








**Anisotropic vortices on superconducting Nb(110)**Artem Odobesko <sup>1,\*</sup>, Felix Friedrich <sup>1</sup>, Song-Bo Zhang <sup>2</sup>, Soumyajyoti Haldar <sup>3</sup>,  
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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, attenuates 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  $\bar{\Gamma}$  point. Calculations within the Bogoliubov–de Gennes theory using these Fermi contours consistently reproduce the experimental results.

DOI: [10.1103/PhysRevB.102.174502](https://doi.org/10.1103/PhysRevB.102.174502)**I. 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) [1–3] which may potentially be used for applications in quantum computation [4]. Although some success has been achieved on heavy electron iron-based superconductors [5,6], the unambiguous spectroscopic identification of MZMs remains demanding, as their spectroscopic distinction from trivial quasiparticle excitations at experimentally accessible temperatures still constitutes significant challenges [7–9].

In vortices, such trivial excitations occur when the electron mean free path  $\ell$  is much larger than the vortex diameter, i.e., the superconducting coherence length  $\xi$ . As predicted by Caroli, de Gennes, and Matricon (CdGM) in the 1960s [10], Andreev reflection inside the vortex gives rise to a discrete set of bound states. Their separation in energy is given by  $\Delta^2/E_F$ , where  $2\Delta$  is the width of the superconducting gap and  $E_F$  is the Fermi energy, often resulting in values in the  $\mu\text{eV}$  range only [11]. At such low splittings, the CdGM states above and below the Fermi level can hardly be resolved even if measurements are performed at millikelvin temperatures, as they thermally merge into one broad peak which appears to be energetically positioned at zero bias [12–14].

Furthermore, the spatial distribution of specific CdGM states inside the vortex scales with their angular momentum  $\mu$ , resulting in a wave function which peaks at a distance  $r_\mu \approx |\mu|/k_F$  away from the vortex core [11,15]. 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 [16–18]. In fact, the resulting patterns of vortex bound states can be quite complex [19,20]. Furthermore, in the dirty limit ( $\ell \lesssim \xi$ ), scattering processes lead to energetic broadening and eventually the complete quenching of the CdGM states [21]. 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 a 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 twofold anisotropy is observed at zero bias with an intermediate coffee-bean-shaped form (the shape of a roasted *coffea 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 stadiumlike shape around the  $\bar{\Gamma}$  point of the surface Brillouin zone (SBZ). Using this anisotropic Fermi surface as an input, the experimental data are modeled self-consistently by solving the Bogoliubov–de Gennes (BdG) equation.

**II. EXPERIMENTAL PROCEDURES**

Scanning tunneling microscopy (STM) and STS measurements are performed in a home-built setup (base temperature

