

Birman-Schwinger and the number of Andreev states in Bardeen-Cooper-Schrieffer superconductors

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The number of bound states resulting from inhomogeneities in a BCS superconductor is usually established either by variational means or via exact solutions of particularly simple, symmetric perturbations. Here, we propose estimating subgap states using the Birman-Schwinger principle. We derive upper bounds on the number of subgap states for small normal regions and find a suitable Cwikel-Lieb-Rozenblum inequality. We also estimate the number of such states for large normal regions using high dimensional generalizations of the Szegő theorem. The method works equally well for local inhomogeneities of the order parameter and for external potentials.

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I. INTRODUCTION

It is well known that inhomogeneities in a superconducting system may give rise to Andreev bound states. Such bound states form in superconductor–normal metal–superconductor (SNS) junctions and can affect the transmission and noise properties of the junction. The presence of such states in the cores of vortices is of much interest as well. Vortices in *s*-wave superconductors may have Caroli–de Gennes–Matricon (CdGM) states;¹ bound states in vortices in *p* + *ip* superfluids were studied, e.g., in Ref. 2. Zero modes in the core of half-quantum vortices in *p*-wave superconductors^{3,4} are of extensive recent interest. Such modes are described in terms of unpaired Majorana fermions and have non-Abelian braiding statistics.^{5,6} Other inhomogeneities in the system have been of interest as well, for example, stripes and other structures in the pairing function of a superconductor (see, e.g., Refs. 7 and 8).

Often, the bound states are either directly obtained for systems of high symmetry, such as a circular vortex, or idealized planar SNS junctions, or studied using perturbation theory. In addition, multiple scattering and semiclassical (WKB) methods based on the Andreev approximation have been developed.⁹

In this paper, we introduce an alternative view on Andreev states, complementing the above-mentioned methods. Our approach does not assume a particular symmetry, and works even when the Andreev approximation is inadequate (see, e.g., Ref. 10). We base our approach on a simple adaptation of the Birman-Schwinger counting argument to the superconducting scenario. The Birman-Schwinger method has been widely used to study bound states of the Schrödinger equation with a potential. The Birman-Schwinger bound has been introduced by Birman¹¹ and Schwinger¹² as a refinement of previous estimates by Bargmann¹³ on the number of bound states in a potential. For a discussion and review see Ref. 14. Recently the Birman-Schwinger approach was used in the context of estimating the critical temperature of BCS models in Refs. 15–17.

In this paper we establish the following results:

(1) A bound on the number of subgap states in a superconductor containing a normal region. The bound on the number of

states below a given subgap energy *E* is expressed in Eq. (11) and holds for general values of the chemical potential μ , the gap Δ_0 . For example, in the limit of large chemical potential, the inequality is given in the simple form

$$N_E \leq \frac{\sqrt{\mu} \Delta_0^4 \text{vol}(A)}{\pi (\Delta_0^2 - E^2)^{3/2}} + \frac{\Delta_0^2 (\Delta_0^2 - 2E^2) \text{vol}(A)}{8\pi \mu^{3/2} \sqrt{\Delta_0^2 - E^2}}, \quad (1)$$

where $\text{vol}(A)$ is the volume of the normal region. Clearly, the inequality is most effective for energies not very close to the top of the gap.

(2) In studying the bound states of Schrödinger operators with deep potential wells, often Birman-Schwinger inequalities yield poor upper bounds to the number of bound states. In such cases the Cwikel-Lieb-Rozenblum inequality^{18–20} may be used to obtain upper bounds with power-law behavior in line with the semiclassical expectations for deep wells. We establish the Cwikel-Lieb-Rozenblum inequality (20) for the Bogolubov–de Gennes equation. This bound requires more work and has the advantage of retaining a simple form for a spatially varying Δ ; however, for normal regions, and in the typical situation of gap energy being small compared to Fermi energy, it seems to give a worse upper bound to the number of states than the simple Birman-Schwinger inequality.

(3) Finally, using semiclassical tools and the relation to Szegő theory we supply an asymptotic expression for the number of states in large regions and a conjecture (28) for the scaling $l^{d-1} \log(k_F l)$ of the subleading term.

The paper is organized as follows: In Sec. II, we derive a Birman-Schwinger operator which is suitable for the treatment of mean field BCS superconductors. In Sec. III we derive the basic bound on the number of states in a normal region of a superconductor. We proceed to present the Cwikel-Lieb-Rozenblum inequality in Sec. IV, the derivation of which is technical and deferred to the Appendix. In Sec. V we consider the boundary correction to the number of states for asymptotically large normal regions and explain their connection to the theory of Toeplitz operators and Szegő theorems.

II. THE BIRMAN-SCHWINGER PRINCIPLE FOR BCS

To employ this method, we consider a superconductor described by the mean field BCS Hamiltonian:

$$H_{\text{BCS}} = \sum_{\sigma} \int \psi_{\sigma}^{\dagger}(x) \left[u(x) - \mu - \frac{\hbar}{2m} \nabla^2 \right] \psi_{\sigma}(x) dx + \int [\Delta_{\sigma\sigma'}(x, x') \psi_{\sigma}^{\dagger}(x) \psi_{\sigma'}^{\dagger}(x') + \text{H.c.}] dx dx', \quad (2)$$

where Δ is the superconducting order parameter, μ is the chemical potential, $u(x)$ is a local potential, and m is the effective electron mass. Δ is related to the anomalous Green's function through a self-consistency condition. Here we will assume that $u(x)$ and Δ are given, and represent the effective values of these parameters, which are, in principle, measurable directly.

To diagonalize the BCS Hamiltonian we use the Bogolubov–de Gennes (BdG) equation

$$H_{\text{BdG}} \begin{pmatrix} \psi_e \\ \psi_h \end{pmatrix} = E \begin{pmatrix} \psi_e \\ \psi_h \end{pmatrix}, \quad H_{\text{BdG}} = \begin{pmatrix} h & \Delta \\ \Delta^* & -h \end{pmatrix}, \quad (3)$$

where ψ_e, ψ_h are the electron and hole parts of the quasiparticle wave function, and E is the quasiparticle excitation energy measured relative to the Fermi energy. The solutions of this equation come in $+E, -E$ pairs (unpaired states may exist at $E = 0$). We will mostly consider $h = -\nabla^2 - \mu + u(x)$ (throughout, we take $\frac{\hbar^2}{2m} = 1$).

