Ubiquitous V-Shape Density of States in a Mixed State of Clean Limit Type II Superconductors

N. Nakai,[1,*] P. Miranović,[2] M. Ichioka,[1] H. F. Hess,[3] K. Uchiyama,[4] H. Nishimori,[4] S. Kaneko,[4] N. Nishida,[4] and K. Machida[1]

[1]*Department of Physics, Okayama University, Okayama 700-8530, Japan*
[2]*Department of Physics, University of Montenegro, Podgorica 81000, Montenegro*
[3]*NuQuest Research LLC, La Jolla, California 92037-5801, USA*
[4]*Department of Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan*

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It is demonstrated theoretically and experimentally that the low energy density of states $N(E)$ is described by a singular V-shape form $N(E) = N_0(H) + \alpha|E| + O(E^2)$ for all clean superconductors in a vortex state, irrespective of the underlying gap structure. The linear term $\alpha|E|$ which has not been recognized so far is obtained by exactly evaluating the vortex contribution. Based on microscopic Eilenberger theory $N(E)$ is evaluated for the isotropic gap, line, and point-node gaps to yield a V-shape $N(E)$. Scanning tunneling spectroscopy-STM experiments on $NbSe_2$ and YNi_2B_2C give direct evidence for this. We provide arguments on the significance of this finding and on the relevance to other experiments.

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Much attention has been focused on exotic superconductors, ranging from high T_c cuprates, Ce, and U based heavy Fermion materials, filled skutterdites such as $PrOs_4Sb_{12}$ to cobaltites $Na_xCoO_2 \cdot yH_2O$ [1,2]. The identification of the Cooper-pair symmetry consists of two parts: its parity and the gap structure. The former is responsible for the spin structure of a pair which is either singlet or triplet. This can be probed by directly measuring the spin susceptibility through a NMR Knight shift experiment under an applied field. The latter gap structure is related to the orbital symmetry of a Cooper pair. This can be probed by thermodynamic measurements via a variety of experimental methods, such as temperature (T) dependence of specific heat $C(T)$, thermal conductivity $\kappa(T)$, or nuclear relaxation time $T_1(T)$ in NMR-nuclear quadrupole resonance experiments.

The basic principle of this identification for the gap structure is based on the fact that the energy (E) dependence of the density of states (DOS) $N(E)$ near the Fermi level, which characterizes low-lying excitations of a given gap structure. This $N(E)$ gives rise to a specific power law temperature dependence [2]. For example, the line (point) node gap yields a $C(T)/T \sim T(T^2)$ behavior in specific heat, $\kappa(T) \sim T^2$ (T^3) for thermal conductivity and $T_1^{-1} \sim T^3$ (T^5) in nuclear relaxation time at lower T region. This comes from the fact that the density of states is described by a specific functional form, $N(E) \propto |E|$ for line node and $N(E) \propto E^2$ for point node, through which a simple power counting rule yields specific power law indices in various quantities. Therefore it is decisive to precisely understand the DOS form $N(E)$ in order to identify the gap structure. We have attained a lot of information of the pairing symmetry in various superconductors in this way [2].

We have realized, however, that there is no detailed study to investigate ''the general rule'' for describing $N(E)$ in the mixed state of type II superconductor for various gap structures [3]. Namely, although the above thermodynamic measurements are often performed under an applied field, which is particularly true for T_1 in NMR, one needs to compute the precise functional form of $N(E)$ in the vortex state for various gap structures.

In the previous theoretical work we studied only the full gap case and analyzed $C(T)$ at low T [4]. However, this behavior should be examined with including the contribution of the gap anisotropy. Usually, experimental data taken under a field are often analyzed by simply extending the zero field results discussed above to a finite field ($H > 0$), keeping the same power law of $N(E)$ with a finite residual DOS $N_0(H)$. Namely, it has been implicitly postulated that $N(E) = N_0(H) + \alpha|E|^\gamma$ with $\gamma = 0$ (U-shape) in the full gap, $\gamma = 1$ in the line-node and $\gamma = 2$ in the point-node cases. However, these forms of DOS spectrum should be exactly evaluated by microscopic calculation without ambiguous assumption. The functional form of the DOS is important when we discuss the physical quantities in the mixed state.

