Anisotropic vortices on superconducting Nb(110)

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We investigate the electronic properties of type-II superconducting Nb(110) in an external magnetic field. Scanning tunneling spectroscopy reveals a complex vortex shape which develops from circular via coffee bean-shaped to elliptical when decreasing the energy from the edge of the superconducting gap to the Fermi level. This anisotropy is traced back to the local density of states of Caroli–de Gennes–Matricon states which exhibits a direction-dependent splitting. Oxidizing the Nb(110) surface triggers the transition from the clean to the dirty limit, quenches the vortex bound states, and leads to an isotropic appearance of the vortices. Density functional theory shows that the Nb(110) Fermi surface is stadium-shaped near the Γ point. Calculations within the Bogoliubov-de Gennes theory using these Fermi contours consistently reproduce the experimental results.

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Introduction — In the recent past, we have witnessed a growing interest in the physical properties of vortices in unconventional and topological superconductors, as they allow for the emergence of Majorana zero modes (MZMs) which may potentially be used for applications in quantum computation. Although some success has been achieved on heavy electron iron-based superconductors, the unambiguous spectroscopic identification of MZMs remains demanding, as their spectroscopic distinction from trivial quasiparticle excitations at experimentally accessible temperatures still constitutes significant challenges.

In vortices, such trivial excitations occur when the electron mean free path ℓ is much larger than the vortex diameter, i.e., the superconducting coherence length ξ. As predicted by Caroli, de Gennes, and Matricon in the 1960s, Andreev reflection inside the vortex gives rise to a discrete set of bound states. Their separation in energy is given by ∆²/E_F, where 2∆ is the width of the superconducting gap and E_F is the Fermi energy, often resulting in values in the meV range only. At such low splittings, the CdGM states above and below the Fermi level can hardly be resolved even if measurements are performed at milli-Kelvin temperatures, as they thermally merge into one broad peak which appears to be energetically positioned at zero bias.

Furthermore, the spatial distribution of specific CdGM states inside the vortex scales with their angular momentum µ, resulting in a wave function which peaks at a distance r_µ ≈ |µ|/k_F away from the vortex core. However, the specific spatial and energy distribution of CdGM bound states in a given material depends on various parameters, such as the pairing anisotropy, spin-orbit coupling, Fermi surface anisotropy, or vortex–vortex interactions. In fact, the resulting patterns of vortex bound states can be quite complex. Furthermore, in the dirty limit (ℓ ≪ ξ), scattering processes lead to energetic broadening and eventually the complete quenching of the CdGM states. Thus, detailed investigations of the electronic structure inside superconducting vortices can help to better understand and tell apart trivial from topological states.

In this paper, we present results of a scanning tunneling spectroscopy (STS) study of vortex bound states on clean and oxygen-reconstructed Nb(110) in an external out-of-plane magnetic field. Whereas no bound states are found on the oxygen-reconstructed surface, a well pronounced zero-bias peak appears in the vortex core of clean Nb(110). Differential conductance dI/dU maps measured at constant tip-sample distance reveal that the spatial distribution of the local density of states (LDOS) crucially depends on the bias voltage. While round-shaped vortices are visualized when the bias is set close to the edge of the superconducting gap, a two-fold anisotropy is observed at zero bias with an intermediate coffee bean-shaped form (the shape of a roasted coffee robusta bean, to be precise). The elliptical shape of the LDOS maps is qualitatively explained by the anisotropy of the Fermi surface which exhibits a stadium-like shape around the Γ point of the surface Brillouin zone (SBZ). Using this anisotropic Fermi surface as an input, the experimental data are modeled by solving self-consistently the Bogoliubov-de Gennes (BdG) equation.

Experimental procedures — STM and STS measure-
ments are performed in a home-built setup (base temperature $T = 1.4$ K) which is equipped with a superconducting magnet capable of delivering a magnetic field up to $\mu_0 H = 12$ T along the surface normal. Spectroscopic measurements are conducted by a lock-in technique with $U_{mod} = 0.1 \div 0.2$ meV at a modulation frequency $f = 890$ Hz. Nb(110) was cleaned by a series of high temperature flashes up to $T_B \approx 2400$ °C. As described in detail in Ref. [22], lower flash temperatures result in two intermediate and less-ordered oxygen reconstructions, i.e., NbO$_x$ phase-I at $T_B \leq 1800$ °C and NbO$_x$ phase-II for $2000$ °C $\leq T_B \leq 2300$ °C [23].