For a translationally invariant Δ and $u(x) = 0$, the spectrum of the BdG operator is continuous and consists of the positive and negative energy bands. In an s -wave superconductor these bands are separated from zero by the gap $|\Delta|$. The method will also work for other gap functions, for example in a p -wave superconductor or superfluid with gap $\Delta(p) \sim \Delta_0(p_x + ip_y)$ (as in the Anderson-Brinkman-Morel phase of ^3He). Andreev states in d -wave superconductors have also been of much interest; however, in d -wave superconductors the gap function vanishes on the nodal lines and one needs to differentiate between resonant states and the rest of the spectrum.

To study the introduction of bound states into the system from an inhomogeneous Δ (and possibly also u), we write the perturbed H_{BdG} as $H_0 + W$ where H_0 is translationally invariant. Here W represents the perturbation (inhomogeneous Δ , disorder potential, etc.). We choose a decomposition of the perturbation W into a product $W_1 W_2$, and define the Birman-Schwinger operator:

$$K_E = W_2 \frac{1}{E - H_0} W_1. \quad (4)$$

The key property of K_E is that it has an eigenvalue $\frac{1}{\lambda}$ for each eigenvalue E of $(H_0 + \lambda W)$. Indeed,

$$\begin{aligned} (H_0 + \lambda W)\phi = E\phi &\Rightarrow \frac{1}{\lambda}\phi \\ &= -(H_0 - E)^{-1} W_1 W_2 \phi \Rightarrow \frac{1}{\lambda} (W_2 \phi) \\ &= W_2 (H_0 - E)^{-1} W_1 (W_2 \phi) = K_E (W_2 \phi). \end{aligned} \quad (5)$$

Thus, $W_2 \phi$ is an eigenvector of K_E with eigenvalue $\frac{1}{\lambda}$. The two major differences between the BCS system and the Birman-Schwinger kernel K_E typically used to study bound states in

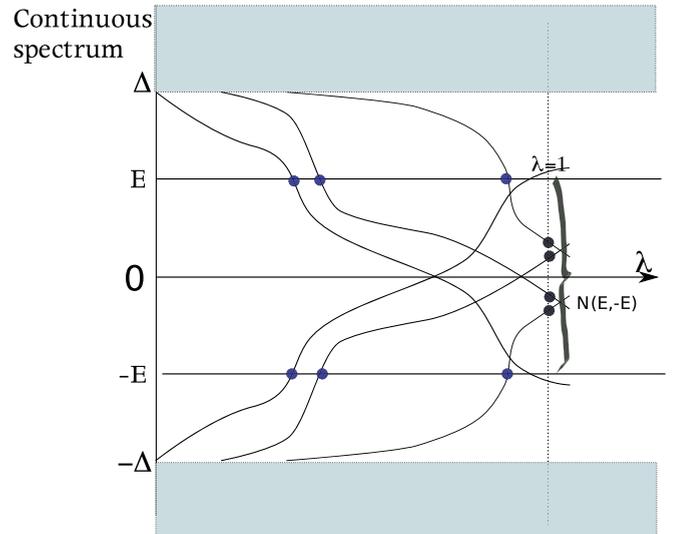


FIG. 1. (Color online) The Birman-Schwinger principle: Continuity of the bound state energy as a function of λ implies that each bound state at $\lambda = 1$ with energy in $(E, -E)$ corresponds to at least one crossing of the E or $-E$ line for some $\lambda \in (0, 1)$.

Schrödinger operators is that H_{BdG} is not bounded below, and that K_E is not Hermitian, but the ideas have been used to estimate the number of states within a spectral gap (see, e.g., Ref. 21).

We now invoke the Birman-Schwinger argument:

Let $N_{E_1, E_2}(V)$ = number of eigenvalues of $H_0 + V$ in the interval (E_1, E_2) , where E_1, E_2 are in the gap; i.e., $|E_1|, |E_2| < \min_p(|\Delta(p)|)$. Assuming that the energy of eigenvalues of $H_0 + \lambda V$ depends continuously on λ as we increase λ from 0 to 1, we see that each eigenvalue for $\lambda = 1$ must have crossed the E_1 or E_2 line for some value of $\lambda \in (0, 1)$, as illustrated in Fig. 1. Thus,

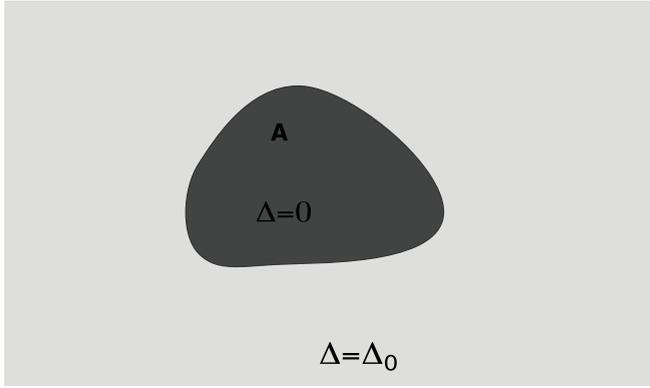
$$\begin{aligned} N(E) &\leq \text{number of crossings for } \lambda \in (0, 1) \\ &= \text{number of eigenvalues of } K_E \text{ larger than } 1. \end{aligned} \quad (6)$$

Note that the inequality sign in (6) is due to the fact that in all cases we consider perturbations that are not strictly positive or negative. The curves in Fig. 1 may be nonmonotonous functions of λ and an in-gap eigenvalue at $\lambda = 1$ may correspond to several crossings. Moreover, in some situations no bound states will be created even for very large λ .

It is important to note that for unpaired zero modes of an unperturbed system such as the $p_x + ip_y$ superconductor (for example in the presence of vortex or boundary), the principle will still work. Such a zero mode is stable as long as it is far from other vortices, and will not shift when adding impurity potentials.

We now find the explicit form of the Birman-Schwinger kernel useful for the study of Andreev bound states in a normal domain of general shape embedded in the superconductor. First, we decompose $\Delta = \Delta_0 + \delta\Delta$, $\delta\Delta = \delta\Delta_1 + \delta\Delta_2$, and note that

$$\begin{pmatrix} 0 & \delta\Delta \\ \delta\Delta^* & 0 \end{pmatrix} = \begin{pmatrix} \delta\Delta_1 & 0 \\ 0 & \delta\Delta_2^* \end{pmatrix} \begin{pmatrix} 0 & \delta\Delta_2 \\ \delta\Delta_1^* & 0 \end{pmatrix}. \quad (7)$$


 FIG. 2. A normal region A inside the superconductor.

