Review of: "Coherent coupling between vortex bound states and magnetic impurities in 2D layered superconductors"

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As per the invitation from *Qeios*, here we make a review on a paper published on *Nature Communications* recently, entitled by “coherent coupling between vortex bound states and magnetic impurities in 2D layered superconductors”[1]. In that paper, the authors performed a comprehensive study on the coupling between vortex bound states and Yu-Shiba-Rusinov (YSR) bound states of magnetic impurities in a conventional type-II superconductor Nb(Se,S)$_2$. By combing scanning tunneling microscope (STM) measurement and Hubbard-corrected density functional calculations, the authors identified an emergent axial particle-hole asymmetry of vortex density of state away from quantum limit temperature, which is originated from the quantum nature of Caroli-de Genne-Matricon (CdGM) vortex bound states.

The CdGM states are a series of quantized superconducting quasiparticles in a vortex, with level spacing proportional to Δ^2/E_F, where Δ is superconducting gap, E_F is Fermi energy[2]. However, the discreteness of the quantized bound states can be observed only under a quantum limit temperature, at which the thermal broadening is much smaller than the ratio of Δ^2/E_F[3]. Under the quantum limit, a signature quantum nature of CdGM states is the particle-hole-asymmetric wavefunction. It is rooted on the rotational symmetry of vortex, that the level of vortex bound states could be marked by the total planar angular momentum ν, *i.e.* $E_\nu \approx \nu\Delta^2/E_F$. In conventional superconductors $\nu = l_z - m/2$, where l_z is the orbital angular momentum that is an arbitrary integer, and m is the vorticity which is equal to 1 or -1 in general conditions. As the wavefunction of the (ν, l_z) component of vortex bound states is proportional to Bessel function $J_{l_z}(x)$, the wavefunction of particle-hole partners oscillates approximately out-of-phase, leads to the particle-hole asymmetric quantum behavior. (This result can be easily verified by checking the l_z of two lowest excitations which are 1 and 0 when $m = 1$).

However, The ratio of Δ/E_F is tiny in most of the conventional superconductors, for instance in Nb(Se,S)$_2$. Thus the level spacing of quantized vortex bound states is several orders of magnitude smaller than the thermal broadening in a real experiment, and a vortex in these materials is far away from the quantum limit. The discrete, oscillating and particle-hole asymmetric wavefunction is quantum in nature, which is generally washed out in experiments away from the quantum limit. A spatial splitting, continuous, and particle-hole symmetric vortex bound states were broadly observed in conventional superconductors by STM[4][5].

Surprisingly, in this paper[1] the authors found that magnetic impurity could mediate the coupling between adjacent vortex bound states, gives rise to the intensity rearrangement of the wavefunction of each (ν, l_z) component. When the band structure is hole like, the intensity of positive-energy bound states moves to the direction of impurity, while at the negative-energy side the intensity moves to the opposite direction of the impurity. But for an electron-like band, the intensity rearrangement is inverted on both positive- and negative-energy bound states. Thus the intensity difference between particle and hole partners polarizes from the vortex center, breaks the “axial symmetry” of the vortex. This hidden quantum asymmetry was revealed in this paper[1] by a detailed theoretical BdG calculation. Remarkably, this emergent axial particle-hole asymmetry becomes more evident at higher temperature away from the quantum limit, while the fast oscillating behavior of the wavefunctions is smeared out by the dominating thermal broadening. It provides a rare opportunity to identify a quantum-nature-related feature at a temperature far away from the quantum limit, which was clearly observed by STM in the paper[1].

We note that the “spatial shift of CdGM state” mentioned in this paper[1] seems mainly the relative rearrangement of the wavefunction intensity on the sides of approaching or departing the impurity. In the view of quantum limit, the magnetic impurity does not qualitatively change the peak position and period of wavefunction oscillation. In Fig. S1 of this paper[1], the authors calculated the impurity-induced particle-hole difference under the quantum limit, however, a detailed demonstration of the influence of the impurity on the wavefunction of each quantized vortex bound states is equally significant for a direct illustration of the axial particle-hole asymmetry. An additional figure of the simulation could be very useful for the readers. Furthermore, to our best knowledge, the picture of the adjacent mixing of vortex bound states induced by impurity is not such clear. The authors are recommended to deliver clearer explanations on the related theoretical modeling and the mechanisms of the axial particle-hole asymmetry as they proposed. Another issue which is worth noting is that the authors mentioned that the discrete nature of CdGM state is revealed by the axial asymmetry at high temperature. Although the axial asymmetry is a direct consequence of the quantum nature, we feel it is a little bit over claim, as no direct observation of the discreteness of the vortex bound states is found here.

As mentioned by one of the referees of this paper[1], that “these findings are novel and provide important insight into the understanding of the relation between the impurities and vortex”, this paper[1] provides interesting information of the influence of impurity on vortex, which may even become an inspiration on the studies of bound states of quantum-limited vortex. Especially, Majorana zero modes (MZM), that is a promising building block for fault-tolerant quantum computation[6], could emerge in a vortex of topological superconductor as the zero-energy vortex bound states[7]. Isolated MZM has been identified in some iron-based superconductors which are under the quantum limit[8]. Recently, a paper published on *Nature Communications* show that vortex MZM can be tuned on by strong and large impurity clusters on LiFeAs[9], owing to native tuning of bulk Dirac fermions, which has a potential to facilitate the manipulation of MZMs in the future. The information of the paper may provide useful information on the detailed analysis of the line profile of higher level vortex bound states which accompany MZM.

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