Experimental results—Figure 1(a) shows the constant-current STM topography image of a clean Nb(110) surface with occasional oxygen-reconstructed patches which appear as dark spots (< 10% of the surface area). The atomic resolution scan reported in Fig. 1(b) confirms the expected lattice constant $a_{[001]} = 330$ pm. Nb is a type-II superconductor with $T_c^{Nd} = 9.2$ K which—if exposed to an external magnetic field—forms an Abrikosov lattice of normal conducting vortices. Tunneling spectra taken far from any vortex show a well-defined superconducting gap with $\Delta = 1.53$ meV [Fig. 1(c)]. We carefully investigate the spatial variation of the electronic structure around vortex cores by mapping the differential conductance $dI/dU$ at various energies $E = eU$ within the superconducting gap. To avoid set-point-related artifacts, all measurements are performed by stabilizing the STM tip at a set-point bias voltage corresponding to an energy far within the normal metallic regime, i.e., at $U_{set} = -100$ mV. After recording the $z$-trace along one scan line at this bias voltage the feedback is switched off, the bias voltage is set to measurement parameters, and the tip is approached towards the surface by a fixed value $\Delta z = 180$ pm. Afterwards the $dI/dU$ signal is measured along the (shifted) $z$-trace. This procedure increases the tunneling current and thereby improves the signal-to-noise ratio. At the same time, it guarantees that the

FIG. 1. (a) Topography of clean Nb(110). (b) Atomic resolution scan with indicated unit cell. (c) Tunneling spectrum of the superconducting gap. (d)-(g) Constant-separation $dI/dU$ maps taken at the voltages marked by colored circles in (c) at $\mu_0 H = 100$ mT. Whereas the vortices appear round-shaped at a bias voltage close to the edge of the gap, they deform into ellipses when approaching zero bias. (h) Stacked representation showing the bias-dependent LDOS inside the vortex in the $[001]$ direction only a vanishing of the peak without any splitting is observed (m). Scan parameters: (a)-(m) $I_{set} = 200$ pA; $T = 1.4$ K (a) $U_{set} = -1$ V; (c) $U_{set} = -10$ mV; (d)-(g) $U_{set} = -100$ mV; (h)-(j) $U_{set} = -10$ mV; (k)-(m) $U_{set} = -7$ mV.
$dI/dU$ maps presented in Figs. 1(d)-(g) are measured at a constant tip-sample separation.

Figures 1(d)-(g) show the Abrikosov lattice formed on clean Nb(110) in a magnetic field $\mu_0 H = 100 \text{ mT}$ at four selected tunneling voltages indicated by colored circles in Fig. 1(e). Some qualitative differences regarding the appearance of the vortices are immediately evident. At $U = -2 \text{ mV}$ [Fig. 1(d)], i.e., at an energy which corresponds to the maximum DOS at the coherence peak, the vortices appear as dark circular regions with a diameter of about 50 nm. As we approach the Fermi level, the vortices split along the [100] direction [Fig. 1(e)], and eventually deform into ellipses [Fig. 1(f)-(g)]. Furthermore, due to the vanishing of the superconducting gap and the enhanced quasiparticle LDOS inside the vortex, the vortices appear brighter than the surrounding superconducting area in Fig. 1(e)-(g).

A more detailed, stacked representation of the energy-dependent vortex shape is presented in Fig. 1(h) for positive bias voltages. As can be expected for particle–hole symmetric excitations in superconductors, the behavior is equivalent to the scenario described in panels (d)–(g) for negative bias. Again, the vortex appears as a circular region of reduced LDOS at the coherence peaks ($U = 2 \text{ mV}$). As the voltage is reduced the LDOS intensity becomes (i) larger inside the vortex than in the surrounding superconducting region, it (ii) splits along [100] direction ($1.2 \text{ mV} \geq U \geq 0.7 \text{ mV}$), and eventually (iii) elongates along the [001] direction ($U \leq 0.7 \text{ mV}$). Figure 1(i) presents the $dI/dU$ map of a vortex measured at the Fermi level ($U = 0 \text{ mV}$). Its shape clearly deviates from a circle (hatched line) and rather corresponds to an ellipse (thick white line) with the semi-major $a$ and semi-minor $b$ axes oriented along the [001] and [100] direction, respectively. The ratio $b/a$ amounts to $\approx 0.55$. We would like to emphasize that the orientation of the ellipse does not depend on the presence of defects, such as step edges, and stays the same at higher magnetic fields.