Here we calculate the density of states $N(E)$ averaged over a unit cell of a vortex lattice in type II superconductors with full gap, point- and line-node gap structures. Our microscopic computation takes into account exact quasiparticle contributions due to vortices, which are not captured by Ginzburg-Landau and London theories. The results are of the general form $N(E) = N_0(H) + \alpha|E| + O(E^2)$ for all cases, i.e., $\gamma = 1$, showing that this singular V-shape DOS is universal independent of the underlying original gap structure.

We measured the DOS $N(E)$ for two superconductors; $NbSe_2$ [5] and YNi_2B_2C [6] by performing scanning tunneling spectroscopy (STS) at low temperatures. We integrate the measured local DOS (LDOS) over a certain area around a vortex core. The former material is known to posses an anisotropic gap without node while the latter is

speculated to be a pointlike nodal gap. Thus these materials provide an excellent testing ground to check the theoretical prediction. Indeed both give rise to a V-shape DOS in common. This study may be useful in understanding vortices recently produced in ultracold Fermionic superfluids in ^{6}Li atomic gases [7].

Theory.—The quasiclassical theory is valid in the case of $k_F\xi \gg 1$, which is satisfied in almost all type II superconductors. k_F is the Fermi wave number and ξ is the BCS coherence length which is the length scale of our unit. We introduce the pair potential $\Delta(\mathbf{r})$, the vector potential $\mathbf{A}(\mathbf{r})$, and the quasiclassical Green's functions $g(i\omega_n, \mathbf{r}, \hat{\mathbf{k}})$, $f(i\omega_n, \mathbf{r}, \hat{\mathbf{k}})$, and $f^\dagger(i\omega_n, \mathbf{r}, \hat{\mathbf{k}})$, where $\mathbf{r}$ is the center-of-mass coordinate of the Cooper pair and the direction of the momentum $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$. The Eilenberger equation is given by

$$\begin{aligned}\left\{\omega_n + \frac{i}{2}\mathbf{v}_F \cdot \left(\frac{\nabla}{i} + \frac{2\pi}{\phi_0}\mathbf{A}(\mathbf{r})\right)\right\} f &= \Delta(\mathbf{r}, \hat{\mathbf{k}}) g, \\ \left\{\omega_n - \frac{i}{2}\mathbf{v}_F \cdot \left(\frac{\nabla}{i} - \frac{2\pi}{\phi_0}\mathbf{A}(\mathbf{r})\right)\right\} f^\dagger &= \Delta^*(\mathbf{r}, \hat{\mathbf{k}}) g,\end{aligned} \tag{1}$$

where $g = [1 - f^\dagger f]^{1/2}$, $\mathrm{Re}\, g > 0$, $\mathbf{v}_F = v_F\hat{\mathbf{k}}$ is Fermi velocity, and ϕ_0 is a flux quantum [8,9]. The applied field $\mathbf{H}$ is along the $\mathbf{z}$ direction. With the symmetric gauge, the vector potential is written as $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{H} \times \mathbf{r} + \mathbf{a}(\mathbf{r})$, and an internal field $\mathbf{h}(\mathbf{r})$ is given by $\mathbf{h}(\mathbf{r}) = \nabla \times \mathbf{a}(\mathbf{r})$. By the numerical calculation Eq. (1) is self-consistently solved with the assumption $V_0(\hat{\mathbf{k}}, \hat{\mathbf{k}}') = V_0\varphi(\hat{\mathbf{k}})\varphi(\hat{\mathbf{k}}')$ and $\Delta(\mathbf{r}, \hat{\mathbf{k}}) = \Delta(\mathbf{r})\varphi(\hat{\mathbf{k}})$, considering the self-consistent conditions for $\Delta(\mathbf{r})$ and $\mathbf{a}(\mathbf{r})$;

