[5,9] However, for the above-chosen impurity parameter corresponding to $NbSe_2$, the calculations show that the broadening of the levels is dominated by mean-free-path effects and no significant changes arise as a consequence of (small) vortex interaction. On the other hand, more extended calculations are required in order to explain Hess *et al.*'s data[2] on the density of states in the core region at $B=1$ T as well as the interesting features they found at the boundary of the Wigner-Seitz cell of a dense vortex lattice.

In conclusion, we found that Kramer and Pesch's bound-state solution of the quasiclassical equations is able to qualitatively explain all observed peculiarities of the density of states in a vortex core. The occurrence of such effects has been shown to depend sensitively on a sufficiently low impurity content. While our results yield further evidence that these phenomena may well be explained by standard BCS theory, a quantitative explanation has not yet been achieved and requires further experimental and theoretical progress.

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