Quantum rotor in nanostructured superconductors

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Despite its apparent simplicity, the idealized model of a particle constrained to move on a circle has intriguing dynamic properties and immediate experimental relevance. While a rotor is rather easy to set up classically, the quantum regime is harder to realize and investigate. Here we demonstrate that the quantum dynamics of quasiparticles in certain classes of nanostructured superconductors can be mapped onto a quantum rotor. Furthermore, we provide a straightforward experimental procedure to convert this nanoscale superconducting rotor into a regular or inverted quantum pendulum with tunable gravitational field, inertia, and drive. We detail how these novel states can be detected via scanning tunneling spectroscopy. The proposed experiments will provide insights into quantum dynamics and quantum chaos.

The classical rotor, a macroscopic particle of mass $m$ confined to a ring, is one of the most studied system in classical mechanics. In a gravitational field the rotor becomes a pendulum with its stable equilibrium at the bottom. Counter-intuitively, the pendulum can also be stabilized at the top by subjecting the pivot to an appropriate drive\textsuperscript{1}, in a state referred to as an inverted pendulum. Further interest in classical rotors arose from the fact that if one applies periodic kicks to the pendulum, its dynamics becomes chaotic. In contrast to classical rotors, quantum rotors are harder to realize\textsuperscript{2}. However, with quantum effects coming into play, quantum rotors furnish even more abundant phenomena than their classical counterparts. For example, the quantum kicked rotor\textsuperscript{3} is one of the most featured models of quantum chaos\textsuperscript{4} and has various applications\textsuperscript{5–9}.

Here we show how a quantum rotor can be obtained in nanostructured superconductors. The idea is to trap quasiparticle excitations in a ring-shaped confinement, i.e. a Mexican hat potential, where quasiparticles can form Andreev bound states\textsuperscript{10}. The desired potential can be achieved in e.g. annular S-N-S junction [see Fig. 1(a)], a superconducting film with a ring-shaped surface etch [“blind” ring\textsuperscript{11}; see Fig. 1(b)], or under a perpendicularly magnetized ferromagnetic disk [Fig. 1(c)] where screening currents suppress the superconducting order parameter mostly within a ring right under the edge of the disk\textsuperscript{12,13}. Very recently, it became possible to “draw” the suppression of superconductivity practically at will by locally applying electric field in a ferroelectric/superconductor (FE/SC) bilayer via scanning (AFM) tip [see in Fig. 1(d) and Ref. 14 for details]. On the other hand, to harbor the Andreev bound states, the ring region should preferably be in the clean limit. As discussed later in this manuscript, favorable conditions for experimental detection of the rotor states include: (1) a wide enough ring region, in the order of several coherence lengths, and (2) a sufficiently large ring radius when compared to the ring width, so that the tunneling through the central potential hill is suppressed. Thus, for conventional superconductors such as Pb or Nb, if a ring is fabricated with its width greater than the e-beam lithography resolution (on the order of several tens of nanometers), the ring radius would be on the order of several hundreds of nanometers. It would not be trivial to make these conventional superconductors with such long mean free paths, although recent experiments by the Roditchev lab\textsuperscript{15} show that several monolayers of Pb, when deposited onto a Si substrate, become crystalline and exhibit longer mean free paths than bulk Pb. In this respect, graphene-superconductor hybrid is ideal for the realization of our proposal\textsuperscript{16–18}. Indeed, superconductor can be nanostructured with a periodic array of ring perforations (using e.g. e-beam lithography) and covered with a graphene flake[see Fig. 1(e)], so that graphene harbors proximity-induced superconductivity with normal regions above the rings. In such a case, the high crystal quality of graphene and therefore the long mean free path ($\sim$μm) would guarantee the appearance of the quantum rotor and facilitate its observation. Notably, this would be the very first realization of a superconducting quantum rotor in real space, different from the ones realized in Josephson junctions using the superconducting U(1) phase space\textsuperscript{19,20}.
Results