To further simplify the system we assume an s -wave superconductor. This will be described by $\Delta = \Delta_0$ outside the region and $\Delta = 0$ inside (Fig. 2). Thus we write $\delta\Delta_1 = \sigma_x \chi_A(x)$ and $\delta\Delta_2 = -\Delta_0 \mathbf{I} \chi_A(x)$, where \mathbf{I} is the identity matrix, and $\chi_A(x)$ is the characteristic function of the region A , so $\chi_A(x) = 1$ if $x \in A$ and 0 otherwise. The Birman-Schwinger operator (4) can be written explicitly. Assuming real Δ_0 for simplicity, we find

$$K_{A,E}(x,x') = \frac{\Delta_0}{\sqrt{\Delta_0^2 - E^2}} (\sigma_x E - \Delta_0) \chi_A(x) \text{Im } g_+(x-x') \times \chi_A(x') - i \Delta_0 \sigma_y \chi_A(x) \text{Re } g_+(x-x') \chi_A(x'), \quad (8)$$

where

$$g_{\pm}(x-x') = \frac{e^{\pm i k_{\pm} |x-x'|}}{4\pi |x-x'|}, \quad (9)$$

where $k_{\pm} = \sqrt{\mu \pm i \sqrt{\Delta_0^2 - E^2}}$, and $\text{Re } k > 0$.

Note that from the numerical point of view studying the Birman-Schwinger kernel (8) has an immediate advantage: The kernel is only supported on the region A . Thus, computation of the spectrum of bound states requires merely finding the eigenvalues of this operator restricted to the region A . Since the operator in (8) is known analytically, one can numerically compute eigenvalues by simply discretizing the region A .

Let us proceed and consider limits where the application of these ideas is particularly interesting

III. NORMAL REGIONS

Here we use $K_{A,E}$ to obtain an upper bound to the number of states. The basic inequality is

$$\begin{aligned} N_E(V) &\leq \sum_{\lambda | \mu_n(\lambda) = E_1 \text{ or } E_2 \text{ for some } \lambda \in (0,1)} 1 \\ &\leq \sum_{\lambda | \mu_n(\lambda) = E_1 \text{ or } E_2 \text{ for some } \lambda \in (0,1)} \frac{1}{\lambda^2} \\ &\leq \sum_{\lambda \text{ eigenvalue of } K_{E1}} \frac{1}{\lambda^2} + \sum_{\lambda \text{ eigenvalue of } K_{E2}} \frac{1}{\lambda^2} \\ &\leq \text{Tr} K_{E1}^* K_{E1} + \text{Tr} K_{E2}^* K_{E2}. \end{aligned} \quad (10)$$

The last inequality is due to the fact that K_E is, as opposed to the usual Birman-Schwinger case, not self-adjoint; therefore we used that for a compact operator $\sum_{\text{eigenvalues}} |\lambda|^p \leq \sum_{\text{singular values}} |s|^p$ for $p \geq 1$ (Schur-Lalesco-Weyl theorem).

This allows us to write a simple inequality for the number of subgap states. Plugging $K_{E,A}$ from (8) in (10) we find

$$N(E) \leq 4\Delta_0^2 \int_{A \times A} dx dx' \left(\frac{\Delta_0^2 + E^2}{\Delta_0^2 - E^2} |\text{Im } g_-(x-x')|^2 + |\text{Re } g_+(x-x')|^2 \right). \quad (11)$$

As $E \rightarrow 0$ the number of states $N_V(E)$ goes to zero; thus, the estimate (11) is effective only when the expression on the right-hand side of (11) is less than 1 in that limit. Let us estimate the size of the region A where this holds, assuming a typical gap much smaller than k_F . Using that for $E \rightarrow 0$, $k_{\pm} \sim \sqrt{\mu} \pm i \frac{\Delta_0}{\sqrt{\mu}}$, we see that

$$N(E) \leq \frac{\Delta_0^2}{4\pi^2} \int_{A \times A} dx dx' \frac{e^{-\sqrt{\frac{\Delta_0^2 - E^2}{\mu}} |x-x'|}}{|x-x'|^2} \times \left(\frac{2E^2}{\Delta_0^2 - E^2} \sin^2(\sqrt{\mu} |x-x'|) + 1 \right), \quad (12)$$

and so the decay is set by coherence length $\xi = \frac{\sqrt{\mu}}{\Delta_0}$. This means that we need the condition $\frac{1}{\pi} \sqrt{\mu} \Delta_0 \text{Vol}(A) < 1$ to make (11) effective at low energies.

Much like for the Schrödinger equation in 3D, we see that for a small enough normal region, the right-hand side of (11) will be less than 1, and so no subgap states will be present below this energy E .

Numerically, we have checked the utility of this approximation for simple situations on a lattice compared to the exact result. The agreement is fairly good for E small, $E < 0.25\Delta_0$.

Let us estimate the leading volume dependence of the bound (11). We write

$$g_{\pm}(r) = \frac{e^{\pm i k_{\pm} |r|}}{4\pi |r|} = \frac{e^{-ar \pm ib|r|}}{4\pi |r|} \quad (13)$$

with

$$\begin{aligned} a &= (\mu^2 + \Delta_0^2 - E^2)^{1/4} \sin \left[\frac{1}{2} \arctan \frac{\sqrt{\Delta_0^2 - E^2}}{\mu} \right], \\ b &= (\mu^2 + \Delta_0^2 - E^2)^{1/4} \cos \left[\frac{1}{2} \arctan \frac{\sqrt{\Delta_0^2 - E^2}}{\mu} \right]. \end{aligned} \quad (14)$$

By (11) we have $N(E) \leq N_1$, where

$$N_1 = 4\Delta_0^2 \int_{A \times A} dx dx' \left(\frac{\Delta_0^2 + E^2}{\Delta_0^2 - E^2} |\text{Im } g_-(x-x')|^2 + |\text{Re } g_+(x-x')|^2 \right). \quad (15)$$

Now, we change to variables $x, x' \rightarrow x, r = (x' - x)$. Taking the r integral over all space we get that $N_1 \leq N'_1$ with

$$N'_1 = 16\pi \Delta_0^2 \text{vol}(A) \int_0^\infty r^2 d\left(\frac{\Delta_0^2 + E^2}{\Delta_0^2 - E^2} |\text{Im } g_-(r)|^2 + |\text{Re } g_+(r)|^2\right) = \Delta_0^2 \text{vol}(A) \int_0^\infty dr \frac{e^{-2ar}}{\pi} \times \left(\frac{\Delta_0^2 + E^2}{\Delta_0^2 - E^2} \sin^2(br) + \cos^2(br)\right).$$