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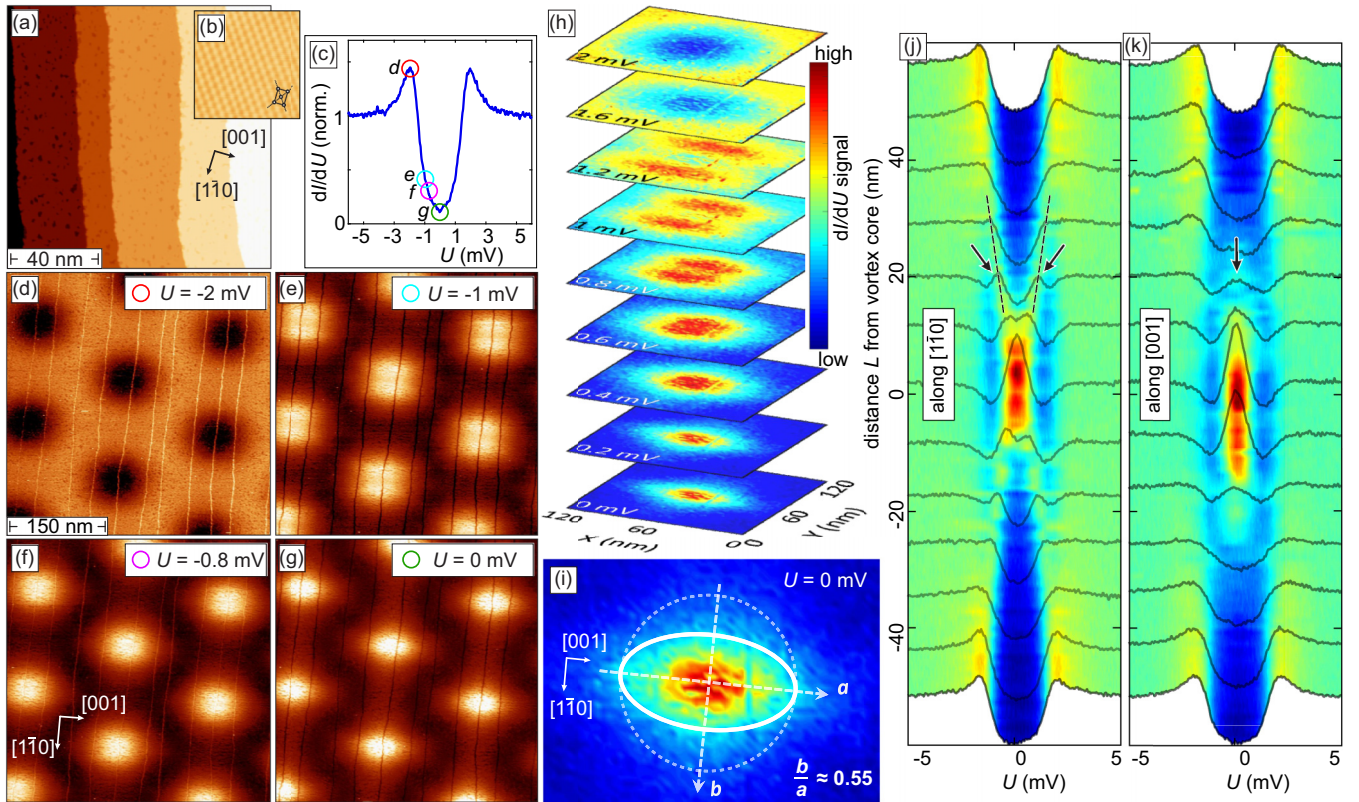


FIG. 1. (a) Topography of clean Nb(110). (b) Atomic resolution scan with the indicated unit cell. (c) Tunneling spectrum of the superconducting gap. (d)–(g) Constant-separation  $dI/dU$  maps taken at the voltages marked by colored circles in (c) at  $\mu_0 H = 100$  mT. Whereas the vortices appear round 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 energy window from 0 to 2 mV. (i) Fermi level ( $U = 0$  V)  $dI/dU$  map revealing an elliptical shape elongated along the [001] direction with a compression  $b/a = 0.55 \pm 0.1$ . (j), (k) Waterfall plot of tunneling spectra taken along the lines labeled  $b$  and  $a$  in (i), respectively. With increasing distance from the vortex core along the  $[1\bar{1}0]$  direction the zero-bias peak splits into two ridges, resulting in the appearance of an X-shaped feature as indicated by two arrows and dashed lines in (j). In contrast, along the [001] direction only a vanishing of the peak without any splitting is observed (k). Scan parameters: (a)–(k)  $I_{\text{set}} = 200$  pA;  $T = 1.4$  K (a)  $U_{\text{set}} = -1$  V; (c)  $U_{\text{set}} = -10$  mV; (d)–(g)  $U_{\text{set}} = -100$  mV; (h)–(i)  $U_{\text{set}} = -10$  mV; (j)–(k)  $U_{\text{set}} = -7$  mV.

