Influence of the quantum zero-point motion of a vortex on the electronic spectra of \textit{s}-wave superconductors

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We compute the influence of the quantum zero-point motion of a vortex on the electronic quasi-particle spectra of \textit{s}-wave superconductors. The vortex is assumed to be pinned by a harmonic potential, and its coupling to the quasi-particles is computed in the framework of BCS theory. Near the core of the vortex, the motion leads to a shift of spectral weight away from the chemical potential, and thereby reduces the zero bias conductance peak; additional structure at the frequency of the harmonic trap is also observed.

I. INTRODUCTION

Recent work on ‘deconfined quantum critical points\textsuperscript{1-4}’ between superfluid and insulating phases has pointed out the central role played by the quantum fluctuations of the vortex excitations of the superfluid state\textsuperscript{5,6}. However, this work has largely been carried out using convenient model Hamiltonians, with little direct connection to the microscopic Bardeen-Cooper-Schrieffer (BCS) theory of the superconducting state. It is the purpose of this paper to begin an exploration of the quantum fluctuations of vortices in the BCS theory. We will examine the theory of a single vortex in an \textit{s}-wave superconductor, fluctuating harmonically in a trapping potential. Our primary focus will be on the influence of this quantum motion on the electronic local density of states (LDOS). Modern scanning tunneling microscopy (STM) can provide detailed measurements of the LDOS in the vicinity of a vortex, and so can, in principle, detect signatures of vortex fluctuations.

Existing \textit{s}-wave superconductors have a large coherence length, $\xi$, and consequently a large effective mass which is expected to scale as the cross-section area of the vortex core $\sim \xi^2$. As a result, the vortex zero-point motion is small, and its signatures in the LDOS are probably indetectable. However, should a small coherence length \textit{s}-wave superconductor be discovered in the future, the results here should be useful.

We will also develop some basic formalism for application to \textit{d}-wave superconductors. Naturally, the cuprate superconductors are prime candidates for observing vortex zero-point motion with their small values of $\xi$, and also indications of proximity to a superconductor-insulator transition (possibly of the ‘deconfined’ or ‘Landau-forbidden’ variety) at finite doping. However, the application of the formalism of the present paper to \textit{d}-wave superconductors is far from straightforward: the anisotropic gap and loss of rotational invariance makes the numerics much more demanding, and the presence of gapless nodal quasiparticles leads to new physics. We therefore defer full discussion of the \textit{d}-wave case to a second paper\textsuperscript{7} (hereafter referred to as II).

In a general sense, our analysis can be viewed as a study of the influence of the phase of the superconducting order parameter on the vortex LDOS. However, rather than integrating over the phase fluctuations explicitly, we are encapsulating them in a collective co-ordinate, the position of the vortex.

An important limitation of the calculation presented here is that, in determining the coupling between the moving vortex and the electronic excitations, we expand in gradients of the pairing amplitude of the electrons. The applicability of such an expansion places a lower bound on the value of the coherence length, and so we are not able to properly explore the limit of extremely short coherence lengths. A separate computation which does not make this gradient expansion, while working in an effective low energy theory, will be presented in paper II.

We will begin in Section II by setting up the general formalism which couples a moving vortex to the electronic quasiparticles. Rather than considering a vortex lattice and its oscillations, we will use a simple Einstein model for the vortex lattice phonons, and so work with a single vortex moving in a harmonic potential. The electronic self-energy corrections from the vortex motion will be computed in Section III for an \textit{s}-wave superconductor. The rotation symmetry of this case is an important aide in our numerical computations, and we are able to obtain good numerical convergence for a significant range of parameters.

II. GENERAL FORMALISM

We will develop the general formalism for a two dimensional \textit{s}- or \textit{d}-wave superconductor. In principle, similar considerations apply to three-dimensional superconductors, but we will not present them here. Complete numerical results for \textit{s}-wave superconductors appear in the following section, while those for \textit{d}-wave superconductors appear in paper II.

To model the zero-point fluctuations of a vortex in a superconductor with either \textit{s}- or \textit{d}-wave symmetry we use the following Bogoliubov-de Gennes like action as a
starting point:
\[ S = \int d^2r \, d\tau \left( \bar{\psi} \! \psi \right) \left( \partial_\tau + H_{\text{BdG}} \right) \left( \psi \! \bar{\psi} \right) + \int d\tau \, V(R(\tau)) \, , \] (1)
where (with \( \hbar = 1 \))
\[ H_{\text{BdG}} = \begin{pmatrix} \left( -\frac{1}{2m_e} \partial_r^2 - E_F \right) & \hat{\Delta}(r - R(\tau)) \\ \hat{\Delta}^*(r - R(\tau)) & \left( -\frac{1}{2m_e} \partial_r^2 - E_F \right) \end{pmatrix} \, . \] (2)
Here \( \psi(r, \tau) \) and \( \bar{\psi}(r, \tau) \) are conjugate Grassman fields for electrons with mass \( m_e \), \( E_F = k_F^2/2m_e = m_e v_F^2/2 \) is the Fermi energy and \( \hat{\Delta}(r - R(\tau)) \) is the gap operator for superconducting electrons in the presence of a vortex at position \( R(\tau) \) in the plane. The vortex is allowed to move in imaginary time \( \tau \) and to account for the interaction between vortices in a vortex lattice we put our vortex in a harmonic oscillator potential \( V(R) \) with equilibrium position \( R = 0 \).

For a superconductor with \( s \)-wave symmetry the gap operator can be taken to be a simple scalar \( \Delta(r) \). Assuming there is a vortex at the center of the plane we can choose a gauge such that the phase of the order parameter is equal to the polar angle of the position vector, i.e. (with a slight abuse of notation) \( \Delta(r) = \Delta(r) e^{i\theta} \).