This last integral can be carried out analytically, yielding

$$N'_1 = \frac{\Delta_0^2}{4\pi a} \text{vol}(A) \left(\frac{1}{2} + \frac{\frac{2E^2}{\Delta_0^2 - E^2} b^2}{\sqrt{\mu^2 + \Delta_0^2 - E^2}}\right). \quad (16)$$

Finally, we can write N'_1 as

$$N'_1 = \frac{\text{vol}(A) \Delta_0^2 ((2\Delta_0^2 - E^2) \sqrt{\mu^2 + \Delta_0^2 - E^2} + \mu E^2)}{4\pi (\Delta_0^2 - E^2) (\mu^2 + \Delta_0^2 - E^2)^{\frac{3}{4}} \sin\left(\frac{1}{2} \tan^{-1} \sqrt{\frac{\Delta_0^2 - E^2}{\mu}}\right)}. \quad (17)$$

The upper estimate N'_1 in (16) is in fact a good approximation to N_1 whenever the size of A is larger than $1/a$ the decay scale for the Green's function.

The most physically common situation for BCS is $\mu \gg \Delta_0$. In this limit we have

$$N'_1 \sim \frac{\sqrt{\mu} \Delta_0^4 \text{vol}(A)}{\pi (\Delta_0^2 - E^2)^{3/2}} + \frac{\Delta_0^2 (\Delta_0^2 - 2E^2) \text{vol}(A)}{8\pi \mu^{3/2} \sqrt{\Delta_0^2 - E^2}}. \quad (18)$$

Taking μ fixed and Δ_0 large, while keeping $\alpha = \Delta_0/E$ fixed, we get

$$N'_1 \sim \frac{(2 - \alpha^2) \Delta_0^{3/2}}{2\sqrt{2}\pi(1 - \alpha^2)^{5/4}} + \frac{(\alpha^2 + 2)\mu\sqrt{\Delta_0}}{4\sqrt{2}\pi(1 - \alpha^2)^{7/4}}. \quad (19)$$

IV. CWIKEL-LIEB-ROZENBLUM INEQUALITY

Often, the estimate (10) may be quite poor because of large contributions from small eigenvalues of $K_{E,A}$. This behavior may sometimes be remedied by considering other inequalities, such as the celebrated Cwikel-Lieb-Rozenblum inequality.¹⁸⁻²⁰

To do so we consider the BdG equation with a gap function $\Delta_0 + \Delta_1(x)$. Using the ideas in Refs. 18 and 22 and adapting to the superconducting scenario we find that the inequality

$$N(0, E) \leq C \frac{\mu^{1/2} |\Delta_0|^2}{(|\Delta_0|^2 - E^2)^2} \int_{|\Delta_1(x)| \geq \frac{|\Delta_0|^2 - E^2}{4|\Delta_0|}} dx \times [\Delta_0^{3/2} |\Delta_1(x)|^{3/2} + |\Delta_1(x)|^3] \quad (20)$$

is valid for $\mu \geq \frac{\sqrt{\Delta_0^2 - E^2}}{18\sqrt{2}}$, with C a constant of order 1. The details of this calculation are given in the Appendix.

For the case $\mu < \frac{\sqrt{\Delta_0^2 - E^2}}{18\sqrt{2}}$, the inequality is changed to

$$N(0, E) \leq \frac{2^{-3/4} C}{3(\Delta_0^2 - E^2)^{3/4}} \int_{|\Delta_1(x)| \geq \frac{|\Delta_0|^2 - E^2}{4|\Delta_0|}} dx \times [\Delta_0^{3/2} |\Delta_1(x)|^{3/2} + |\Delta_1(x)|^3]. \quad (21)$$

The bounds (20) and (21) are closely related to the bound of Ref. 22 on the number of bound states of perturbed Dirac operators. The main technical difference with Ref. 22 is the presence of a chemical potential and thus the presence of a nonvanishing Fermi surface (technically, these change the weak norms appearing in the Cwikel inequalities for singular numbers).

Note that the denominator $(|\Delta_0|^2 - E^2)^2$ in (20) shows that this bound is only useful for $E < |\Delta_0|$. However, most of our interest here is actually with states that are not too close to the top of the gap itself. The reason for this is that in practice, if the BCS self-consistency is taken into account, the first states that are affected are those with energy very close to the gap. Such states will often be washed out from the spectrum, since the gap function may decrease slightly in the vicinity of the normal region.

In the case of a system defined by a normal region $\Delta_1(x) = -\Delta_0 \chi_A(x)$, we have $N(E) \leq N_{\text{CLR}}$ with

$$N_{\text{CLR}} = C \frac{2\mu^{1/2} |\Delta_0|^5}{(|\Delta_0|^2 - E^2)^2} \text{vol}(A). \quad (22)$$

Let us compare the simple CLR and BS estimates. Consider the large μ limit (22) vs (18). We have

$$N'_1/N_C \sim \frac{\sqrt{\Delta_0^2 - E^2}}{\Delta_0} < 1. \quad (23)$$

We conclude that for the typical BCS situation, the simple Birman-Schwinger bound (18) is more effective in dealing with normal regions.

V. ASYMPTOTIC REGIME, SZEGÖ THEOREM

Here we are interested in the large l behavior of the eigenvalues of $K_{E,lA}$, where lA is the region A rescaled by a factor l (i.e. $lA = \{\mathbf{x} : l^{-1}\mathbf{x} \in A\}$). In this limit semiclassical methods are often useful. To study the eigenvalues of $K_{E,lA}$, it is convenient to characterize the behavior of $\text{Tr} f(K_{E,lA})$ for various functions f . We immediately see, since in our situation $[H_0(p), \Delta]$ is supported only on the boundary of the system, that in the volume term we may commute the χ_A terms in the perturbations W_i and the free propagator. This gives the asymptotic leading term for the number of subgap states as the number of eigenvalues of $K_{E,lA}$ larger than 1. The semiclassical approximation expresses it as an integral over the classical phase space:

$$N(E, 0) \sim l^d \text{vol}(A) \int \Theta\{[H_0(p) - E]^{-1} \sigma_x - 1\} d^d p, \quad (24)$$

where Θ is the Heaviside step function.

We may view the operator $K_{E,A}$ as a higher dimensional block of a Toeplitz operator: The kernel depends only on $x - x'$; however, the x, x' indices are restricted to be in A . This is equivalent to chopping a "block" from a regular matrix.