Unusual quasiparticle energy dispersion. In what follows, we focus on the case of strongly deformed order parameter on the ring, typical for systems of Fig. 1(a), (d) and (e). Nevertheless, our findings can be generalized to any other realization of the Mexican hat potential. We begin our theoretical analysis of those bound states with a simplified model - a step-wise superconducting order parameter with radial symmetry $\Delta(r)$, which vanishes between an inner radius $R_{in}$ and outer radius $R_{out}$, but it is otherwise constant and finite. We solve the Bogoliubov-de Gennes (BdG) equation in cylindrical coordinates, and separate the rapidly varying degrees of freedom from the slow ones\textsuperscript{21} by writing the solutions in the form:

$$\begin{bmatrix} u_l \\ v_l \end{bmatrix} = \begin{bmatrix} f_l \\ g_l \end{bmatrix} H_l^{(1)}(k_F r) + c.c.,$$

where $u_l$ and $v_l$ are BdG wave functions, $k_F$ is the Fermi wave vector, $r$ is the radial coordinate, $H_l^{(1)}$ is the Hankel function, and $f_l, g_l$ are slowly varying envelope functions. Next, we insert the WKB-approximated asymptotic form of the Hankel function and change variables\textsuperscript{22,27} from $r$ to $x$, defined by $r^2 = x^2 + b^2$. Here $b$ is the WKB turning point $b = \sqrt{b^2 - 1/4}/k_F$, and $l$ is the angular momentum quantum number. For large $l$, the impact parameter is approximately $b \approx l/k_F$. We obtain:

$$\begin{bmatrix} -iv_F \partial_x \hat{\Delta}(x) \\ i\nu_F \partial_x \hat{\Delta}(x) \end{bmatrix} \begin{bmatrix} f_l \\ g_l \end{bmatrix} = \epsilon \begin{bmatrix} f_l \\ g_l \end{bmatrix},$$

where $\hat{\Delta}(x) \equiv \Delta(r(x))$. This maps our two dimensional (2D) problem onto a one dimensional (1D) problem. The 1D order parameter is given by

$$\begin{cases} \Delta_0 & \text{if } |x| < x_{in} \\ 0 & \text{if } x_{in} < |x| < x_{out} \\ \Delta_x & \text{if } |x| > x_{out} \end{cases}$$

where $x_{in} = \sqrt{R_{in}^2 - b^2}$ and $x_{out} = \sqrt{R_{out}^2 - b^2}$. In the quasiclassical picture, the quasiparticles move along a chord in the $x$ direction. The distance $b$ of the chord from the center of the 2D ring potential is roughly proportional to the $l$. This is consistent with the classical picture that a particle with higher angular momentum is localized further away from the pivot. Each orbit with different angular momentum is mapped on a chord of different length. As shown in Fig. 2(a), the $l = 0$ state $(b = 0)$ resides in the most narrow well, with two segments separated by the central hill. As the distance $b$ and the angular momentum increases, the chord length of the bound state (or, equivalently, the width of the potential well) also increases. The bound state energy decreases accordingly as long as $b < R_{in}$. Once $b$ reaches $R_{in}$, the two segments of the chord merge into one wide potential well, causing the energy to drop to a local minimum $\epsilon(b_0)$, where $b_0 \approx k_F R_{in}$. As $b$ is increased further, the length of the chord shrinks and energy increases again. Therefore, the dispersion $\epsilon(l)$ must have a local minimum at a non-zero angular momentum. This is non-trivial and contradicts classical intuition: for such a dispersion faster “rotation” does not always correspond to higher energy. Although very different in origin, such a quantum effect was found earlier in the roton dispersion in superfluid $^4\text{He}$\textsuperscript{24–27}.