The \( d \)-wave case is more difficult and it is customary to express the gap operator in terms of a non-local order parameter with a center of mass coordinate \( r \) and a relative coordinate \( r' \). Expanding in powers of \( r' \) and keeping only terms up to second order we can eliminate \( r' \) and write the gap operator with \( d_{x^2-y^2} \) symmetry (see Appendix A) as
\[ \hat{\Delta} = \{ \partial_x, \{ \partial_y, \Delta(r) \} \} - \{ \partial_y, \{ \partial_x, \Delta(r) \} \}, \] (3)
where \( \{a, b\} = (ab + ba)/2 \). This equation is equivalent to a gap operator with \( d_{xy} \) symmetry as derived by Simon and Lee. For a vortex at the origin we again take \( \Delta(r) = \Delta(r) e^{i\theta} \). In Appendix A we will discuss issues of gauge invariance associated with the above expressions and the important comments made on this issue in Ref. 5. A choice of gauge is made in Eq. 6, and no additional term is needed to preserve gauge invariance of the Bogoliubov-de Gennes equations.

Integrating out the electronic degrees of freedom in the action given in Eq. 1 one obtains an effective action for the vortex degrees of freedom. Expanding in powers of the velocity of the vortex we obtain for the effective vortex action (for simplicity at zero temperature) in the imaginary frequency formalism (see Appendix B)
\[ S^\text{Vortex}_{\text{eff}} = \frac{m_v}{2} \int \frac{d\omega}{2\pi} R^\dagger(i\omega) \begin{pmatrix} \omega^2 - \omega_0^2 & \omega \omega_0 \\ -\omega \omega_0 & \omega^2 + \omega_0^2 \end{pmatrix} R(i\omega) \, . \] (4)
While the term proportional to \( \omega \) can be identified to be the Magnus force, the term proportional to \( \omega^2 \) is just the vortex kinetic energy and defines the mass of the vortex, \( m_v \). For a BCS-superconductor with \( s \)-wave symmetry \( m_v \) is of the order of \( m_e(k_F\xi)^2 \). With \( m_v \) given, we have defined \( \omega_0 \) by \( V(R) = m_v \omega_0^2 R^2/2 \). For a vortex in a vortex lattice, the characteristic frequency is the plasma frequency
\[ \omega_p = \sqrt{4\pi^2 \rho_s/m_v A_0} \, , \] (5)
where \( \rho_s \) is the superfluid stiffness and \( 1/A_0 \) is the density of vortices. The frequency \( \omega_0 \) is approximately given by \( \omega_0 \approx (5/2)\omega_0 \). Finally, in a Galilean invariant superfluid, \( \omega_c = 2\pi \rho_s/m_v \) and in a dual picture can be identified to be the ‘cyclotron’ frequency. For a superfluid on a lattice, however, it has recently been argued that \( \omega_c \) is reduced and the density of the Mott insulator has to be subtracted from the superfluid stiffness when the superfluid is close to a nearby Mott insulating state.\(^{2,3,4,5}\)

