Local density of states of a strongly type-II *d*-wave superconductor: The binary alloy model in a magnetic field

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We calculate self-consistently the local density of states (LDOS) of a *d*-wave superconductor considering the scattering of the quasiparticles off randomly distributed impurities and off externally induced vortices. The impurities and the vortices are randomly distributed but the vortices are preferably located near the impurities. The increase of either the impurity repulsive potential or the impurity density only affects the density of states slightly. The dominant effect is due to the vortex scattering. The results for the LDOS agree qualitatively with experimental results considering that most vortices are pinned at the impurities.

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Experimental evidence suggests that the pairing symmetry in high temperature superconductors (HTSC) is *d* wave.[1] A good description of the nonconventional superconducting phase is obtained using a standard BCS approach but a clear understanding of the normal phase of these materials remains a hard challenge. If we apply a strong enough magnetic field, these materials (being strongly type-II superconductors) will enter a vortex phase. Scanning tunneling microscopy (STM) studies of HTSC have revealed a very different quasiparticle structure from that predicted by the pure *d*-wave BCS single vortex models.[2] In a pure *d* wave there are extended gapless states, a fourfold symmetric shape of the local density of states (LDOS) and a zero-bias conductance peak. Experimentally, however, the following are observed: (i) the absence of zero energy peaks, (ii) the absence of coherence peaks close to the vortex, (iii) low-energy states with an energy ∼5.5 meV for YBCO and ∼7.7 meV for BSCCO, and (iv) the absence of fourfold symmetric star-shaped LDOS.[2] The coherence peaks are recovered about 10 Å from the core center[3] and the core states are localized decaying exponentially with distance (∼22 Å).[3] Possible reasons for the failure of the pure *d*-wave theory to explain the experimental results have included a mixed pairing of the type $d_{x^2-y^2}+id_{xy}$, considering that the vortices have antiferromagnetic cores such that localized magnetic order coexists with superconductivity or charge order fluctuations.[4,5]

Recently, a pure *d*-wave pairing for a vortex lattice has yielded results that are in good qualitative agreement with experiments.[6] Indeed a calculation of the local density of states shows that close to the vortex position the coherence peaks disappear, there are significant low energy peaks, and there is no zero energy enhancement of the density of states.[6] However, in most systems disorder is present, for instance, in the form of impurities. The presence of the impurities affects the quasiparticles (QP) in two ways: the QP scatter off the impurities due to potential scattering (if they are nonmagnetic) and the impurities pin the vortices also affecting the density of states of the QP, particularly at low energies.

The separate effects of the scattering of the quasiparticles from the impurities and from the vortices have been studied before. The details of the impurity disorder are relevant and a consistent picture of the various possible scenarios has been obtained.[7] Studies of the superfluid stiffness due to the presence of the impurities have revealed that, even though it gets lower, the decrease is smaller than expected. The reason is that the order parameter is only significantly affected very close to the impurities and largely unaffected elsewhere. Therefore the order parameter is very nonhomogeneous and a fully self-consistent calculation is required.[8] Considering exclusively the effect of the scattering off homogeneously distributed vortices (no impurities) it has been shown that in the lattice case the low energy states are extended Bloch states[9] instead of Dirac-Landau levels.[10] Also, it was shown that the quasiparticles, besides feeling a Doppler shift caused by the moving supercurrents,[11] also feel a quantum "Berry-like" term due to a half-flux, $\phi_0/2$, Aharonov-Bohm scattering of the quasiparticles by the vortices. The effect of a random vortex distribution was considered taking random and statistically independent scalar and vector potentials.[12] A finite density of states was predicted at zero energy. Also, by considering randomly pinned discrete vortices the density of states was calculated, displaying low energy peaks and no coherence peaks. However at low energies a power law deviation from a finite zero energy value was found, where both the zero energy value and the exponent depend on the magnetic field and on the Dirac anisotropy.[6] Also, it was found that even though the low energy states are strongly peaked at the vortex cores, they appear to remain extended. An approximate scaling of the density of states was found at low energies.[6]