The above reasoning for an unusual dispersion relation is further verified by both analytic and numerical solutions using BdG equations. For $l < b_0 \approx k_F R_{in}$ and $\epsilon \ll \Delta_0 \leq \Delta_x$, the quasiparticle dispersion $\epsilon_n(l)$ can be obtained analytically by matching the solutions at $x = x_{out}$, $x_{in} = x_{out} - x_{out}$ as

$$\epsilon_n = \frac{v_F}{2} \left( \frac{n + 1}{4} \right) + \sin^{-1} \left( \tan(2\text{tan}(2q x_{in})) \right).$$

Here $q = \frac{\Delta_0}{\Delta_x}$, $\xi$ is the coherence length, and $v_F$ is the Fermi velocity. For $l > b_0$, we obtain

$$\epsilon_n = \frac{v_F}{2} \pi \left( n + \frac{1}{2} \right).$$

The energy levels obtained here coincide with Andreev's result\textsuperscript{29} for a normal slab in contact with two superconductors. Note that $\epsilon_n$ depends on $l$ through $x_{in}(l)$ and $x_{out}(l)$ [see Fig. 2(c)]: it decreases with $l$ for $l < b_0$ and then increases for $l > b_0$ as in the case of bound states inside a vortex core\textsuperscript{22,27}. We confirmed this analytic result numerically by solving BdG with B-splines basis (see Methods) and direct diagonalization, as shown in Fig. 2(c).

Quantum rotor. In a realistic system [cf. Fig. 1(c)] one likely finds a smooth suppression of the order parameter. Nevertheless, $\epsilon(l)$ still has a local minimum at non-zero angular momentum, as we show in Fig. 3(a) [for $r = (R_{out} + R_{in})/2 = 1.25\xi$]. The low-lying excitations around the dispersion minimum can then be approximated by a quadratic function $\epsilon(l) \approx (l_0^2 - l^2)/2I$, where $l_0$ is the angular momentum of the local minimum, and $I$ is the effective inertia. The magnitude of $I$ is consistent with $m r^2$, i.e. the inertia
Figure 2 | Andreev bound states and their energy dispersion. (a) Quasiclassical trajectories of the Andreev bound states in the radially step-like order parameter. The bound states are depicted as electrons (solid arrow) being Andreev reflected as a hole (dashed arrow). Here $b$ denotes the distance of the linear reflection path from the center of the 2D potential. (b) Example of a line profile of the order parameter corresponding to panel (a). Panel (c) shows the quasiparticle dispersion of lowest energy states for the step-like potential featured in panel (b).

Numerical verification of the rotor state. To confirm these predictions, we solve numerically the BdG equations on a discrete square lattice. Note that in order to compare these results with the quasiclassical limit, we have to consider large systems (e.g. $500 \times 500$ lattice points). For the size of our nanostructured ring, we take the radius $R = 100a$ and width $W = 30a$, where $a = 1$ is the lattice constant. Here we chose this particular combination of $R$ and $W$ in order to have only one peak for $l = 0$ and a well defined rotor peak for $l = b_0$. If $W$ is larger, multiple overlapping peaks make the analysis cumbersome. The value of the superconducting order parameter is chosen to be $\Delta = 0.1t$, where $t$ is the hopping amplitude, giving a coherence length on the order of the ring width, $\xi \sim 20a$.

We compare in Fig. 3 the local density of states (LDOS) in the middle of planar and ring S-N-S junctions of same width. As seen from the graph, the LDOS is modified only within the superconducting gap due to multiple Andreev reflections at the normal/superconducting interface. For both situations there is a main peak around $E/\Delta = 0.55$ which is mainly given by paths of length $W$ and corresponds to the state with $l = 0$. Interestingly, for the ring geometry an additional peak appears at low energies. This peak is the low-lying state with $l = l_0$ discussed in previous section and is given by the longest chords in the ring. In other words, this peak corresponds exactly to the rotor state.

Discussion

In this Section, we present further implications of the existence of the rotor state, and its manifestations in the presence of applied drive. These effects are interesting in their own right, but also essential for the experimental verification of the rotor state.