Diagrammatically, the above propagator to the effective vortex action is just the RPA propagator which includes the Berry phase term. To determine the effect of the vortex motion on the electronic spectrum we can use the RPA propagator and calculate the self energy correction to the electronic eigenstates in the GW approximation.\(^{10}\) Let us first expand the gap operator \( \Delta(r - R(\tau)) \) in Eq. 1 to leading order in \( R(\tau) \). Then \( S \) can be written as \( S \approx S_0 + S_{\text{int}} \) with
\[ S_0 = \int d\tau \, d^2r \left( \bar{\psi} \! \psi \right) \left( \partial_\tau + H^0_{\text{BdG}} \right) \left( \psi \! \bar{\psi} \right) \] (6)
and \( H^0_{\text{BdG}} \) obtained from Eq. 2 by setting \( R = 0 \). To leading order the coupling of the vortex to the electronic degrees of freedom is described by
\[ S_{\text{int}} = -\int d\tau \, d^2r \, R(\tau) \left( \bar{\psi} \! \psi \right) \begin{pmatrix} 0 & \partial_\tau \Delta^* \\ \partial_\tau \Delta & 0 \end{pmatrix} \left( \psi \! \bar{\psi} \right) \, . \] (7)
Let us now go to a basis which diagonalizes the Bogoliubov-de Gennes Hamiltonian \( H^0_{\text{BdG}} \): It is well-known that if \( \Psi_t(r) \equiv [u_t(r), v_t(r)]^T \) (with, say, \( t > 0 \) is an eigenstate of \( H^0_{\text{BdG}} \) with eigenvalue \( \epsilon_t \), then \( [-v_t^*(r), u_t^*(r)]^T \) is an eigenstate of \( H^0_{\text{BdG}} \) with eigenvalue \( -\epsilon_t \). Defining
\[ U_\ell(r) = \begin{pmatrix} u_\ell(r) & -v_\ell(r) \\ v_\ell(r) & u_\ell(r) \end{pmatrix} \] (8)
we can write
\[ \begin{pmatrix} \psi_\ell(r, \tau) \\ \bar{\psi}_\ell(r, \tau) \end{pmatrix} = \sum_{\ell > 0} U_\ell(r) \begin{pmatrix} \chi_+ \ell(\tau) \\ \chi_- \ell(\tau) \end{pmatrix} \] (9)
such that
\[ \int d^2r \, U^\dagger_\ell(r) H^0_{\text{BdG}} U_\ell(r) = \sigma_z \epsilon_\ell \delta_{\ell,\ell'} \, , \] (10)
where $\sigma_z$ (like $\sigma_x$ which we will use below) is just a usual Pauli matrix. While it is customary to restrict the energies $\epsilon_\ell$ to values greater zero\textsuperscript{10} for which we use quantum numbers $\ell > 0$, we prefer to subsume the ‘spin’ index into the index $\ell$ and define for $\ell > 0$
\[ \Psi_{-\ell}(r) \equiv [u_{-\ell}(r), v_{-\ell}(r)]^T \equiv [-v_\ell^*(r), u_\ell^*(r)]^T \] such that $\epsilon_{-\ell} = -\epsilon_\ell$. With this notation,
\[ \begin{pmatrix} \psi_\ell^*(r, \tau) \\ \psi_\ell(r, \tau) \end{pmatrix} = \sum_\ell \Psi_\ell(r) \chi_\ell(\tau) \] (11)
and $\mathcal{S}_0$ reduces to
\[ \mathcal{S}_0 = \int d\tau \sum_\ell \tilde{\chi}_\ell(\partial_\tau + \epsilon_\ell) \chi_\ell, \] (12)
where the sum is now over all quantum numbers $\ell$ including the ‘spin’ index. In the new basis, $\mathcal{S}_{int}$ can be written as
\[ \mathcal{S}_{int} = -\int d\tau \sum_{\ell, \ell'} \mathbf{R}(\tau) \cdot \mathbf{M}_{\ell, \ell'} \tilde{\chi}_\ell \chi_{\ell'} , \] (13)
where the transition matrix elements
\[ \mathbf{M}_{\ell, \ell'} = \int d^2 r \left( \left( u_\ell^* \partial_\tau \Delta v_{\ell'} + v_{\ell'}^* \partial_\tau \Delta^* u_\ell \right) \right) \] (14)
are like $\mathbf{R}(\tau)$ vectors in the two-dimensional plane. It is convenient to also define $M^\pm \equiv (M^x \pm i M^y)/2$ such that
\[ M^+_{\ell, \ell'} = \left( M^-_{\ell, \ell'} \right)^* = \int d^2 r \left( u_\ell^* \partial_\tau \Delta v_{\ell'} + v_{\ell'}^* \partial_\tau \Delta^* u_\ell \right), \] (15)
with $\partial_\tau \equiv (\partial_x + i \partial_y)/2$. We can now calculate the self energy in the GW approximation\textsuperscript{10} for which we obtain
\[ \Sigma_\ell(i\omega) = \sum_{\ell', \mu} \frac{A_{\ell, \ell'}^\mu}{\omega + [\omega, \text{sgn}(\epsilon_{\ell'}) + \epsilon_\ell] - \alpha \omega_c/2}, \] (16)
with
\[ A_{\ell, \ell'}^\mu = \frac{|M_{\ell, \ell'}^\mu|^2}{m_c \omega_v}. \] (17)
Here, $\alpha = \pm$ and $\omega_v = \sqrt{\omega_0^2 + \omega_\tau^2}/4$ is the vortex (‘magnetoplasma’) frequency in an Einstein model. As should be expected, the self energy satisfies $\Sigma_{-\ell}(i\omega) = -\Sigma_\ell(-i\omega)$.

If our system is infinitely large and boundary effects can be neglected we can make use of the Hellmann-Feynman theorem
\[ \int d^2 r \Psi_\ell^+ \partial_\tau \mathcal{H}_{BDG}^0 \Psi_{\ell'} = (\epsilon_{\ell'} - \epsilon_\ell) \int d^2 r \Psi_\ell^+ \partial_\tau \Psi_{\ell'} \] (18)
and write $M^\alpha_{\ell, \ell'}$ as
\[ M^\alpha_{\ell, \ell'} = (\epsilon_{\ell'} - \epsilon_\ell) U^\alpha_{\ell, \ell'}, \] (19)
with
\[ U^+_{\ell, \ell'} = \left( U^-_{\ell', \ell} \right)^* = \int d^2 r \Psi_\ell^+ \partial_\tau \Psi_{\ell'}. \] (20)

In our numerical calculation presented below, however, we will, of course, consider a system of finite size such that boundary effects need to be included. We will see that calculating $M^\alpha_{\ell, \ell'}$ using the Hellmann-Feynman theorem will turn out to be easier than calculating these transition matrix elements directly.

### III. VORTEX IN AN s-WAVE SUPERCONDUCTOR

For a vortex in an $s$-wave superconductor centered at the origin we choose $\Delta(r) = \Delta(r) e^{i\theta}$ with $\Delta(r)$ the bulk gap and $\xi = v_F / \pi \Delta_0$ is the coherence length. $\mathcal{H}_{BDG}^0$ is rotationally invariant such that angular momentum is a good quantum number. Following Caroli, de Gennes, and Matricon\textsuperscript{12} we denote angular momentum by $\mu = \pm 1/2, \pm 3/2, \ldots$ and write
\[ \begin{pmatrix} u_\mu^\alpha(r) \\ v_\mu^\alpha(r) \end{pmatrix} = \frac{\exp[-i(\mu - \sigma_z/2)\theta]}{\sqrt{2\pi}} \begin{pmatrix} f_{\mu, +}(r) \\ f_{\mu, -}(r) \end{pmatrix}. \] (21)