The theory describing the asymptotic properties of blocks of Toeplitz matrices is based on various Szegő theorems and appears in numerous problems in physics. Most famously, the strong (two-term) Szegő limit theorem was initially used in the celebrated computation of the spontaneous magnetization for the 2D Ising model by Onsager (see, e.g., Ref. 23). The Szegő limit theorem also plays a special role in entanglement entropy studies; see in particular Refs. 24 and 25.

To try and describe the next term, we turn to a higher dimensional generalization of the Szegő limit theorem, which has been extensively studied by Widom.²⁶ Denote $\mathcal{G}_E(p) = (H_0(p) - E)^{-1}\sigma_x$. Given a unit vector direction n_x , we can define an operator acting on functions of a single variable, with kernel

$$\mathcal{G}_{E,n_x,p_\perp}(s-t) = \int e^{ip_{||}(s-t)} \mathcal{G}_E(p_\perp + n_x p_{||}) dp_{||}. \quad (25)$$

Using Ref. 26 we see that

$$\begin{aligned} & \text{Tr} f(K_{E,lA}) \\ & \sim \frac{l^d \text{vol}(A)}{(2\pi)^d} \int f[\mathcal{G}_E(p)] d^d p \\ & \quad + \frac{l^{d-1}}{(2\pi)^{d-1}} \int_{\partial A} dx \int_{p_\perp \cdot n_x = 0} d^{d-1} p_\perp \text{tr} \\ & \quad \times [f(\chi_+ \mathcal{G}_{E,n_x,p_\perp} \chi_+) - \chi_+ f(\mathcal{G}_{E,n_x,p_\perp}) \chi_+] \\ & \quad + o(l^{d-1}), \end{aligned} \quad (26)$$

where n_x is the normal to ∂A at x . For the case of an s -wave superconductor the operator $\mathcal{G}_{E,n_x,p_\perp}$ can be computed explicitly:

$$\begin{aligned} & \mathcal{G}_{E,n_x,p_\perp}(s-t) \\ & = -\sqrt{\frac{\pi \Delta_0^2}{2(\Delta_0^2 - E^2)}} \text{Im} \left(\frac{e^{-|s-t|k_+(p_\perp)}}{k_+(p_\perp)} \right) (\Delta_0 + z\sigma_x) \\ & \quad + i\sqrt{\frac{\pi}{2}} \Delta_0 \text{Re} \left(\frac{e^{-|s-t|k_+(p_\perp)}}{k_+(p_\perp)} \right) \sigma_y, \end{aligned} \quad (27)$$

where $k_\pm(p_\perp) = \sqrt{p_\perp^2 - \mu \pm i\sqrt{\Delta_0^2 - E^2}}$, and $\text{Re} k_\pm > 0$ [here $i\sigma_y = (0, 1, -1, 0)$].

In our case, we are interested in the number of eigenvalues above 1. Thus we need to solve this problem for $f(\lambda) = \Theta(\lambda - 1)$. However, for this function the arguments leading to (26) are no longer applicable, but rather, due to the discontinuous nature of f , the area term as written in (26) is divergent. We conjecture that in such a case, the boundary term should be modified to

$$\begin{aligned} & \frac{l^{d-1}}{(2\pi)^{d-1}} \int_{\partial A} dx \int_{p_\perp \cdot n_x = 0} d^{d-1} p_\perp \text{tr} [f(\chi_{l+} \mathcal{G}_{E,n_x,p_\perp} \chi_{l+}) \\ & \quad - \chi_{l+} f(\mathcal{G}_{E,n_x,p_\perp}) \chi_{l+}] + o(l^{d-1}), \end{aligned} \quad (28)$$

where $\chi_{l+}(s) = \theta(0 < s < l)$. In analogy to the appearance of logarithmic corrections when considering similar expressions for the entanglement entropy of fermions in d dimensions, we expect this term to scale as $O(l^{d-1} \log l)$, which also seems to be consistent with a preliminary numerical investigation.

In this case (as well as for any isotropic superconductor), this integral is independent of the direction n_x , and so we have that the boundary term is given by

$$\frac{l^{d-1} \log l}{(2\pi)^{d-1}} \text{vol}(\partial A) m_f(E) \quad (29)$$

for some function $m_f(E)$. The transformation $f \rightarrow m_f$ is independent of the shape, and we believe it can be studied using Wiener-Hopf methods for specific cases.

Finally, we remark that it has been argued that there is a minigap present in the local density of states if the shape of the normal region corresponds to a chaotic ‘‘Andreev billiard.’’^{27–30} The minigap is of order $\Delta_0 \log(k_F l)$, and its nature depends on τ_E/τ_D , where τ_D is dwell time in the normal region and τ_E is the Ehrenfest time. This question has recently been revisited in Ref. 31. To arrive at this result, the strategy is to consider the BdG equation within the Andreev approximation and analyze possible classical trajectories. It would be of interest to see whether such a result may come out of a Birman-Schwinger-like analysis.

VI. CONCLUSIONS AND OUTLOOK

To summarize, in this paper we studied the bound states in superconductors using a Birman-Schwinger approach. The advantage of the method is its validity for general perturbations, and beyond the Andreev approximation. Our main results are stated in the following equations: The bound on subgap states (11), the Cwikel-Lieb-Rozenblum type inequality for BdG (20), and the asymptotic expression for the number of states in large regions with the conjecture (28) for the scaling $l^{d-1} \log(k_F l)$ of the subleading term. For most physical situations the Birman-Schwinger bound (11) seems a better bound than the CLR bound (20), since it gives a lower upper bound for large Fermi energy μ .

In the same way it is possible to study the effect of adding disorder potentials, as well as spatially varying or momentum dependent Δ . Because of the wide interest in the properties of vortices in such systems it is also of great interest to understand whether the Birman-Schwinger methods can be useful in the study of bound states in vortices. Indeed, it is not immediately clear how this should be done: The presence of core states in vortices seems to be mainly due to the phase winding around the vortex core (see, e.g., Ref. 32), and arguably less sensitive to the suppression of order parameter in the core. Since the phase winding is of a topological nature (i.e., it is discrete) it cannot be considered as a perturbation which is turned on in a continuous way from zero, as in the case we have considered. The present approach may be utilized to understand the interplay between the topological and nontopological state binding. To do so, one should take as the unperturbed vortex an idealized radially symmetric vortex, and then add phase gradients and order parameter suppression as perturbations, and study the additional bound states introduced in this manner.