$T = 1.4$  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  $U_{\text{mod}} = 0.1$ – $0.2$  meV at a modulation frequency  $f = 890$  Hz. Nb(110) was cleaned by a series of high-temperature flashes up to  $T_{\text{fl}} \approx 2400$  °C. As described in detail in Ref. [22], lower flash temperatures result in two intermediate and less-ordered oxygen reconstructions, i.e.,  $\text{NbO}_x$  phase I at  $T_{\text{fl}} \leq 1800$  °C and  $\text{NbO}_x$  phase II for  $2000$  °C  $\leq T_{\text{fl}} \leq 2300$  °C [23].

### III. 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  $T_c^{\text{Nb}} = 9.2$  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  $U_{\text{set}} = -100$  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  $dI/dU$  maps presented in Figs. 1(d)–1(g) are measured at a constant tip-sample separation.

Figures 1(d)–1(g) show the Abrikosov lattice formed on clean Nb(110) in a magnetic field  $\mu_0 H = 100$  mT at four selected tunneling voltages indicated by the colored circles in Fig. 1(c). Some qualitative differences regarding the appearance of the vortices are immediately evident. At  $U = -2$  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  $[1\bar{1}0]$  direction [Fig. 1(e)], and eventually deform into ellipses [Figs. 1(f) and 1(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 Figs. 1(e)–1(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 Figs. 1(d)–1(g) for negative bias. Again, the vortex appears as a circular region of reduced LDOS at the coherence peaks ( $U = 2$  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 the  $[1\bar{1}0]$  direction ( $1.2$  mV  $\geq U \geq 0.7$  mV), and eventually (iii) elongates along the  $[001]$  direction ( $U \leq 0.7$  mV). Figure 1(i) presents the  $dI/dU$  map of a vortex measured at the Fermi level ( $U = 0$  mV). Its shape clearly deviates from a circle (hatched line) and rather corresponds to an ellipse (thick white line) with the semimajor  $a$  and semiminor  $b$  axes oriented along the  $[001]$  and  $[1\bar{1}0]$  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(j) and 1(k) 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  $[1\bar{1}0]$  direction [marked by two black arrows and hatched lines in Fig. 1(j)], a behavior expected for CdGM state [17,24], no such splitting is detected along  $a$ , i.e., the major axes along the  $[001]$  direction [Fig. 1(k)].

A detailed investigation of the electronic structure inside vortices observed on ordered clean Nb(110), the less-ordered NbO<sub>x</sub> phase II, or the disordered NbO<sub>x</sub> phase I [22] reveals that the existence and shape of zero-bias peak (ZBP) features critically depends on the surface quality. Figure 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 a vortex, clearly presenting a superconducting gap. Evidently, the spectral features observed around zero bias exhibit marked, surface structure-dependent differences. Whereas the ZBP intensity measured on clean Nb(110) (blue) clearly exceeds the normal conducting DOS, indicating the presence of CdGM states in the vortex core, the ZBP is less pronounced on the NbO<sub>x</sub> phase II (green) and essentially absent for the NbO<sub>x</sub> phase I (red).

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<sub>x</sub> phase I presented in Figs. 2(b)–2(d), which remains circular throughout the entire energy