In this work we study the *combined* effects on the quasiparticle spectrum of the scattering off impurities and vortices induced by an external magnetic field. We model the disorder using the binary alloy model[14] where the impurities are distributed randomly over the lattice sites. At each impurity site it costs an energy U to place an electron (it acts as a local shift on the chemical potential). The impurities are randomly distributed over a $L\times L$ periodic two-dimensional lattice and play the role of pinning centers for the vortices. It is favorable that a vortex is located in the vicinity of an impurity.[15] Taking into account a given distribution of the positions of the impurities $\{\mathbf{r}_i^p\}_{i=1,N_p}$, the distribution of the positions of

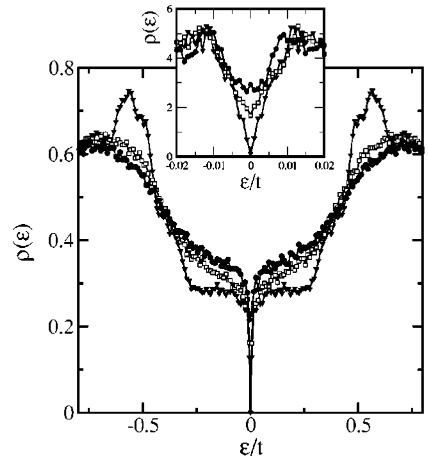

FIG. 1. Quasiparticle density of states for a 20×20 sites system with 4% of impurities, with $U=5t$, $\epsilon_F=1.2$, and $V=-2.3t$. We consider three cases: no vortices (▼), four vortices pinned at locations ensuring the minimization of the total vortex energy (□), and four vortices located at random (●). For each case the density of states is averaged over 100 configurations.

the vortices $\{\mathbf{r}_i^v\}_{i=1,N_v}$ is chosen in such a way it minimizes the total vortex energy given by $\mathcal{E}=\mathcal{E}_v+\mathcal{E}_p$, where $\mathcal{E}_v=\mathcal{U}_v\Sigma_{\mathbf{r}_i^v,\mathbf{r}_j^v}K_0(|\mathbf{r}_i^v-\mathbf{r}_j^v|/\lambda)$ is the repulsive interaction energy between the vortices in the London regime and $\mathcal{E}_p=\mathcal{U}_p\Sigma_{\mathbf{r}_i^v,\mathbf{r}_j^p}f(|\mathbf{r}_i^v-\mathbf{r}_j^p|/r_p)$ is the pinning energy associated with the impurities acting as pinning centers for the vortices. The interaction between the vortices is not significantly screened since the penetration length is very large. In the equations above $\mathcal{U}_v=(\phi_0/4\pi\lambda)^2$ is the energy of interaction between two vortices, $K_0(r)$ stands for the zero-order Hankel function, $\mathcal{U}_p<0$ is the pinning strength created by an impurity, and $f(r/r_p)$ is a rapidly decreasing function for $r/r_p>1$. In our model we assume that the pinning energy is much larger than the interaction between vortices $|\mathcal{U}_p|\gg\mathcal{U}_v$ and $r_p\sim\delta$ where δ is the lattice constant. In that case, as $N_v\ll N_p$ each vortex is preferably pinned in the close vicinity of an impurity. As we take the London limit, which is valid for low magnetic field and over most of the H-T phase diagram in extreme type-II superconductors such as cuprates, we assume that the size of the vortex core is negligible and place each vortex core at the center of a plaquette. So in the limit of the strong pinning described above, each vortex will be pinned in the center of one of the four plaquettes surrounding a site hosting an impurity. The plaquettes selected by the vortices are those minimizing the interaction energy $\mathcal{E}_v$ between the vortices.