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APPENDIX : CWIKEL-LIEB-ROZENBLUM FOR BDG

1. Estimates on singular values

To control the spectrum of the Birman Schwinger operators, we will use the following inequality ($p > 2$) (theorem XI.22 in Ref. 33):

$$s_n(\hat{a}b) \leq n^{-1/p} C_{p,d} \|a\|_p \|b\|_{p,w}, \quad (\text{A1})$$

where s_n is the n th singular value of the operator $\hat{a}b = a(x)b(i\nabla)$, i.e., the n th largest eigenvalue of the operator $\sqrt{(\hat{a}b)^\dagger \hat{a}b}$. Here $C_{p,d}$ is a constant, $\|a\|_p = (\int dx |a(x)|^p)^{1/p}$ is the L^p norm, and the value $\|b\|_{p,w}$ is defined as follows (page 30 in Ref. 34). Defining

$$M_b(t) = \text{vol}(x | |b(x)| > t), \quad (\text{A2})$$

$\|b\|_{p,w}$ is given by

$$\|b\|_{p,w} = \inf \left\{ C : M_b(t) < \frac{C^p}{t^p} \forall t \right\}. \quad (\text{A3})$$

Note $\|b\|_{p,w}$ is not strictly speaking a norm, since it does not satisfy a triangle inequality. It is called weak since $L^p \subset L^p_w$.

To familiarize ourselves with computing $\|b\|_{p,w}$ consider first the following example.

Example: Let us compute $\|b\|_{3,w}$ for $b(x) = (x^2 + c)^{-1/2}$ assuming $c > 0$. We have

$$\begin{aligned} M_b(t) &= \text{vol}(x | (x^2 + c)^{-1/2} > t) \\ &= \text{vol}\left(x^2 < \frac{1}{t^2} - c\right) \theta\left(\frac{1}{t^2} - c > 0\right). \end{aligned} \quad (\text{A4})$$

In 3D this gives

$$M_b(t) = \frac{4\pi}{3} \left| \frac{1}{t^2} - c \right|^{3/2} \theta\left(\frac{1}{t^2} - c > 0\right) \leq \frac{4\pi}{3} \frac{1}{t^3}. \quad (\text{A5})$$

Since the above inequality approaches equality for $t \rightarrow 0$, the infimum in (A3) is given by $\|b\|_{3,w} = (\frac{4\pi}{3})^{1/3}$. Note that $\|b\|_{3,w}$ does not depend on c .

In the derivation of the Cwikel-Lieb-Rozenblum inequality we will need the $\|b\|_{3,w}$ estimate for

$$b(i\nabla) = [(-\nabla^2 - m)^2 + c]^{-1/2}, \quad (\text{A6})$$

with $m, c > 0$. Here we show that

$$\|b\|_{3,w} \leq c^{-1/4} (v_3)^{1/3} \max \left[1, \left(\frac{324m^2}{c} \right)^{1/12} \right]. \quad (\text{A7})$$

As in the example above, we define

$$\begin{aligned} M_b(t) &= \text{vol}(x | ((x^2 - m)^2 + c)^{-1/2} > t) \\ &= \text{vol}\left((x^2 - m)^2 < \frac{1}{t^2} - c\right) \theta\left(\frac{1}{t^2} - c > 0\right). \end{aligned} \quad (\text{A8})$$

Let $v_d = \frac{\pi^{d/2}}{\Gamma(d/2+1)}$ be the volume of a d -dimensional sphere. Then,

$$M_b(t) = \begin{cases} v_d (m + \sqrt{\frac{1}{t^2} - c})^{d/2} & \text{if } 0 < t < (m^2 + c)^{-1/2}, \\ v_d \left[(m + \sqrt{\frac{1}{t^2} - c})^{d/2} - (m - \sqrt{\frac{1}{t^2} - c})^{d/2} \right] & \text{if } (m^2 + c)^{-1/2} < t < \frac{1}{\sqrt{c}}, \\ 0 & \text{if } t > \frac{1}{\sqrt{c}}. \end{cases} \quad (\text{A9})$$

From the small t behavior, we see that to bound M_b uniformly as in the definition (A3) the power has to be at least $1/t^{d/2}$, i.e., $p \geq d/2$. In the first sector we see also that the constant has to be at least v_d . However, v_d may not be good enough since the bound in the region 2 may be different. Let us estimate it.

For $(m^2 + c)^{-1/2} < t < \frac{1}{\sqrt{c}}$,

$$\begin{aligned} &v_d \left[\left(m + \sqrt{\frac{1}{t^2} - c} \right)^{d/2} - \left(m - \sqrt{\frac{1}{t^2} - c} \right)^{d/2} \right] \\ &= v_d \int_{-1}^1 ds \partial_s \left(m + s \sqrt{\frac{1}{t^2} - c} \right)^{d/2} = \frac{dv_d}{2} \sqrt{\frac{1}{t^2} - c} \\ &\quad \times \int_{-1}^1 ds \left(m + s \sqrt{\frac{1}{t^2} - c} \right)^{d/2-1} \leq \frac{dv_d}{t} (2m)^{d/2-1}, \end{aligned}$$

where we use that in this region $m \geq \sqrt{\frac{1}{t^2} - c}$.

Now we have to write this as bounded by a $1/t^{d/2}$ expression. If $d/2 < 1$ we are done, but if not, $d/2 - 1 > 0$, as in the $d = 3$ case, using $\frac{1}{t\sqrt{c}} > 1$ we have

$$\begin{aligned} \frac{dv_d}{t} (2m)^{d/2-1} &\leq \frac{dv_d}{t} (2m)^{d/2-1} \frac{1}{t^{d/2-1} (\sqrt{c})^{d/2-1}} \\ &= \frac{dv_d (2m)^{d/2-1}}{(\sqrt{c})^{d/2-1} t^{d/2}}. \end{aligned} \quad (\text{A10})$$

Combining all these results we see that (for $d > 2$)

$$M_b(t) \leq \max \left[1, \frac{d(2m)^{d/2-1}}{(\sqrt{c})^{d/2-1}} \right] \frac{v_d}{t^{3/2}}.$$

And thus we see that in this case we are in the weak $L_w^{3/2}$ space; i.e., $\|b\|_{3/2,w} \leq [v_d \max(1, \frac{3(2m)^{1/2}}{c^{1/4}})]^{2/3}$.