There is only one bound state for each angular momentum $\mu$, but there are also extended states, such that we also include a radial quantum number $n^\mu$. It should be noted that while $\ell$ is a collective label for $\mu$ and $n$, $-\ell$ collectively labels $-\mu$ and $n$. Making the above ansatz, the Bogoliubov-de Gennes equations reduce to

\[ \begin{pmatrix} \sigma_z \frac{1}{2m_e} \left( -\frac{d}{dr} \right)^2 - \frac{1}{r} \frac{d}{dr} + \frac{(\mu - \sigma_z/2)^2}{r^2} - \frac{\hbar^2}{v_F^2} \right) + \sigma_z \Delta(r) \right) \left( \begin{array}{c} f_{\mu, +}(r) \\ f_{\mu, -}(r) \end{array} \right) = \epsilon_\mu \left( \begin{array}{c} f_{\mu, +}(r) \\ f_{\mu, -}(r) \end{array} \right). \] (22)

$\epsilon_\mu$ much smaller than the bulk gap $\Delta_0$ and large coherence lengths $\xi$. As was shown by Caroli, de Gennes, and
Matricon, the bound state energies are then given by
\[ \epsilon_\mu = E_1 \mu, \quad \text{with} \quad E_1 \approx \frac{\Delta_0^2}{E_F}. \] (23)

Also, the radial part of the wave function is well approximated by
\[ f_{\mu, \pm}(r) = C_\mu \exp \left( -2 \int_0^r \frac{\Delta(r')}{v_F} \right) J_{\mu+1/2}(k_F r), \] (24)

where \( J_m(x) \) are ordinary Bessel functions of the first kind and integer order \( m = \mu \mp 1/2 \). The constants \( C_\mu \) are independent of the \( \pm \) index and are all of order \( \sqrt{k_F/\xi} \). It should be noted that \( f_{\mu+1, +}(r) \approx f_{\mu, -}(r) \) which we will use for an estimate of the matrix elements \( A_{\mu', \mu; n'}^{\mu, \mu} = \delta_{\mu', \mu+1} A_{\mu; n}^{\mu, \mu} \). With the radial quantum number included we have

\[ M_{\mu n, \mu'; n'}^{\mu, \mu} = \frac{1}{2} \delta_{\mu', \mu+1} \int_0^\infty dr \left\{ \left[ \rho \partial_r \Delta - \Delta(r) \right] J_n^{\mu, +}(r) J_n^{\mu', -}(r) + \left[ \rho \partial_r \Delta + \Delta(r) \right] f_n^{\mu, -}(r) f_n^{\mu', +}(r) \right\}. \] (25)

Using the above, we obtain \( A_{\mu}^+ \approx v_F^2/(4\pi^2 m_e \omega_0 \xi^4) \).

Since the mass of a vortex in a BCS superconductor, \( m_v \), is of the order \( m_e(k_F \xi)^2 \), it follows
\[ A_{\mu}^+ \approx A \equiv \frac{1}{4\pi v_F m_e^2(\omega_0/\Delta_0)^5}. \] (26)

The fact that if we keep \( \omega_0/\Delta_0 \) constant, the self energy increases with the fifth power of \( 1/\xi \) as \( \xi \) decreases is quite remarkable. For large \( \xi \), the self energy correction is very small and the motion of the vortex obviously has practically no influence on the spectrum. However, as \( \xi \) decreases, the self energy correction becomes more and more important and we expect a dramatic change of the spectrum within a small range of the coherence length \( \xi \).

Let us now consider the local density of states (LDOS) (in the more general case and with \( \ell \) including the ‘spin’ index) is given by
\[ \rho(r, \omega) = -\frac{1}{\pi} \text{Im} \sum \varepsilon \left\{ \frac{|u_r(r)|^2}{\omega - \varepsilon - \Sigma_{\varepsilon}(\omega) + i0^+} \right\}. \] (27)

For the case of an \( s \)-wave order parameter as considered here, the only bound state wave function which does not vanish at \( r = 0 \) is \( u_{\mu=1/2}(r) \). We can therefore actually calculate the LDOS at the vortex center and obtain
\[ \rho(0, \omega) = \frac{|u_{\mu=1/2}(0)|^2}{\omega_1^2} \left\{ (\omega_0 + \omega_e + E_1)^2 \delta(\omega - \epsilon_{1/2}) + A \delta(\omega - \epsilon_{1/2} - \omega_1) \right\}, \] (28)

with \( \omega_1 = \sqrt{(\omega_0 + \omega_e + E_1)^2 + 2A} \) which for large coherence lengths \( \xi \) is close to the vortex frequency \( \omega_v \). While there is just a peak with weight \( |u_{\mu=1/2}(0)|^2 \) at the unperturbed energy \( \epsilon_{1/2} \) in the absence of the matrix element \( A \), as \( \xi \) decreases \( A \) increases and we also find two satellite peaks shifted from this position by \( \pm \omega_1 \).

To obtain the LDOS away from the vortex center and to calculate the LDOS at arbitrary energy we follow Gygi and Schlüter and evaluate the eigenenergies and eigenvectors of \( \mathcal{H}_{\text{BdG}} \) numerically. First we replace the system of infinite size by a disk of finite radius \( R_0 \). We then expand the quasi-particle amplitudes \( f_{n, \pm} \) into Fourier-Bessel series: Denoting the \( j \)’th zero of the ordinary Bessel function \( J_m \) by \( \alpha_{mj} \), we introduce the functions
\[ \phi_{mj}(r) = \frac{\sqrt{2}}{R_0|J_{m+1}(\alpha_{mj})|} J_m(\alpha_{mj} r/R_0), \] (29)

which are eigenfunctions to the kinetic energy operator and satisfy the normalization condition
\[ \int_0^{R_0} dr r \phi_{mj}(r)\phi_{mj'}(r) = \delta_{jj'} \]. (30)