$$\Delta(\mathbf{r}) = N_0 2\pi T \sum_{\omega_n>0}^{\omega_c} V_0 \langle \varphi(\hat{\mathbf{k}}) f(i\omega_n, \mathbf{r}, \hat{\mathbf{k}})\rangle_{\hat{\mathbf{k}}}, \tag{2}$$

$$\mathbf{j}(\mathbf{r}) = \frac{\pi\phi_0}{\kappa^2\Delta_0\xi^3} 2\pi T \sum_{\omega_n>0}^{\omega_c} i\langle \hat{\mathbf{k}}\, g(i\omega_n, \mathbf{r}, \hat{\mathbf{k}})\rangle_{\hat{\mathbf{k}}}, \tag{3}$$

where $\mathbf{j}(\mathbf{r}) = \nabla \times \nabla \times \mathbf{a}(\mathbf{r})$, N_0 is density of states at the Fermi level in the normal state. $\langle \cdots \rangle_{\hat{\mathbf{k}}}$ means the average over the direction of $\hat{\mathbf{k}}$. The cutoff energy is set as $\omega_c = 20T_c$. Δ_0 is uniform gap at $T = 0$. We use the high κ for the Ginzburg-Landau parameter. The angle dependence of the pair potential $\varphi(\hat{\mathbf{k}})$ specifies various gap structures with isotropic, line-node, or point-node gaps.

The LDOS at an energy E is given by

$$N(E, \mathbf{r}) = N_0 \langle \mathrm{Re} g(i\omega_n \to E + i\eta, \mathbf{r}, \hat{\mathbf{k}})\rangle_{\hat{\mathbf{k}}}, \tag{4}$$

where g is calculated by Eq. (1) with $i\omega_n \to E + i\eta$. We set $\eta = 0.01\Delta_0$. The total DOS $N(E)$ is the spatial average of the LDOS, i.e., $N(E) = \langle N(E, \mathbf{r})\rangle_{\mathbf{r}}$. The self-consistent calculation is performed within the vortex-lattice unit cell, which is divided into 81×81 mesh points. We assume that vortices form a triangular lattice. The cylindrical Fermi surface is chosen for the s-wave and the line-node case. And we use the spherical Fermi surface for the point-node case.

We display the DOS $N(E)$ for the s-wave case with the isotropic gap in Fig. 1(a). It is seen from this that the DOS has a V-shape form with a singularity at $E = 0$, namely,

$$N(E) = N_0(H) + \alpha\frac{|E|}{\Delta_0} + O(E^2), \tag{5}$$

where $N_0(H)$ is the energy independent term, corresponding to the zero-energy DOS which is only a function of the field H. This yields the Sommerfeld T-linear coefficient $\gamma_0(H)$ in the specific heat as $\gamma_0(H) \equiv \lim_{T\to 0} C(T)/T = (2\pi^2/3)N_0(H)$. We confirm that the sharp V-shape DOS is easily smeared by the thermal broadening effect. Impurities also affect smearing of the sharp edge of the V-shape DOS which becomes round by finite mean free path effect due to impurities. The linear slope $\alpha(H)$ in $N(E)$ is field dependent; For the s wave in Fig. 1(a), $\alpha(H)$ is small at lower fields. As H increases $\alpha(H)$ takes a maximum around $H/H_{c2} \sim 0.3$ and then becomes smaller again towards H_{c2}, continuing to a flat DOS in the normal state. This nonmonotonic behavior of the slope is the same also for the point-node case, but is contrasted with that in the line-node case; both are discussed below.