Quantum pendulum. It is well-known that superconducting properties can be strongly affected by an electric current. An applied $dc$ current in our system leads to the following effective Hamiltonian for the low-lying states:

$$H = \frac{(l-l_0)^2}{2l} + v_s k,$$

where $k = (k_F \cos \theta, k_F \sin \theta)$ and $v_s$ is the superfluid velocity corresponding to the applied transport current. The equation of motion then exhibits nonlinear dynamics:

$$\dot{\theta} - \frac{k_F v_s}{I} \sin \theta = 0.$$

For our choice of coordinates, this corresponds to an inverted pendulum. Nevertheless, the "gravitational" force drives the system away from the $\theta = 0$ (up) unstable equilibrium point. To analyze the behavior of this quantum pendulum, we use the effective Hamiltonian in Eq. (6), and show that the thermally averaged zero energy local density of states, $g(r) = \int_{-\infty}^{\infty} \sum_n |\psi_n(r)|^2 \delta(E_n) \phi(r) \phi^*(r) \frac{1}{4T \cosh^2(\epsilon/2T)} dc$, has a peak at the bottom position, $\theta = \pi$ [see Fig. 4(c)]. Hence in the presence of an applied $dc$ current our system becomes the quantum analogue of a pendulum in a gravitational field.

Numerical results with applied current. We next show the full numerical solutions of the BdG equations on a discrete lattice in the presence of an external $dc$ current. A supercurrent is applied to the system in $y$-direction by imposing a phase gradient, $\partial \phi/\partial y$, on the superconducting order parameter.
identical to an effective potential 30,31 injecting a of states (LDOS) calculated for a quantum rotor, for the same parameters as in (a). (c) The calculated LDOS for a quantum pendulum, obtained by injecting a dc current in the indicated direction (vᵣ = 1.0 m/s). The finite transport current is effectively equivalent to gravity in the classical pendulum picture.

The dashed line in Fig. 5(a) shows the calculated LDOS(E) for the case without applied current, taken at the bottom position of the ring (at θ = π). One notices two main peaks, largest of which corresponds to the state with \( l = 0 \), whereas the smaller one is the state with \( l = L \).

The solid curve in Fig. 5(a) is calculated at the same place on the ring, but now in the presence of the current along the y-direction. According to Fig. 4, a pendulum state is expected. We indeed observe that the rotor peak is split into pendulum states since there is a phase difference along the chords which contribute to those states. However, because the chiral symmetry is not broken, states with opposite chirality are located at top and bottom locations respectively, as shown in the LDOS map in Fig. 5(b) [for energy corresponding to the lowest energy peak in Fig. 5(a)]. In other words, the two pendulum states at \( φ = π \) and \( φ = 0 \) are degenerate in energy, but the application of a small perpendicular magnetic field breaks the chiral symmetry and selects only one of them [as shown in Fig. 5(c)]. The LDOS maps for all the energies and other field/current configurations can be found in the Supplementary Material.

Inverted pendulum. Finally, we return to Eq. (6) to point out that although the inverted pendulum is unstable, it can be driven to stability by horizontal or vertical pivot motion (cart-pole or Kapitza pendulum, respectively)36. If the pivot is vibrated with an amplitude \( A \cos \omega t \), and the frequency \( \omega \) is much higher than the pendulum’s natural frequency \( \omega_N \), i.e. more precisely \( \omega \gg \frac{R}{A} \omega_N \), where \( \omega_N = \sqrt{\frac{h}{M} v_f} / l \), the effect of the fast pivot motion will be identical to an effective potential 30,31 \( V_{\text{eff}} = \frac{1}{4} IR^2 a^2 \omega^2 \sin^2 \theta \). For such a case, which in a system of Fig. 1(c) [(d)] can be realized by an ac in-plane magnetic [electric] field, we calculated the local density of states [see Fig. 6] and indeed observed a peak at the top position \( \theta = 0 \) of the pendulum, corresponding to the inverted pendulum state. Note, however, that the peak at \( \theta = π \) for a regular pendulum state remains, which is different from the classical case. Quantum mechanics allows the particle to reside in both potential wells, while classical mechanics forces the particle to choose either bottom or top localization. Finally we note that while the inverted pendulum state is stabilized by a high frequency drive, low-frequency drives are also of interest as they lead to the classically chaotic regime. Therefore, the quantum rotor proposed here is a testbed for further studies of quantum chaos32. Applying pulsed current to our device would transform the superconducting rotor into a pendulum with pulsed gravity, i.e. another quantum chaotic system 32.