Truncating the Fourier-Bessel series for the quasi-particle amplitudes \( f_{n, \pm} \) at large \( N_0 \), we have
\[ \begin{pmatrix} f_{n, +}(r) \\ f_{n, -}(r) \end{pmatrix} = \sum_{j=1}^{N_0} \begin{pmatrix} c_{mj}^+ \phi_{\mu+1/2,j}(r) \\ d_{mj}^- \phi_{\mu-1/2,j}(r) \end{pmatrix}. \] (31)

With these approximations the Bogoliubov-de Gennes equations can be solved by solving the following matrix eigenvalue problem:
\[ \begin{pmatrix} T^- & \Delta \\ \Delta^T & T^+ \end{pmatrix} \Psi_n = \epsilon_n \Psi_n. \] (32)

Here \( T^\pm \) and \( \Delta \) are \( N_0 \times N_0 \) matrices with matrix elements
\[ T_{jj'}^{\pm} = \mp \frac{1}{2m_e} \left( \frac{\alpha_{j+1/2,j}^2 - k_F^2}{R_0^2} \right) \delta_{jj'}, \] (33)
\[ \Delta_{jj'} = \int_0^{R_0} dr r \phi_{\mu-1/2,j}(r) \Delta(r) \phi_{\mu+1/2,j'}(r) \] (34)
and $\Psi^\mu_n$ is given by $\Psi^\mu_n = (c_1 \cdots c_{N\sigma}, d_1 \cdots d_{N\sigma})^T$. Having calculated these eigenvectors we can express the matrix elements $M^\mu_{\mu, n, \mu + 1, n'}$ which determine the $A^\mu_{\mu, n, n'}$ as

$$M^\mu_{\mu, n, \mu + 1, n'} = \frac{1}{2} \sum_{j,j'} \left( C^\mu_{j,j'} \frac{\partial \mu_{j,j'}(r)}{\partial \mu_{j,j'}(r) \phi_{\mu_{j,j'}(r)}, \phi_{\mu_{j,j'}(r)}} + d^\mu_{j,j'} e_{n, n'} d \right),$$

where we have defined

$$K^{(\mu)}_{j,j'} = \int_0^{R_0} dr \left[ r \partial_r \Delta + \Delta(r) \right] \phi_{\mu_{j,j'}(r)} \phi_{\mu_{j,j'}(r)},$$

and

$$L^{(\mu)}_{j,j'} = \int_0^{R_0} dr \left[ r \partial_r \Delta + \Delta(r) \right] \phi_{\mu_{j,j'}(r)} \phi_{\mu_{j,j'}(r)},$$

Alternatively, as discussed at the end of the preceding section, we can also make use of the Hellmann-Feynman theorem which when including boundary terms reads for the s-wave case considered here.

$$M^\mu_{\mu, n, \mu + 1, n'} = (\epsilon - \epsilon) U^\mu_{\mu, n, \mu + 1, n'} - \frac{R_0}{2m_e} \int_0^{R_0} d\theta \partial_r \Psi^\mu_{\mu, n, \mu + 1, n'} |_{r=R_0}.$$  

Expressing all wave functions in terms of their Fourier-Bessel components both integrals can be done analytically and we obtain

$$M^\mu_{\mu, n, \mu + 1, n'} = \frac{1}{2} \sum_{j,j'} \left[ C^\mu_{j,j'} \frac{\partial \mu_{j,j'}(r)}{\partial \mu_{j,j'}(r) \phi_{\mu_{j,j'}(r)}, \phi_{\mu_{j,j'}(r)}} + d^\mu_{j,j'} \right] C^\mu_{n, n'} d \left( n, n' \right),$$

with the matrix elements $K^{(m)}_{j,j'}$ and $L^{(m)}_{j,j'}$ given by

$$K^{(m)}_{j,j'} = \text{sign}(m + 1/2) (-1)^{j-j'} \frac{2 \alpha_{m,j} \alpha_{m+1,j'}}{R_0 (\alpha^2_{m,j} + \alpha^2_{m+1,j'})},$$

$$L^{(m)}_{j,j'} = \text{sign}(m + 1/2) (-1)^{j-j'} \frac{\alpha_{m,j} \alpha_{m+1,j'}}{m_e R_0^2}.$$  

For simplicity and to avoid too many parameters which do not change the essential physics, we have neglected the electromagnetic vector potential in our above considerations and will not calculate the pair potential self-consistently. Neglecting the vector potential is safe in the extreme type II case where the London penetration length is much larger than the coherence length which we are considering here. Although there are significant deviations from the tanh-behavior of $\Delta(r)$ for small temperatures, corrections to the LDOS are expected to be small and can easily be incorporated. Once all eigenenergies and eigenvectors of $H^0_{BdG}$ are determined, the matrix elements $A^\mu_{\mu, n, n'}$ and then the LDOS can be calculated.

In STM experiments the local tunneling conductance $G = \partial I/\partial V$ can be measured as a function of gate voltage $V$. If we are at very low temperature and have a tip with a constant density of states (DOS) the tunneling conductance is essentially equal to the LDOS of the probe. At finite temperature, each peak in the LDOS becomes broadened with the derivative of the Fermi function $f(\omega) = 1/(e^{\omega/T} + 1)$ such that

$$G(r, \omega = eV) = -\frac{G_0}{\rho_0} \int d\omega \rho(r, \omega + \omega') f'(\omega').$$

Here we have expressed the normalization constant in terms of the DOS of a free 2-dimensional electron gas (per spin direction), $\rho_0 = m_e/2\pi$, and the corresponding tunneling conductance, $G_0$.