The Cwikel estimates require $p > 2$ let us estimate $\|b\|_{3,w}$. Since $t^{-3/2} < t^{-3}$, say, for $t < 1$, we need to deal with the large t behavior of M_b . Let us use the following.

Lemma: If $M_b < Ct^{-\alpha}$, and $M_b = 0$ for $t > t_0$, then we have, for any $\alpha_1 > \alpha$ that

$$\|b\|_{\alpha_1,w} \leq (t_0^{\alpha_1 - \alpha} C)^{1/p}. \quad (\text{A11})$$

Proof: For $t < t_0$ we have

$$M_b(t) \leq Ct^{-\alpha} < Ct^{-\alpha} (t_0/t)^{\alpha_1 - \alpha} < Ct^{-\alpha_1} t_0^{\alpha_1 - \alpha},$$

and $M_b = 0$ for $t > t_0$; therefore $M_b < Ct_0^{\alpha_1 - \alpha} t^{-\alpha_1}$ for all $t > 0$. \square

In our case M_b drops to zero when $t = c^{-1/2}$. Therefore, for $b(x) = [(x^2 - m)^2 + c]^{-1/2}$ we have, for $p > 3/2$,

$$\|b\|_{p,w} \leq c^{-1/2} c^{\frac{3}{4p}} \left\{ v_d \max \left[1, \frac{3(2m)^{1/2}}{c^{1/4}} \right] \right\}^{1/p}, \quad (\text{A12})$$

and in particular,

$$\|b\|_{3,w} \leq c^{-\frac{1}{4}}(v_3)^{1/3} \max \left[1, \left(\frac{324m^2}{c} \right)^{1/12} \right]. \quad (\text{A13})$$

2. Derivation of the main inequality

Here we repeat almost exactly the analysis of Cancelier, Levy-Bruhl, and Nourrigat, ‘‘Remarks on the Spectrum of Dirac Operators.’’²² The main difference between our work and theirs is the presence of the chemical potential, which appears in the estimates such as (A30).

Assume $\|V - V_\lambda\| \leq |\Delta_0|\lambda/4$, then

$$\begin{aligned} \|(H_0 + V)u\| &\leq \Delta_0\sqrt{1-\lambda}\|u\| \\ \Rightarrow \|(H_0 + V_\lambda)u\| &\leq \Delta_0\sqrt{1-\lambda/2}\|u\|. \end{aligned} \quad (\text{A14})$$

To check this note that

$$\begin{aligned} \|(H_0 + V_\lambda)u\|^2 &\leq \|(H_0 + V)u\|^2 + 2\|(H_0 + V)u\|\|(V_\lambda - V)u\| \\ &\quad + \|(V - V_\lambda)u\|^2 \\ &\leq \left[|\Delta_0|^2(1-\lambda) + |\Delta_0|^2\frac{\lambda}{2}\sqrt{1-\lambda} + |\Delta_0|^2\frac{\lambda^2}{16} \right] \|u\|^2 \\ &\leq |\Delta_0|^2 \left(1 - \lambda + \frac{\lambda}{2}\sqrt{1-\lambda} + \frac{\lambda^2}{16} \right) \|u\|^2 \\ &\leq |\Delta_0|^2 \left[1 - \frac{\lambda}{2} \right] \|u\|^2. \end{aligned} \quad (\text{A15})$$

The last inequality can be checked by differentiation. Thus we have

$$\begin{aligned} \|(H_0 + V_\lambda)u\|^2 - |\Delta_0|^2 \left[1 - \frac{\lambda}{2} \right] \|u\|^2 &\leq 0 \\ \Rightarrow \langle u | (H_0^2 - |\Delta_0|^2) + [H_0, V_\lambda]_+ + \left(V_\lambda^2 + |\Delta_0|^2\frac{\lambda}{2} \right) | u \rangle &\leq 0. \end{aligned}$$

Noting that for BdG $H_0^2 = (-\nabla^2 - \mu)^2 \mathbf{1} + |\Delta_0|^2 \mathbf{1}$, we get for such u 's:

$$\langle u | (-\nabla^2 - \mu)^2 + |\Delta_0|^2\frac{\lambda}{2} + S_\lambda | u \rangle \leq 0, \quad (\text{A16})$$

where $S_\lambda = [H_0, V_\lambda]_+ + V_\lambda^2$. Therefore we are interested in the number of bound states of $(-\nabla^2 - \mu)^2 + |\Delta_0|^2\frac{\lambda}{2} + S_\lambda$. These are given by a Birman-Schwinger method. Observing the Birman Schwinger kernel,

$$K_{\text{BdG}} = \frac{1}{[(-\nabla^2 - \mu)^2 + |\Delta_0|^2\frac{\lambda}{2}]^{1/2}} S_\lambda \frac{1}{[(-\nabla^2 - \mu)^2 + |\Delta_0|^2\frac{\lambda}{2}]^{1/2}}. \quad (\text{A17})$$

We now note that the S_λ contains several terms, of the following forms (there are also matrix indices, but let us ignore these, since we are going to add the estimate for each element). We also assume Δ_0 real for simplicity; also, here the perturbation is actually of the form $-\Delta_1(x)\sigma_x$, so we appropriately define Δ_λ as we defined V_λ .

Next we use the Cwikel inequalities (A1) for $p = 3$ and the standard inequalities for singular numbers:

Fan's inequality:

$$\mu_{n+m+1}(A+B) \leq \mu_{n+1}(A) + \mu_{m+1}(B) \quad (\text{A18})$$

and

$$\begin{aligned} \mu_n(AB) &\leq \|B\| \mu_n(A), \\ \mu_{n+m+1}(AB) &\leq \mu_{n+1}(A) \mu_{m+1}(B) \end{aligned} \quad (\text{A19})$$

to deal with the different terms in K_{BdG} .

We get estimates for the n th singular number of three different forms [here b is as above in (A6)]:

(i)

$$\begin{aligned} A_1 &= \Delta_0 \frac{1}{[(-\nabla^2 - \mu)^2 + |\Delta_0|^2\frac{\lambda}{2}]^{1/2}} \sqrt{\Delta_\lambda(x)} \\ &\quad \times \sqrt{\Delta_\lambda(x)} \frac{1}{[(-\nabla^2 - \mu)^2 + |\Delta_0|^2\frac{\lambda}{2}]^{1/2}}, \end{aligned} \quad (\text{A20})$$

$$s_n(A_1) \leq \Delta_0 \left(\|\sqrt{\Delta_\lambda}\|_{3,C_{3,d}} \|b\|_{3,w} \frac{1}{(n/2)^{1/3}} \right)^2. \quad (\text{A21})$$

Here we used standard inequalities for the singular values of sums and products of operators as in (A19), to have $s_n(AB) \leq s_{\lfloor n/2 \rfloor}(A) s_{\lfloor n/2 \rfloor}(B)$.