In Fig. 1(b) we exhibit the results for the line-node case described by the pair function $\varphi(\theta, \phi) = \sqrt{2}\cos 2\theta$. At $H = 0$, $N(E) = \alpha|E|/\Delta_0$ without a constant term in the low energy range as expected. In the vortex state this expression is valid except that we must add a field dependent $E = 0$ value, that is, $N(E) = N_0(H) + \alpha|E|/\Delta_0$. At first sight this result seems "apparent" because the original zero field DOS has a V shape and it is simply shifted upwards. However, this is not the case because the V-shape DOS is obtained even when the original gap structure is not a V shape as already shown in the s-wave case. The field dependence of $\alpha(H)$ in the line-node case is

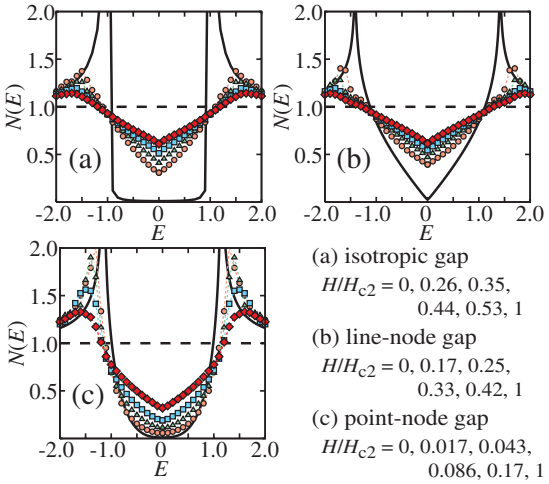

FIG. 1 (color online). Averaged density of states $N(E)$ of (a) the isotropic gap, (b) the line-node gap, and (c) the point-node gap. H increases from bottom to top at $E = 0$.

seen to be a monotonic decreasing function with H where the maximum slope occurs at $H = 0$. In Fig. 1(c) we show the V-shape DOS for the point-node case at $H > 0$. It is seen that at low fields the linear portion of $|E|$ is limited to low energies around $E = 0$. But as H increases a V-shape DOS feature manifests itself for wider energy ranges, so that the form in Eq. (5) is evident.

This ubiquitous V-shape DOS can be understood in terms of the LDOS. We show the so-called spectral evolution for the s-wave case in Fig. 2(a) where the spectral weight $N(E, r)$ in Eq. (4) is displayed in a plane of the distance r from the vortex core and the energy E/Δ_0. The zero-energy peak at the core site is split into two peaks as moving away from the core, that is, the two ''trajectories'' are given by $r = \beta|E|$. This spectral evolution agrees with the STS observation on $NbSe_2$ shown in Fig. 2(b). The total DOS is obtained by integrating this spectral weight spatially for each energy, namely,

$$N(E) = N_0 + \int_0^\infty dr r \delta(r - \beta|E|) = N_0 + \beta^2|E|. \quad (6)$$

The first term comes from the zero-energy peak at $r = 0$. This argument is applicable for the d-wave case where instead of the circular symmetry for the s-wave case the fourfold symmetry must be taken into account, which amounts to modifying the coefficient β^2, but the $|E|$ dependence remains unchanged. Thus it is understood that the V-shape DOS is universal, independent of the underlying original gap structure.

Experiment.—$NbSe_2$ is a typical anisotropic s-wave superconductor with a gap ranging from 0.7 to 1.3 meV, $T_c = 7.2$ K, and $H_{c2}(T = 0) = 3.2$ T, whose layered structure and van der Waals surfaces are ideal for STM-STS experiments [5]. When an external field is applied to the c axis, the vortices form a triangular lattice. A series of differential conductance spectra $\sigma(r, V)$ are taken along a line that extends radially through a vortex. Such an example taken at 50 mK and 0.025 T is shown in Fig. 2(b). The overall features and numerous details of the LDOS agree very well with the theoretical calculations shown in Fig. 2(a) (also see Ref. [10]).