In our numerical calculations we have chosen $k_F R = 400$. For the vortex (Einstein) frequency we use $\omega_{\nu} = 0.2 \Delta_0$ and for simplicity we set $\omega_c = 0$. Setting the temperature equal to $T = 0.006 E_F$ we obtain smooth curves for the tunneling conductance with well distinguished bound state peaks. In Fig. 1 we show plots of the tunneling conductance $G(r, \omega)$ at the vortex center and at several distances away from it for $k_F \xi = 10$ and $m_e = m_e(k_F \xi)^2 = 100 m_e$. The plots are almost indistinguishable from plots for the tunneling conductance with the same parameters but a static vortex (this amounts to taking the limit $m_e \to \infty$). As we decrease the coherence length (and/or the vortex mass) the influence of the moving vortex on the electronic spectrum becomes more and more pronounced. In Fig. 4 we show the tunneling conductance for $k_F \xi = 5$ and $m_e = m_e(k_F \xi)^2 = 25 m_e$. Now one can clearly see two satellite peaks at the center of the vortex, shifted from the central peak by $\pm \omega_1$ which is of the order of the vortex frequency $\omega_\nu$. In units of the Fermi energy the temperatures chosen in Figs. 1 and 2 are the same. However, in units of the bulk gap $\Delta_0$, the temperature in the latter figure is smaller than that in the former by a factor of two. As a result of this, the height of the zero bias peak is actually larger in Fig. 2 than in Fig. 1 even though spectral weight is shifted to the satellite peaks in Fig. 2. In fact, the quantum zero-point motion does lead to a reduction of the zero bias conductance peak as can be seen by comparing the results of Fig. 4 with those calculated for the same parameters, but with a static vortex. This case is shown in Fig. 5.

IV. CONCLUSIONS

We presented a first determination of the influence of the vortex zero-point motion in a simple model based upon BCS theory. For s-wave superconductors, a comprehensive computation was possible, with good convergence of finite-size effects, and the ability to explore a wide range of parameters as $T \to 0$. We found two important effects in the electronic LDOS: (i) a suppression in the strength of the zero-bias peak at the vortex core,
FIG. 1: Tunneling conductance $G = \partial I / \partial V$ for a superconductor with $s$-wave symmetry as a function of $\omega$ at the vortex center $r = 0$ (upper curve) and $k_F r = 4, 8, \ldots, 20$ for $k_F \xi = 10$ and $m_v = m_e (k_F \xi)^2 = 100 m_e$. Each curve is offset by 2 units for clarity. We have chosen $\omega_c = 0.2 \Delta_0$ and have for simplicity set $\omega_c = 0$. The temperature is $T = 0.006 E_F$ and this finite temperature leads to a broadening of the conductance peaks. As can be seen in the figure, there are no satellite peaks. For these parameters, the tunneling conductance of the static vortex case, without the self energy correction, has an almost identical appearance.

and (ii) the appearance of satellite peaks at frequencies of order $\pm \omega_v$, where $\omega_v$ is the vortex oscillation frequency.

An extension of our results to $d$-wave superconductors appears in paper II. There we will introduce a model designed specifically to study the influence of the low energy quasiparticles, and present implications for experiments on the cuprate superconductors.

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APPENDIX A: BOGOLIUBOV-DE GENNES EQUATIONS FOR A $d$-WAVE SUPERCONDUCTOR

In this appendix we derive local Bogoliubov-de Gennes equations for a superconductor with $d$-wave symmetry. These are applied to the vortex zero point motion, as in Section II while complete numerical results are deferred to paper II.

As a starting point we use the following generalized Bogoliubov-de Gennes equations,

$$
\begin{pmatrix}
\hat{\mathcal{H}}_0 & \hat{\Delta} \\
\hat{\Delta}^* & -\hat{\mathcal{H}}_0^*
\end{pmatrix}
\begin{pmatrix}
\hat{u}_\ell(r) \\
\hat{v}_\ell(r)
\end{pmatrix}
= \epsilon_\ell
\begin{pmatrix}
\hat{u}_\ell(r) \\
\hat{v}_\ell(r)
\end{pmatrix}
.$$  (A1)

Here,

$$\hat{\mathcal{H}}_0 = \frac{1}{2m_e} (-i \partial_r + \mathbf{A}(\mathbf{r}))^2 - E_F$$  (A2)

is the effective single particle Hamiltonian, $\mathbf{A}(\mathbf{r})$ is the vector potential, and the gap operator $\hat{\Delta} = \Delta(\mathbf{r})$ is de-
To obtain local Bogoliubov-de Gennes equations we use this order parameter and expand the rhs of Eq. (A4) up to second order in \( \mathbf{r}' \) which certainly is a good approximation if the dominant contribution to \( \Delta(\mathbf{r}, \mathbf{r}') \) comes from small \( \mathbf{r}' \) which we will assume here. Within this approximation, it is straightforward to show that

\[
\hat{\Delta} = \frac{(\partial_x^2 - \partial_y^2)\Delta}{4k_F^2} + \frac{\partial_x \Delta \partial_x - \partial_y \Delta \partial_y}{k_F^2} + \frac{\Delta(\partial_x^2 - \partial_y^2)}{k_F^2},
\]

which can also be written as

\[
\hat{\Delta} = \left\{ \partial_x, \{\partial_x, \Delta(\mathbf{r})\} \right\} - \left\{ \partial_y, \{\partial_y, \Delta(\mathbf{r})\} \right\}
\]

(A8)

where \( \{a, b\} = (ab + ba)/2 \) denotes a symmetrized product and we have defined \( \Delta(\mathbf{r}) \) as

\[
\Delta(\mathbf{r}) = \frac{\pi}{4} k_F^2 \int_0^{\infty} dr' r'^3 \Delta(\mathbf{r}, \mathbf{r}') \cdot
\]

(A9)