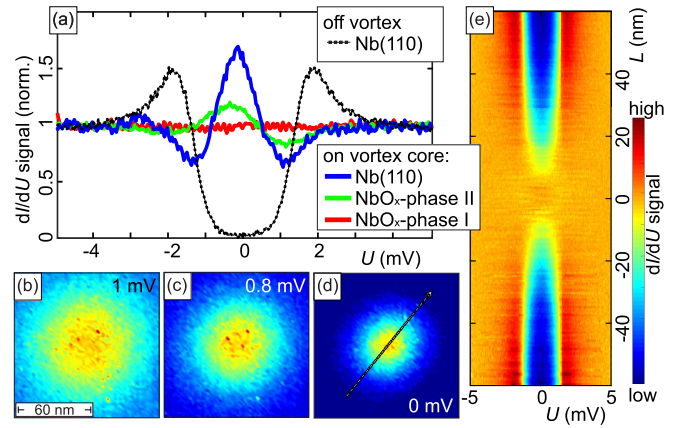


FIG. 2. (a) Tunneling spectra measured on different Nb surfaces in an external magnetic field: (black) the fully gapped tunneling spectrum of clean Nb(110) far away from any vortex; (blue) intense zero-bias peak in the center of the vortex on clean Nb(110); (green) less intensive peak in a vortex core on NbO<sub>x</sub> phase II; (red) Ohmic behavior in vortex core on NbO<sub>x</sub> phase I. Stabilization parameters:  $U_{\text{set}} = -7$  mV,  $I_{\text{set}} = 100$  pA. (b)–(d) show differential conductance  $dI/dU$  maps of a single vortex on NbO<sub>x</sub> phase I imaged at (b)  $U = 1$  mV, (c)  $U = 0.8$  mV, and (d)  $U = 0$  mV. (e) Tunneling spectra measured along the line in (d). No zero-bias feature is observed. Stabilization parameters:  $U_{\text{set}} = -5$  mV,  $I_{\text{set}} = 100$  pA,  $\mu_0 H = 100$  mT,  $T = 1.5$  K.

range within the superconducting gap. Furthermore, the tunneling spectra presented in Fig. 2(e) which were taken along the line in Fig. 2(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<sub>x</sub> phase I is consistent with a crossover from the clean to dirty limit, where additional scattering leads to a reduction of the electron mean free path. As it becomes shorter than the size of the vortex, the vortex core bound states blur and eventually disappear [21]. If we assume for the clean Nb(110) surface a mean free path close to the bulk value,  $\ell^{\text{Nb}} \geq 100$  nm [25], it clearly exceeds the coherence length  $\xi^{\text{Nb}} \approx 38$  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.

#### IV. DISCUSSION

Anisotropic vortices were first observed by Hess *et al.* on superconducting NbSe<sub>2</sub> [19,20]. Three scenarios were discussed as potential reasons: (i) vortex-vortex interactions, (ii) anisotropic pairing, and (iii) an anisotropy of the Fermi surface [16,17,24]. 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  $\lambda^{\text{Nb}} \approx 39$  nm and  $\xi^{\text{Nb}} \approx 38$  nm are at least four times smaller than the Abrikosov lattice constant ( $\approx 160$  nm) observed at  $\mu_0 H = 100$  mT. Therefore, we rule out that scenario (i) is responsible for the observed elliptical shape in Nb.

The twofold 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  $[1\bar{1}0]$ . 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 ( $\Delta = 1.53$  meV) [26,27], insufficient to explain the strong anisotropy observed in Fig. 1(i).

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] 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. [22]. 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  $\bar{\Gamma}$ ,  $\bar{N}$ ,  $\bar{S}$ , and  $\bar{H}$  can be recognized [22]. Since STM is most sensitive to electronic states in the vicinity of the  $\bar{\Gamma}$  point of the SBZ, with other states decaying exponentially with increasing  $k_{\parallel}$  [33,34], 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 [35,36]. 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 with the thermal broadening set to  $k_B T \simeq 0.26\Delta_0$ , where  $\Delta_0$  is the pairing potential in the absence of a magnetic field, equivalent to an effective temperature of about 2 K, in good agreement with the energy resolution of our experiment. We present the results in Figs. 3(d) and 3(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 [see Fig. 3(e)], in good qualitative agreement with experimental