In order to deduce the spatially averaged DOS over a unit cell, the data are collected along the line paths that extend out in three different directions from a vortex as shown in Fig. 3. The normalized DOS are inferred by the ratio of conductance, $\sigma(r, V)/\sigma(r, V = 5\ \text{meV})$, and are shown as a color scale image. These data are weighted by radius and summed to emulate an integration over the unit cell. This is essentially a polar coordinate integration: $N(E) = \int N(E, r, \theta) r dr d\theta$. The resulting averaged DOS are displayed in Fig. 4(a) for two fields $H = 0.1$ and 0.4 T along with the DOS at a zero field showing the s-wave gap function. A definite V shape in the DOS at finite fields is evident between -0.6 and 0.6 meV, and confirmed by the better fit attained by $\sigma(V) = \sigma_0 + \alpha|V| + \beta V^2$ (solid line) over that of a simpler parabolic form $\sigma(V) = \sigma_0 + \beta V^2$ (dashed line) as shown in Fig. 4(b). Furthermore, we note that the zero bias offset σ/σ_N (σ_N is the normal state conductance) corresponding to the Sommerfeld coefficient $\gamma(H)/\gamma_N$ at low T nicely matches the specific heat experiments [11] to within 5%.

Similar analyses have been performed on YNi_2B_2C whose gap structure is speculated to be pointlike nodes and $\sigma(r, V)$ has been measured at 460 mK [6]. The samples have $T_c = 15.6$ K and $H_{c2}(T = 0) = 8$ T. When the external field is applied to the c axis of this tetragonal system, a square vortex lattice is formed. At $T = 450$ mK, STS data are collected for various spatial points and bias voltages to yield the average DOS $N(E)$. The results are shown in Figs. 4(c) and 4(d) for $H = 0$, 0.07, and 0.3 T. The conductance data sets for finite fields are seen to posses a V-shape dependence. Although it is difficult from these

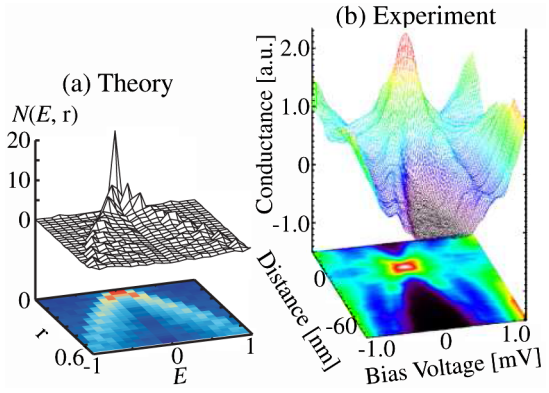

FIG. 2 (color online). (a) Theoretical calculation of LDOS $N(E, r)$, showing very similar subgap peak structures to (b). (b) The spectral evolution $N(E, r)$ in $NbSe_2$ at 0.025 T along 109 nm length that intersects a vortex as measured by STM-STS.

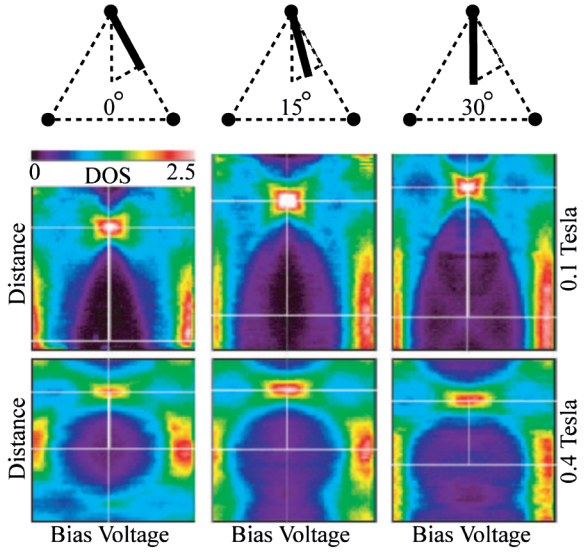

FIG. 3 (color online). Spectral evolution along 3 paths (black solid lines) for $NbSe_2$ with respect to the vortex lattice for $H = 0.1$ and 0.4 T. The LDOS data between the 2 horizontal white lines are used in the integration.