Eq. (A9) is equivalent to the gap operator derived by Simon and Lee\(^\text{[8]}\) for a \( d_{xy} \)-wave superconductor. It was later claimed by Vafek \textit{et al} in\(^\text{[9]}\) that this gap operator would not preserve the gauge invariance of the Bogoliubov-de Gennes equations and an additional term was introduced to fix this problem. The implicit assumption underlying this claim is that \( \Delta(\mathbf{r}) \) (as well as \( \hat{\Delta} \)) should transform under a gauge transformation as \( \Delta(\mathbf{r}) \rightarrow e^{2i\chi(\mathbf{r})} \Delta(\mathbf{r}) \). Using our approach, it is however easy to see that although the gap operator \( \Delta \) is gauge invariant the above assumption does not hold: Working to the same order as before it follows from Eq. (A4) that under a gauge transformation we have \( \Delta(\mathbf{r}, \mathbf{r}') \rightarrow e^{2i\chi(\mathbf{r})}(1 + i \partial_x \partial_y \chi_{\alpha\beta} r'_\alpha r'_\beta/4)\Delta(\mathbf{r}, \mathbf{r}') \). Plugging this into Eq. (A7), it is a straightforward exercise to show that under this transformation the gap operator \( \hat{\Delta} \) does indeed transform as \( \hat{\Delta} \rightarrow e^{2i\chi(\mathbf{r})}\hat{\Delta} \) such that the local Bogoliubov-de Gennes equations are gauge invariant. The transformation properties of \( \Delta(\mathbf{r}) \) are more complicated but this is no problem because the gap operator is a combination of derivatives and \( \Delta(\mathbf{r}) \) and only this combination has to transform as \( \hat{\Delta} \rightarrow e^{2i\chi(\mathbf{r})}\hat{\Delta} \). It should also be noted that the derivation of the gap operator and the above argument about its gauge transformation become exact in the limit where \( \Delta(\mathbf{r}, \mathbf{r}') \) becomes more and more peaked at smaller and smaller \( \mathbf{r}' \).

**APPENDIX B: EFFECTIVE ACTION OF A VORTEX IN A BCS SUPERCONDUCTOR**

In this appendix we present a simple and straightforward derivation of the effective action describing vortex dynamics in a clean two-dimensional BCS superconductor. These complement the results of Ref.\(^\text{[3]}\) which presented the corresponding results using a low energy theory for a \( d \)-wave superconductor.

Our starting point is the Bogoliubov-de Gennes-like action given in Eq. (1) without the harmonic oscillator.
potential $V(R)$,
\[ S = \int d^2r \, d\tau \left( \bar{\psi}_1 \psi_1 \right) \left( \partial_\tau + i\mathcal{H}_{\text{BdG}} \right) \left( \bar{\psi}_1 \psi_1 \right). \] (B1)

In contrast to alternative derivations of an effective vortex action we have seen, we will not expand $\mathcal{H}_{\text{BdG}}$ in powers of $R$. Instead, we diagonalize the Bogoliubov-de Gennes Hamiltonian $\mathcal{H}_{\text{BdG}}$ at every instant in imaginary time $\tau$ in terms of its eigenfunctions. Using the unitary transformation given in Eq. (1) we then obtain
\[ S = \int_0^\beta d\tau \sum_\ell \bar{\chi}_\ell (\partial_\tau + \epsilon_\ell) \chi_\ell + \int_0^\beta d\tau \sum_{\ell,\ell'} \bar{\chi}_\ell Q_{\ell,\ell'} \chi_{\ell'}. \] (B2)

Here, $Q_{\ell,\ell'} \equiv Q_{\ell,\ell'}(\tau)$ is given by
\[ Q_{\ell,\ell'} = -\hat{R}(\tau) \cdot \int_{|r| \leq R_0} d^2r \left[ u_\ell^* (r - R(\tau)) \partial_\tau v_{\ell'} (r - R(\tau)) + v_{\ell'}^* (r - R(\tau)) \partial_\tau u_\ell (r - R(\tau)) \right]. \] (B3)

When shifting $r$ by $R(\tau)$, boundary terms which finally will lead to a Berry phase need to be considered carefully. We have therefore restricted the integration over space to $|r| \leq R_0$ and will only at the end of the calculation take the limit $R_0 \to \infty$. Doing the mentioned shift $r \to r + R(\tau)$, we get $Q_{\ell,\ell'}(\tau) = Q_{\ell,\ell'}(0) + Q_{\ell,\ell'}(1)(\tau)$ with
\[ Q_{\ell,\ell'}(0) = -\hat{R} \cdot \int_{|r| \leq R_0} d^2r \left[ u_\ell^* \partial_\tau v_{\ell'} + v_{\ell'}^* \partial_\tau u_\ell \right], \] (B4)
and
\[ Q_{\ell,\ell'}(1)(\tau) = \oint_{|r| = R_0} (dr \times R) \cdot \hat{e}_z \left( \hat{R} \cdot \left[ u_\ell^* \partial_\tau v_{\ell'} + v_{\ell'}^* \partial_\tau u_\ell \right] \right). \] (B5)

To obtain an effective action for the vortex, we can now integrate out the fermionic degrees of freedom. It is convenient to first transform the imaginary-time integral in Eq. (B2) in a Matsubara sum over fermionic frequencies $\omega_n = (2n + 1)/\beta$. The effective action for the vortex is then given by
\[ S_{\text{Vortex}} = -\text{Tr} \ln \left( 1 + \frac{1}{\beta} G Q \right). \] (B6)