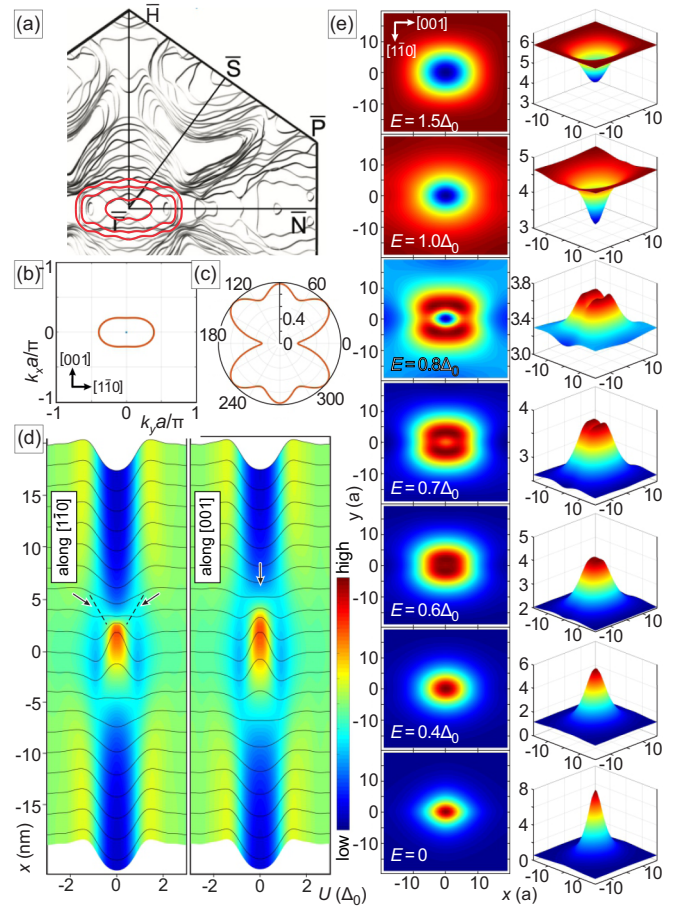


FIG. 3. (a) Calculated Fermi surface of Nb(110). Red lines denote pockets around the  $\bar{\Gamma}$  point. (b) Hypothetical Fermi surface and (c) Fermi velocity of the dominant Fermi contour. (d) Calculated LDOS along the two principal directions crossing the vortex core. (e) Excitation energy-dependent LDOS profiles after thermal broadening with  $k_B T \simeq 0.26\Delta_0$ .

observations in Figs. 1(h)–1(k). Close inspection of Fig. 3(d) also reveals a weak splitting of a zero-bias peak along the  $[1\bar{1}0]$  direction highlighted by two black arrows (left panel). The peak splitting is absent along the [001] direction, as can be recognized in Fig. 3(d) (right panel) and indicated by a single arrow. This nonsplitting is a combined effect of the lower slope of the distance-dependent energy splitting along the [001] direction and thermal broadening, as specified in Ref. [23]. Simulations suggest that the splitting may be detectable at effective temperatures below about 600 mK [23]. Regardless of the temperature, however, the vortex remains anisotropic with a coffee-bean-shaped feature at excitation energies below the superconducting gap.

Our analysis confirms that the anisotropy of the Fermi surface is responsible for the spatial structure of the excited states within the vortices. Depending on details of the anisotropy of the Fermi surface, 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. These spectral details observed on a conventional superconductor may help to clarify the nature of bound states detected inside vortex cores of more exotic superconductors. Since

Nb(110) is clearly a trivial superconductor where—depending on the crystallographic direction analyzed—splitting or non-splitting zero-bias peaks may be observed, the observation of non-splitting zero-bias peaks in materials claimed to be topological superconductors is obviously insufficient to safely identify Majorana zero modes (MZMs). Instead, we propose that future experiments should try to tune the disorder, for example, by dosing the surface under study with dilute amounts of adsorbates. In contrast to trivial CdGM states, MZMs are topologically protected and should therefore be largely insensitive to surface disorder. Conversely, zero-bias peaks originating from CdGM states will attenuate as soon as the surface impurity-induced reduction of the mean free path  $\ell$  falls short of the coherence length  $\xi$ , i.e., the dirty limit is reached.

## V. 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 ellipse 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 states inside the vortex core by, for example, introducing a disorder.

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