Once the impurity positions $\{\mathbf{r}_i^p\}_{i=1,N_p}$ are fixed and the correlated vortex positions $\{\mathbf{r}_i^v\}_{i=1,N_v}$ are determined we are able to calculate the quasiparticle spectrum using the Bogoliubov-de Gennes (BdG) equations $\mathcal{H}(\mathbf{r})\Psi_n(\mathbf{r})=\epsilon_n\Psi_n(\mathbf{r})$, where $\Psi_n^\dagger(\mathbf{r})=(u_n^*(\mathbf{r}),v_n^*(\mathbf{r}))$. It is convenient[4,6] to perform a unitary gauge transformation. After carrying out this gauge transformation the Hamiltonian reads

$$\mathcal{H}=\begin{pmatrix}\hat{h}_A & \hat{\Delta}\\ \hat{\Delta}^\dagger & -\hat{h}_B^\dagger\end{pmatrix}, \quad (1)$$

where

$$\hat{h}_\mu=-t\sum_{\boldsymbol{\delta}}e^{i\mathcal{V}_{\boldsymbol{\delta}}^\mu(\mathbf{r})}\hat{s}_{\boldsymbol{\delta}}-\epsilon_F+\mathcal{U}(\mathbf{r}),$$

$$\hat{\Delta}=\sum_{\boldsymbol{\delta}}e^{i\mathcal{A}_{\boldsymbol{\delta}}(\mathbf{r})+i\pi\delta_y}\Delta(\mathbf{r},\mathbf{r}+\boldsymbol{\delta})\hat{s}_{\boldsymbol{\delta}}.$$

The phase factors are given by $\mathcal{V}_{\boldsymbol{\delta}}^\mu(\mathbf{r})=\int_{\mathbf{r}}^{\mathbf{r}+\boldsymbol{\delta}}\mathbf{k}_s^\mu\cdot d\mathbf{l}$ and $\mathcal{A}_{\boldsymbol{\delta}}(\mathbf{r})=\frac{1}{2}\int_{\mathbf{r}}^{\mathbf{r}+\boldsymbol{\delta}}[\mathbf{K}_s^A(\mathbf{l})-\mathbf{k}_s^B(\mathbf{l})]\cdot d\mathbf{l}$, where the vector $\hbar\mathbf{k}_s^\mu(\mathbf{r})=m\mathbf{v}_s^\mu(\mathbf{r})=\hbar\nabla\phi^\mu-(e/c)\mathbf{A}(\mathbf{r})$ is the superfluid momentum vector of the effective $\mu=A,B$ supercurrent. This quantity can be calculated for an arbitrary configuration of vortices, such as

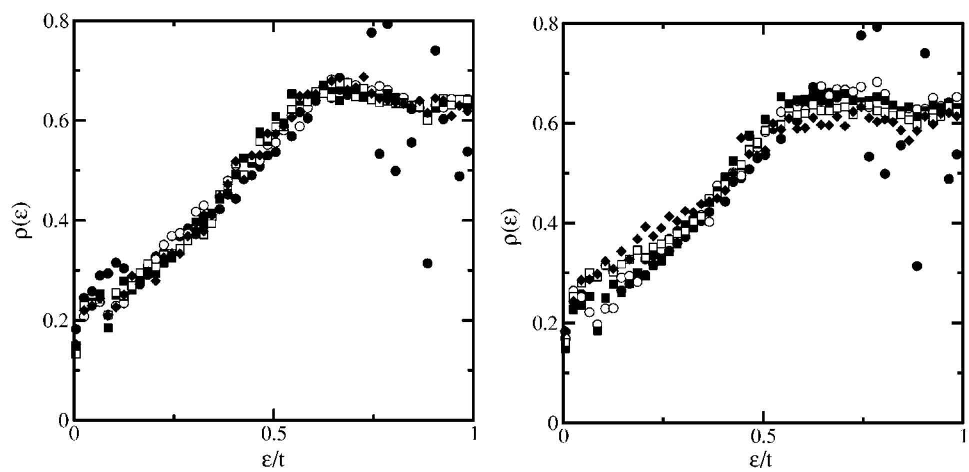

FIG. 2. Quasiparticle density of states for 20×20 sites. Left panel: system with 2% of impurities, four vortices pinned at locations ensuring the minimization of the total vortex energy and $U=2t$ (○), $5t$ (■), $10t$ (□), and $100t$ (♦). The case of four vortices pinned at random in a system without impurity is also presented (●). Right panel: system with four vortices pinned at locations ensuring the minimization of the total vortex energy, $U=5t$, and the following percentages of impurity: 0% [vortices pinned at random] (●), 1% (○), 2% (■), 4% (□), and 6% (♦).