Here, $G$ is a diagonal matrix Green function with matrix elements $1/(i\omega_n - \epsilon_\ell)$, $Q$ has as its matrix elements the Fourier transforms of $Q_{\ell,\ell'}(\tau)$, and the trace is over both $\omega_n$ and all $\ell$. Expanding the logarithm in the effective vortex action up to second order we obtain $S_{\text{eff}} \approx S_{\text{Vortex}} = S_{\text{eff},1} + S_{\text{eff},2}$, with
\[ S_{\text{eff},1} = \sum_\ell f(\epsilon_\ell) Q_{\ell,\ell}(0), \] (B7)
and
\[ S_{\text{eff},2} = \frac{1}{2} \sum_{\omega_m, \ell, \ell'} \frac{f(\epsilon_{\ell'}) - f(\epsilon_{\ell})}{\omega_m - \epsilon_{\ell'} + \epsilon_{\ell'}} |Q_{\ell,\ell'}(i\omega_m)|^2. \] (B8)

Here, $f(\epsilon) = 1/(e^{\beta\epsilon} + 1)$ is the Fermi function and the $\omega_m = 2\pi m / \beta$ are bosonic Matsubara frequencies. While $Q_{\ell,\ell'}^{(0)}$ does not give a contribution to Eq. (B7) due to its antisymmetry, we have not included $Q_{\ell,\ell'}^{(1)}(i\omega_m)$ into Eq. (B8) because it only contributes at higher order. Identifying
\[ j(r) = \frac{1}{2m_s} \sum_\ell \left[ u_\ell^* \partial_\tau v_{\ell'} + v_{\ell'}^* \partial_\tau u_\ell \right] \] (B9)
as the current and using well-known vector identities we can rewrite $S_{\text{eff},1}$ as
\[ S_{\text{eff},1} = \frac{2m_s i}{\beta} \sum_{\omega_m} i\omega_m \left( R(\omega_m) \times R(-i\omega_m) \int_0^\beta dr \cdot j \right) \] (B10)
\[ - \oint d\tau \left( R(-i\omega_m) j \right) \cdot \hat{e}_z. \]

Now, using $j = \rho_s v_s = \rho_s \theta/2m_s R$, where $\rho_s$ is the superfluid stiffness and $v_s$ the superfluid velocity, we arrive at
\[ S_{\text{eff},1} = -\pi \rho_s \frac{1}{\beta} \sum_{\omega_m} \omega_m \left( R(\omega_m) \times R(-i\omega_m) \right) \cdot \hat{e}_z. \] (B11)

This is the Magnus force whose interpretation as a geometrical Berry phase is most transparent when transforming back to imaginary time. Defining
\[ S(\Gamma) = \frac{1}{2} \int_0^\beta d\tau \left( \hat{R} \times \hat{R} \right) \cdot \hat{e}_z = \frac{1}{2} \int_\Gamma (dR \times R) \cdot \hat{e}_z \] (B12)
as the area enclosed by the loop $\Gamma$ we can recast Eq. (B11) into
\[ S_{\text{Vortex}} = -i2\pi \rho_s S(\Gamma), \] (B13)
which agrees with the result by Ao and Thouless who emphasized the robustness of the Berry phase. Let us now consider $S_{\text{Vortex}}$ which we rewrite as
\[ S_{\text{Vortex}} = \frac{1}{2\beta} \sum_{\omega_m, \ell, \ell'} \frac{f(\epsilon_{\ell'}) - f(\epsilon_{\ell})}{\omega_m - \epsilon_{\ell'} + \epsilon_{\ell'}} \omega_m^2 |U_{\ell,\ell'} \cdot R(\omega_m)|^2, \] (B14)
with
\[ U_{\ell,\ell'} = \int d^2r \left[ u_\ell^* \partial_\tau v_{\ell'} + v_{\ell'}^* \partial_\tau u_\ell \right]. \] (B15)

Neglecting the small $\omega_m$ in the denominator of Eq. (B14) and noticing that after summation over $\ell$ and $\ell'$ the term proportional to $(R(\omega_m) \times R(-i\omega_m)) \cdot \hat{e}_z$ has to vanish we obtain
\[ S_{\text{Vortex}} = \frac{m_v}{2} \frac{1}{\beta} \sum_{\omega_m} \omega_m^2 |R(\omega_m)|^2 = \frac{m_v}{2} \int_0^\beta d\tau \hat{R}^2(\tau), \] (B16)
where the mass of the vortex, $m_v$, is given by

$$m_v = \frac{1}{2} \sum_{\omega_m, \ell, \ell'} \frac{f(\epsilon_\ell) - f(\epsilon_{\ell'})}{\epsilon_\ell - \epsilon_{\ell'}} |U_{\ell, \ell'}|^2.$$

(B17)

Using the formalism described in the main body of this paper this equation can be used to calculate the mass of a vortex in a superconductor with $s$- or $d$-wave symmetry. To summarize, we can write the vortex action as

$$S_{\text{Vortex eff}} = m_v \frac{1}{2} \beta \sum_{\omega_m} \mathbf{R}^\dagger(i\omega_m) \begin{pmatrix} \omega_m^2 & \omega_c & \omega_m^2 \\ -\omega_c & \omega_m^2 & \omega_c \\ \omega_m^2 & -\omega_c & \omega_m^2 \end{pmatrix} \mathbf{R}(i\omega_m),$$

(B18)

with $\omega_c = 2\pi \rho_s / m_v$ which when taking the limit of zero temperature and putting the vortex in a harmonic oscillator potential turns into Eq. (4). While the vortex mass can in principle be calculated microscopically it can also be treated as a phenomenological constant.

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16. Actually, $\mu$ is minus the angular momentum of a given eigenstate. The minus sign is due to the fact that we are considering a vortex of positive vorticity but prefer to have $\epsilon_\mu$ positive if $\mu$ is positive.