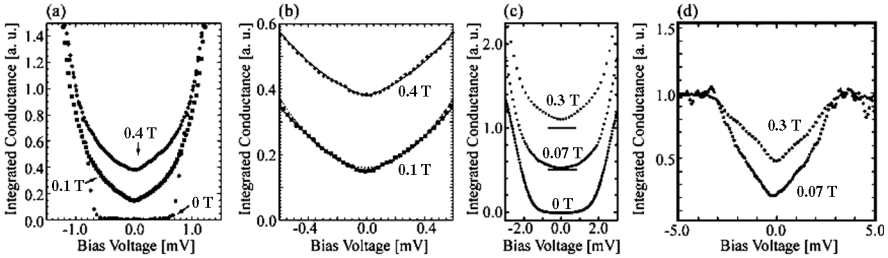

FIG. 4. (a) Spatially averaged DOS $N(E)$ over a unit cell at $H = 0$, 0.1, and 0.4 T for $NbSe_2$. (b) Same data but over ± 0.6 mV range inside the gap. The solid lines with $a + b|V| + c|V|^2$ are seen better fitting curves than the dashed line with a quadratic form $a + c'|V|^2$. (c) DOS $N(E)$ averaged over a unit cell at $H = 0$, 0.07, and 0.3 T for YNi_2B_2C. (d) DOS $N(E)$ averaged over circular area with diameter 10 nm around a core in YNi_2B_2C.

data to determine the precise functional form $\sigma(V) = \sigma_0 + \alpha|V|^\eta$, it contains a linear term $\eta = 1$.

As is clear from the above argument leading to Eq. (6), we could see a V-shape tunneling conductance if we restrict our integration region to a narrower region around a core. This procedure emphasizes the contribution from the vortex core which ultimately yields a V-shape DOS. In fact as shown in Fig. 4(d) which is obtained by integrating over a circular area with diameter 10 nm centered at a core, one can see a clear V-shape conductance curve for both fields.

The ubiquitous V-shape DOS has important consequences on identifying the pairing symmetry, in particular, its gap structure through the T dependences of various thermodynamic quantities as mentioned before. At low temperatures the T dependence is governed by the functional form of DOS. Using the V-shape DOS in Figs. 1 and 4, the simple power law counting tells us the following: specific heat $C(T)/T = \gamma_0(H) + \alpha' T$, nuclear relaxation time $T_1(T)^{-1} \propto T + c'T^3$, and thermal conductivity $\kappa(T) \propto T + c''T^2$. Therefore, in the experiment under magnetic field, we cannot simply assign the origin of the power law behavior as a line node, since the origin may be the V-shape DOS due to the vortex states, not due to the line-node gap structure. The T_1 behavior $T_1(T)^{-1} \propto T^3$ under magnetic fields is a result of the spatial average. If we observe T_1 outside of the vortex core by site selective NMR technique [12], we can unambiguously identify the signal due to the line node.

Simon and Lee [13], and Won and Maki [14] derive a scaling law to describe T and H dependences of various thermodynamic quantities for the line-node d-wave systems. In particular, the latter authors explicitly find a scaling function based on the averaged DOS obtained from the Doppler shift idea [15] whose functional form differs from ours. The Simon-Lee and Won-Maki scaling, which is quite successful for wide range of line-node superconductors (see, for example, Ref. [16]), can be improved and applied to other superconductors with different gap structures by using the obtained V-shape DOS.

In summary, by the self-consistent quasiclassical calculation evaluating the vortex contribution exactly, we have demonstrated the averaged density of states in the mixed state is a V shape, described by $N(E) = N(E = 0) + \alpha_E|E|/\Delta_0 + O(E^2)$. This formula is valid for any underlying gap structures; isotropic, point-node, or line-node gaps. However the α_E is small for the isotropic and point-node gap case in a low field. Two STM experiments on $NbSe_2$ and YNi_2B_2C unambiguously exhibit this behavior in their tunneling conductance. The vortex-lattice geometry does not affect the V shape and just slightly changes α_E. We have discussed several important consequences. In particular, when one identifies the gap symmetry by measuring thermodynamic quantities, careful consideration is needed in the mixed state.

*Electronic address: nakai@mp.okayama-u.ac.jp

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