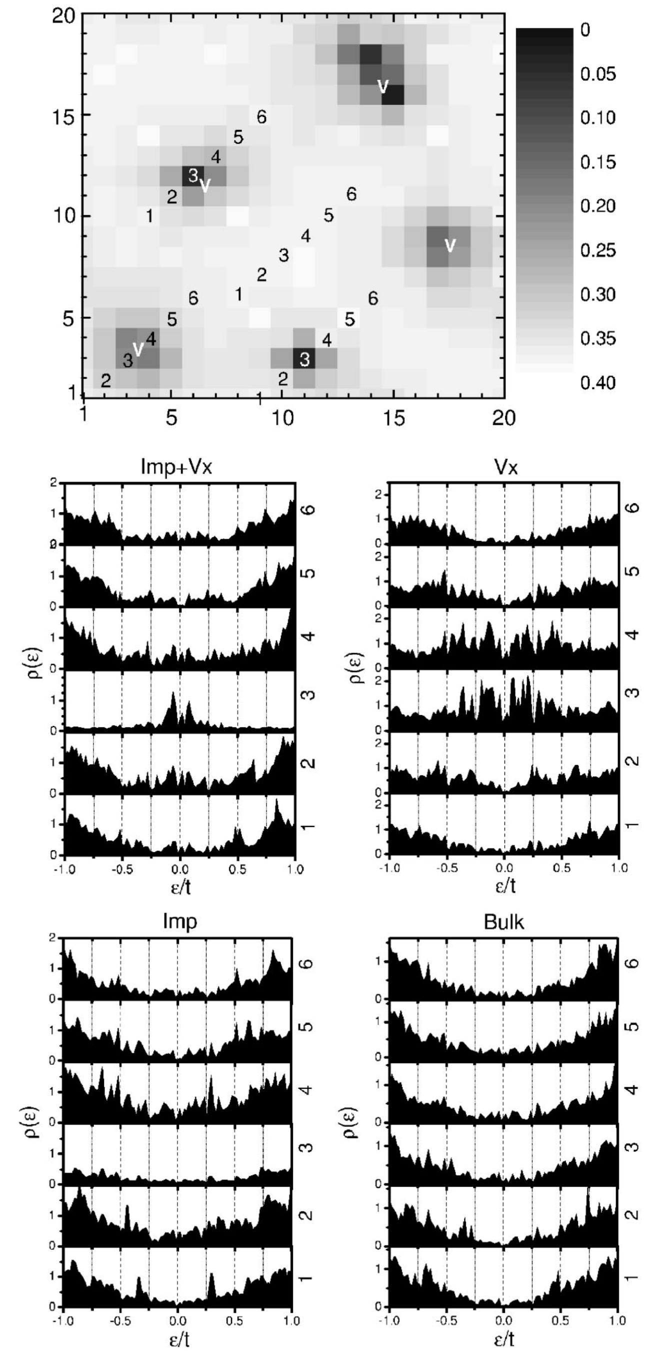

FIG. 3. Quasiparticle local density of states for different points on the lattice. The impurity concentration is 0.75%. We have chosen a particular distribution of the impurities and vortices where we can find the various possibilities of a site far from any impurity or vortex (Bulk), an impurity site with no vortex nearby (Imp), a site close to a vortex and no impurity nearby (Vx) and an impurity site with a vortex attached (Imp+Vx). For each of these four possibilities we have calculated the quasiparticle local density of states along a path of six numbered sites 1,…,6. On the top most pannel the four particular paths are shown on the top of the corresponding profile of the d-wave order parameter $\Delta_d(\mathbf{r})$. The path located on the center of the lattice corresponds to the Bulk case, the one centered on the site (6,12) corresponds to the Imp+Vx case, the one centered on the site (3,3) corresponds to the Vx case, and the one centered on the site (11,3) correspond to the Imp case.