Figures 1(k) and (m) show the spatial evolution of tunneling spectra measured along the axes $b$ and $a$. The spectrum measured at the vortex center is characterized by a strong zero-bias peak, representing CdGM states which are thermally blurred into a single peak [19, 20]. However, along the two high-symmetry axes we observe qualitatively different transitions from the peaked spectrum measured at the vortex center to the fully gapped spectrum far away. Whereas the zero-bias peak splits in energy into two ridges if measured along the [100] direction [marked by two black arrows and hatched lines in Fig. 1(k)], a behavior expected for CdGM state [17, 21], no such splitting is detected along $a$, i.e., the major axes along the [001] direction [Fig. 1(m)].

A detailed investigation of the electronic structure inside vortices observed on ordered clean Nb(110), the less-ordered NbO$_x$ phase-II, or the disordered NbO$_x$ phase-I [22] reveals that the existence and shape of ZBP features critically depends on the surface quality. Fig. 2(a) presents tunneling spectra measured in vortex cores on all three surfaces. For comparison, the black curve in Fig. 2(a) shows the spectrum of superconducting clean Nb(110) far away from any vortex; (blue) intense zero-bias peak in the center of the vortex on clean Nb(110); (green) less intensive peak in a vortex core on NbO$_x$ phase-II; (red) Ohmic behavior in vortex core on NbO$_x$ phase-I. Stabilization parameters: $U_{\text{set}} = -7 \text{ mV}$, $I_{\text{set}} = 100 \text{ pA}$. Panels (b)-(d) show differential conductance $dI/dU$ maps of a single vortex on NbO$_x$ phase-I imaged at (b) $U = 1 \text{ mV}$, (c) $U = 0.8 \text{ mV}$, and (d) $U = 0 \text{ mV}$. (e) Tunneling spectra measured along the line in (d). No zero-bias feature is observed. Stabilization parameters: $U_{\text{set}} = -5 \text{ mV}$, $I_{\text{set}} = 100 \text{ pA}$, $\mu_0 H = 100 \text{ mT}$, $T = 1.5 \text{ K}$.

This reduction of the ZBP is accompanied by a more isotropic appearance of vortices, as evidenced by the $dI/dU$ map of a vortex on the NbO$_x$ phase-I presented in Fig. 2(b-d), which remains circular throughout the entire energy range within the superconducting gap. Furthermore, the tunneling spectra presented in Fig. 2(e) which were taken along the line in (d) across the vortex reveal the absence of any feature potentially related to bound states. These findings suggest that the origin of the anisotropy observed for vortices on the clean Nb(110) surface results from the presence of the CdGM states. Their absence on the less ordered NbO$_x$ phase-I is consistent with a cross-over from the clean to the dirty limit [21]. If we assume for the clean Nb(110) surface a mean free path close to the bulk value, $\ell_{\text{Nb}} \geq 100 \text{ nm}$.
it clearly exceeds the coherence length $\xi^\text{Nb} \approx 38 \text{ nm}$. Since the oxygen-reconstructed surfaces of Nb are less ordered, additional scattering of quasiparticles may substantially decrease the mean free path and quench the CdGM states.

Discussion—Anisotropic vortices were first observed by Hess et al. on superconducting NbSe$_2$ [19, 20]. Three scenarios were discussed as potential reasons: (i) vortex–vortex interactions, (ii) anisotropic pairing, and (iii) an anisotropy of the Fermi surface [19, 21, 24]. The effect of vortex–vortex interactions becomes relevant for spacings comparable with or smaller than the London penetration depth $\lambda$. Under this condition the stray field-mediated interaction between a given vortex and adjacent flux lines may cause a significant distortion of its shape [17]. Furthermore, as the spacing approaches the characteristic coherence length $\xi$, the hybridization of the nearest neighbor quasiparticle wave functions may also affect the LDOS [18]. However, both $\lambda^\text{Nb} \approx 39 \text{ nm}$ and $\xi^\text{Nb} \approx 38 \text{ nm}$ are at least four times smaller than the Abrikosov lattice constant ($\approx 160 \text{ nm}$) observed at $\mu_0 H = 100 \text{ mT}$. Therefore, we rule out that scenario (i) is responsible for the observed elliptical shape in Nb.