In summary, we provided analytical and numerical results for novel quantum rotor states in nanostructured superconductors. Besides being a remarkable example of a quantum analogue of a classical system, the superconducting rotor (i) can be realized in various superconducting systems, (ii) has a tunable inertia and gravitational field, (iii) can be externally manipulated through effective tilt, pulsed gravity, and pivot oscillations, and (iv) can be converted to a quantum pendulum, inverted pendulum, or be driven to a chaotic regime. Hence this quantum rotor has the potential to provide insights into a variety of phenomena which certainly deserve further experimental and theoretical investigation.

Methods
The Bogoliubov-de Gennes (BdG) equations are used to calculate the spectrum and LDOS throughout this work. The BdG equations provide mean field description of superconductivity and are generalized from the Hartree-Fock equations. We first applied the quasiclassical approximation, which separates the fast oscillation mode with length scale \( 1/k_F \). It allowed us to discuss physical quantities varying over the superconducting coherence length, and also provided clear physical picture of the quasiclassical trajectories. For the quasiclassical limit, the numerical calculations are done within the B-spline basis18,36, which is very efficient for inhomogeneous problems such as the one presented here.

We also performed full BdG calculations for a discrete square lattice by using the Chebyshev-BdG method16,37. This method can extract relevant physical quantities, for example LDOS, from large systems (here we used a square lattice with 500 \times 500 grid points) and avoid large matrix diagonalization.

In order to describe inhomogeneous s-wave superconductivity we use a real-space tight-binding formulation. The corresponding Hamiltonian written in Nambu spinor form is the following:

\[
\begin{align*}
\end{align*}
\]

Figure 5 | Realization of the quantum pendulum. (a) Full BdG calculation of the LDOS vs. energy in \( \theta = π \) location on the ring (of width \( W = \xi \) and radius \( R = 5\xi \)), for the quantum rotor (no current) and pendulum state (with current generated via \( \hat{\varepsilon}\phi/\hat{\varepsilon} = 0.0033/\delta t \)). The 2D LDOS for a quantum pendulum is shown for \( E/\Delta = -0.088 \) in the absence (b) and presence (c) of a small perpendicular magnetic field, \( \Phi/\Phi_0 = 0.15 \).
where the coefficients \( \alpha_{ij}^o(\tilde{t}) = \langle \psi_i^+ | \psi_j \rangle \) and \( \alpha_{ij}^o(\tilde{t}) = \langle \psi_i^+ | \psi_j \rangle \) can be obtained by an iterative procedure involving repeated applications of the Hamiltonian on iterative vectors \( |\psi_n\rangle \):

\[
|\psi_{n+1}\rangle = 2\pi |\psi_n\rangle - |\psi_{n-1}\rangle,
\]

where \( |\psi_0\rangle = |\psi_j\rangle \) and \( |\psi_{-1}\rangle = 0 \). The local density of states (LDOS) is then:

\[
N_j(\omega) = -\frac{1}{\pi} \text{Im} \left[ \tilde{G}_j(\omega) \right],
\]

We performed the expansions separately for each grid point and further accelerated our calculations by using graphical processing units (GPUs) to perform the sparse matrix - vector multiplications.

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Author contributions
M.V.M. and F.M.P. are experts in the behavior of the superconducting condensate in an inhomogeneous field (such as the stray field of a magnetic dot), whose analysis within the Ginzburg-Landau theory lead to the idea of B.I. of a new Andreev bound state in such a system. S.-H.L. carried out the analytical and numerical solution of quasiclassical BdG calculations to demonstrate the bound state, and developed the simplified Hamiltonian for it. S.-H.L. and M.V.M. then conceived the analogy to the classical rotator in a gravitational field. L.C. performed the full BdG calculations with Chebychev method. All authors contributed to the final scientific statement of the manuscript.

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