$$\mathbf{k}_\mu(\mathbf{r}) = 2\pi \int \frac{d^2k}{(2\pi)^2}\frac{i\mathbf{k}\times\hat{z}}{k^2+\lambda^{-2}}\sum_i e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_i^{\mu})}. \qquad (2)$$

Here λ is the magnetic penetration length and the sum extends over all vortex positions. $\mathbf{A}(\mathbf{r})$ is the vector potential associated with the uniform external magnetic field $\mathbf{B}=\boldsymbol{\nabla}\times\mathbf{A}$. The vortices A are only visible to the electrons and the vortices B are only visible to the holes. Each resulting μ subsystem is then in an effective magnetic field $\mathbf{B}_{\mathrm{eff}}^{\mu}=-(mc/e)\boldsymbol{\nabla}\times\mathbf{v}_s^{\mu}=\mathbf{B}-\phi_0\mathbf{z}\Sigma_i\delta(\mathbf{r}-\mathbf{r}_i^{\mu})$ where each vortex carries now an effective quantum magnetic flux ϕ_0. For the case of a regular vortex lattice,[4,16] these effective magnetic fields vanish simultaneously on average over a unit magnetic cell containing two vortices, one of each type. More generally, in the absence of spatial symmetries, as it is the case for disordered systems, these effective magnetic fields $\mathbf{B}_{\mathrm{eff}}^{\mu=A,B}$ vanish if the number of vortices of the two types are in equal number, $N_A=N_B$, and equal to the number of elementary quantum fluxes ϕ_0 of the external magnetic field penetrating the system. The sums are over nearest neighbors ($\boldsymbol{\delta}=\pm\mathbf{x},\pm\mathbf{y}$ on the square lattice) and the operator $\hat{s}_{\boldsymbol{\delta}}$ is defined through its action on space-dependent functions, $\hat{s}_{\boldsymbol{\delta}}u(\mathbf{r})=u(\mathbf{r}+\boldsymbol{\delta})$. The energy $\mathcal{U}(\mathbf{r})$ is the impurity potential which takes the value $U>0$ at the sites $\{\mathbf{r}_i^p\}_{i=1,N_p}$ hosting an impurity and zero elsewhere. The operator $\hat{\eta}_{\boldsymbol{\delta}}=e^{i\pi\delta_y}\hat{s}_{\boldsymbol{\delta}}$ carries the symmetry of the d-wave order parameter. The disorder potential induced by the impurities and the inhomogeneous superfluid velocities induced by the vortices strongly affect the pairing potential $\Delta(\mathbf{r},\mathbf{r}+\boldsymbol{\delta})$ defined over the link $[\mathbf{r},\mathbf{r}+\boldsymbol{\delta}]$ of the two-dimensional lattice. Thus for a given configuration of the impurity positions and of the vortex positions the pairing potential $\Delta(\mathbf{r},\mathbf{r}+\boldsymbol{\delta})$ is calculated self-consistently until convergence is obtained for each individual link. On each lattice site we can define the amplitude of the d-wave order parameter as $\Delta_d(\mathbf{r})=\Sigma_{\boldsymbol{\delta}}(-1)^{\delta_y}\Delta(\mathbf{r},\mathbf{r}+\boldsymbol{\delta})$. The amplitude of the order parameter is strongly suppressed in the vicinity of impurities and vortices.

As the effective magnetic fields experienced by the particles and the holes vanish on average, within the gauge transformation we are allowed to use periodic boundary conditions on the square lattice $[\Psi(x+nL,y+mL)=\Psi(x,y)$ with $n,m\in\mathbb{Z}]$. The $L\times L$ original lattice becomes then a magnetic supercell where the impurities are placed at random and where the vortices are placed in such a way as to minimize their total energy. The disorder induced by the impurities in the system is then established over a length L. Thus in order to compute the eigenvalues and eigenvectors of the Hamiltonian (1) we seek for eigensolutions in the Bloch form $\Psi_{n\mathbf{k}}^{\dagger}(\mathbf{r})=e^{-i\mathbf{k}\cdot\mathbf{r}}(U_{n\mathbf{k}}^{*},\ V_{n\mathbf{k}}^{*})$ where $\mathbf{k}$ is a point of the Brillouin zone. We diagonalize then the Hamiltonian $e^{-i\mathbf{k}\cdot\mathbf{r}}\mathcal{H}e^{i\mathbf{k}\cdot\mathbf{r}}$ for a large number of points $\mathbf{k}$ in the Brillouin zone and for many different realizations (around 100) of the random impurity positions and of the correlated vortex positions.