The two-fold rotational symmetry of (110) surfaces of body-centered cubic crystals, such as Nb, certainly implies inequivalent electronic properties along the two high-symmetry directions [001] and [110]. Since both scenarios, (ii) and (iii), are intimately related to the surface electronic structure of the respective superconductor, either of the two effects may—in principle—be responsible for the anisotropic dispersion of bound states inside the vortex. However, experiments performed on crystalline Nb planar tunnel junctions suggest that the anisotropy of the superconducting gap does not exceed 10% of the average value ($\Delta = 1.53 \text{ meV}$) [26, 27], insufficient to explain the strong anisotropy observed in Fig. 1(j).

To explain the experimental observations, we calculate the Fermi surface of clean Nb(110) using the plane-wave-based VASP [28, 29] code within the projector augmented-wave method [30, 31]. The generalized gradient approximation of Perdew-Burke-Ernzerhof [32, 33] is used for the exchange correlation. Details of theory methods and examples of the good agreement between theoretical and measured LDOS can be found in Ref. [24].

The calculated Fermi surface of the Nb(110) surface is plotted in Fig. 3(a). Multiple Fermi surface pockets centered around the various high-symmetry points $\Gamma$, $\overline{N}$, $\overline{S}$, and $\overline{\Gamma}$ can be recognized [22]. Since STM is most sensitive to electronic states in vicinity to the $\Gamma$ point of the SBZ, with other states decaying exponentially with increasing $k \parallel$ [34, 35], we expect that the stadium-shaped contours (red) in Fig. 3(a) contribute most to the measured signal. Therefore, we employ similar contours to approximate the Fermi surface within an effective model described in the following.

In this model, we consider an electron gas on a 2D square lattice, with different effective masses, $m_x / m_y \approx 0.47$, in two principal directions and with an s-wave pairing interaction. In order to mimic a truly anisotropic band structure, we further consider an isotropic spin-orbit interaction, which can be either of Rashba or Dresselhaus type [36, 37]. This spin-orbit interaction results in two split Fermi surfaces. The larger Fermi surface takes a stadium shape and carries a strong anisotropic Fermi velocity, see Fig. 3(b), while the smaller one is circular. We set the chemical potential at a value where the stadium-shaped Fermi surface dominates. Additionally, we apply a quantized magnetic flux and impose magnetic periodic boundary conditions on the lattice. Then, we solve the resulting BdG equations self-consistently on the lattice and calculate the LDOS around a vortex core at a low temperature set to $k_B T \approx 0.26 \Delta_0$, where $\Delta_0$ is the pairing potential in the absence of the magnetic field. We present the results in Figs. 3(d–e) and provide
more details about the simulation in Ref. [23]. At low excitation energies, the LDOS is enhanced at the vortex core with an elliptical shape. This changes to a coffee-bean shape at intermediate excitation energies and to a round shape at high excitation energies, in excellent qualitatively agreement with experimental observations.

Our analysis confirms that the anisotropy of the Fermi surface is carried over to the spatial structure of the excited states within the vortices. Depending on details of the anisotropy of the Fermi surface and the resulting Fermi velocities and the spin-orbit coupling, a distinct anisotropy of the CdGM states can be observed even in a system with an isotropic order parameter.

**Conclusion**—In conclusion, we have presented STS studies of vortex bound states of the clean Nb(110) surface in an external magnetic field. Our results reveal that the vortex shape in dI/dU maps depends on the energy, transforming from circular to a coffee-bean shape, and finally to an ellipses when approaching $E_F$. We provided evidence that the observed energy-dependent spatial distribution originates from Caroli-de Gennes-Matricon states which inherit their anisotropy from the Nb(110) Fermi surface. By oxidizing the Nb(110) surface we could trigger the transition from the clean to the dirty limit, accompanied by the complete disappearance of any anisotropy in the LDOS due to the quenching of the vortex bound states. These findings will be useful in the future for distinguishing trivial from topological vortex bound states by, for example, their spatial distribution or by introducing disorder.

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