(ii)

$$\begin{aligned} A_2 &= \Delta_0 \frac{1}{[(-\nabla^2 - \mu)^2 + |\Delta_0|^2\frac{\lambda}{2}]^{1/2}} \Delta_\lambda(x) \\ &\quad \times \Delta_\lambda(x) \frac{1}{[(-\nabla^2 - \mu)^2 + |\Delta_0|^2\frac{\lambda}{2}]^{1/2}} \end{aligned} \quad (\text{A22})$$

gives, in the same way,

$$s_n(A_2) \leq \left(\|\Delta_\lambda\|_{3,C_{3,d}} \|b\|_{3,w} \frac{1}{(n/2)^{1/3}} \right)^2. \quad (\text{A23})$$

(iii)

$$\begin{aligned} A_3 &= \frac{1}{[(-\nabla^2 - \mu)^2 + |\Delta_0|^2\frac{\lambda}{2}]^{1/2}} (-\nabla^2 - \mu) \\ &\quad \times \Delta_\lambda(x) \frac{1}{[(-\nabla^2 - \mu)^2 + |\Delta_0|^2\frac{\lambda}{2}]^{1/2}}. \end{aligned} \quad (\text{A24})$$

Since $\left\| \frac{1}{[(-\nabla^2 - \mu)^2 + |\Delta_0|^2\frac{\lambda}{2}]^{1/2}} (-\nabla^2 - \mu) \right\| < 1$, we have

$$s_n(A_3) \leq \|\Delta_\lambda\|_{3,C_{3,d}} \|b\|_{3,w} \frac{1}{(n)^{1/3}}. \quad (\text{A25})$$

Combining these estimates and adding them (and noting that $\|\sqrt{\Delta_\lambda}\|_3^2 = \|\Delta_\lambda\|_{3/2}$) we conclude the inequality:

$$\begin{aligned} s_n(K_{\text{BdG}}) &\leq C' \left[\Delta_0 \|\Delta_\lambda\|_{3/2} \|b\|_{3,w}^2 \frac{1}{n^{2/3}} + \|\Delta_\lambda\|_3^2 \|b\|_{3,w}^2 \right. \\ &\quad \left. \times \frac{1}{n^{2/3}} + \|\Delta_\lambda\|_3 \|b\|_{3,w} \frac{1}{n^{1/3}} \right]. \end{aligned} \quad (\text{A26})$$

Now we can get the inequality as follows: We are looking for the largest N for which $s_N \geq 1$. Thus we multiply by $N^{2/3}$ the above inequality:

$$\begin{aligned} N^{2/3} &\leq C' \left[\Delta_0 \|\Delta_\lambda\|_{3/2} \|b\|_{3,w}^2 + \|\Delta_\lambda\|_3^2 \|b\|_{3,w}^2 \right. \\ &\quad \left. + \|\Delta_\lambda\|_3 \|b\|_{3,w} N^{1/3} \right]. \end{aligned} \quad (\text{A27})$$

Thus if N_m satisfies

$$\begin{aligned} N_m^{2/3} &= C' \left[\Delta_0 \|\Delta_\lambda\|_{3/2} \|b\|_{3,w}^2 + \|\Delta_\lambda\|_3^2 \|b\|_{3,w}^2 \right. \\ &\quad \left. + \|\Delta_\lambda\|_3 \|b\|_{3,w} N_m^{1/3} \right], \end{aligned} \quad (\text{A28})$$

the number of bound states must have $N \leq N_m$. Let us bound N_m from above. We write $N_m^{2/3} = A + BN_m^{1/3} \Rightarrow N_m^{1/3} = \frac{B + \sqrt{B^2 + 4A}}{2}$. Since $\sqrt{B^2 + 4A} \leq B + 2\sqrt{A}$, we have $N_m^{1/3} \leq B + \sqrt{A}$. Furthermore, using the generalized mean inequality $(|a| + |b| + |c|)^k \leq 3^{k-1}(|a|^k + |b|^k + |c|^k)$, we have

$$\begin{aligned} N_m &\leq C' [(\Delta_0 \|\Delta_\lambda\|_{3/2} \|b\|_{3,w}^2)^{3/2} \\ &\quad + (\|\Delta_\lambda\|_3^2 \|b\|_{3,w}^2)^{3/2} + (\|\Delta_\lambda\|_3 \|b\|_{3,w})^3] \\ &\leq C'' \|b\|_{3,w}^3 [\Delta_0^{3/2} \|\Delta_\lambda\|_{3/2}^{3/2} + \|\Delta_\lambda\|_3^3]. \end{aligned} \quad (\text{A29})$$

In the BdG context we have $m = \mu$ and $c = \frac{\lambda}{2} |\Delta_0|^2$ in (A6). There are two cases:

(i) $\mu > \frac{\sqrt{\Delta_0^2 - E^2}}{18\sqrt{2}}$: We have

$$\|b\|_{3,w} \leq 2(v_3)^{1/3} \left(\frac{9\mu}{2\lambda^4 |\Delta_0|^4} \right)^{1/6}. \quad (\text{A30})$$

Using (A30) we have

$$\|b\|_{3,w}^3 \leq 8v_3 \left(\frac{9\mu}{2\lambda^4 |\Delta_0|^4} \right)^{1/2}. \quad (\text{A31})$$

So finally

$$N_m \leq C \frac{\mu^{1/2}}{\lambda^2 |\Delta_0|^2} [\Delta_0^{3/2} \|\Delta_\lambda\|_{3/2}^{3/2} + \|\Delta_\lambda\|_3^3] \quad (\text{A32})$$

for some C .

We can now write this explicitly as an integral:

$$N_m \leq C \frac{\mu^{1/2}}{\lambda^2 |\Delta_0|^2} \int_{|\delta\Delta(x)| \geq \frac{|\Delta_0|\mu}{4}} dx [\Delta_0^{3/2} (\delta\Delta_x)^{3/2} + (\delta\Delta_x)^3].$$

The optimal constants in (A1) are not known in general, but the various upper bounds for them are all of order 1. Finally, relating λ and E we get (A20).

(ii) Similarly, for $\mu < \frac{\sqrt{\Delta_0^2 - E^2}}{18\sqrt{2}}$ and using (A13) we get (A21).

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