In Fig. 1 we show the density of states averaged over 100 configurations for a moderate impurity concentration and for a typical value of $U=5t$. We compare the cases with no vortices and with a low vortex density (considering both an energetically favorable distribution of the vortices and a fully random configuration). The self-consistent calculation of the order parameter gives a maximum amplitude, Δ_0, of the order of $0.5t$. It is clear that when there are no vortices present, coherence peaks appear at $\epsilon \sim \Delta_0$. If the vortices penetrate the sample these peaks disappear. Without vortices the density of states vanishes at zero energy as found before and if we include the magnetic field the density of states becomes finite.[6] Also it is clear that if the vortices are fully randomly distributed the DOS is larger than the one where the vortices tend to be pinned at the impurity sites. The results are therefore qualitatively similar to the ones obtained when there are no impurities present ($U=0$).[6] In Fig. 2, we show the influence of the impurity concentration and of the repulsive local potential U. Changing the impurity concentration leads to no qualitative difference except that there is a slight increase in the density of states (DOS). The same happens with the change of U. Both sets of results indicate that the strong effect is the scattering off the vortices.

More detailed information about the scattering of the quasiparticles is obtained calculating the LDOS for a given impurity and vortex configuration. It is defined by

$$\rho(\vec{r},\epsilon) = \sum_n \left[|u_n(\vec{r})|^2 + |v_n(\vec{r})|^2\right]\delta(\epsilon - \epsilon_n).$$

In Fig. 3 we compare the LDOS at four different sites. (i) At a site in the bulk the band-structure profiles are somewhat similar to the case of a vortex lattice.[6] The coherence peaks are evident, the zero-energy density of states is very small (but not strictly zero), and the low-energy peaks are smeared out. (ii) At an impurity site (and no vortex nearby) the same structure is apparent except that since the impurity potential is repulsive the density of states at the impurity site is considerably depleted at low energy (for instance, in the very large U limit the density of states is virtually zero at the impurity site). (iii) In the vicinity of a vortex site (but far from any impurity) the structure is very similar to the case obtained before[6] with no coherence peaks close to the vortex and an enhanced zero-energy density of states near the vortex. (iv) Finally the interesting case of a location where a vortex is bound to an impurity reveals that the coherence peaks are recovered very close to the vortex. Also, the low-energy density of states at the impurity site is increased with respect to the (Imp) case, due to the vortex nearby. However the density of states is considerably smaller than for the case (Vx) of a vortex far from any impurity.

The results obtained previously for the vortex lattice case with no impurities explain qualitatively the DOS results but are not realistic. In the experimental systems disorder is present and its effect must be taken into account. The results show that the dominant effect on the quasiparticle DOS is due to the vortex scattering. The presence of an impurity basically renormalizes the DOS except when the impurity is strongly repulsive where the density of states is significantly depressed near the impurity. This is the unitary limit where a gapped system is predicted in the absence of magnetic field.[7] The quantum effect originated in the Aharonov-Bohm scattering of the quasiparticles circulating around a vortex line has been shown to have considerable effects on the density of states.[16,17] Significant changes with respect to the classical Doppler shift effect[11] occur at low energies.[16] The results obtained in this paper show that the addition of impurity scattering is not very significant and the Berry phase is dominant, as argued before.[4,6] The results are very similar to the ones obtained experimentally with STM in Ref. 3 except for the finite density of states at zero energy in the vicinity of an isolated vortex. The experimental results are therefore more consistent with the situation where all or most of the vortices are pinned to the impurity sites. At these points, even though there is an enhancement of the low-energy density of states with respect to an impurity with no vortex attached, the increase is reduced by the presence of the impurity with respect to the case of a vortex but no impurity nearby.

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