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Approximate solutions for the Bogoliubov–de Gennes equations: Superconductor–normal-metal–supercondcutor junctions and the vortex problem

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We present a method for generating wave functions for inhomogeneous superconductors. The method is based on the Andreev approximation to the Bogoliubov–de Gennes equations. Bound states for the superconductor–normal-metal–superconductor junction and the single vortex are discussed. The following simple expression for the bound-state energy as a function of the angular quantum number μ is derived: $E_\mu = \Delta(r_\mu)$, where $r_\mu = \mu/k_{11} \approx \mu/k_F$ is the classical turning point. The agreement with recently reported exact numerical wave functions and energies is excellent.

This Brief Report has to do with the Bogoliubov–de Gennes (BdeG) equations of space-dependent superconductivity.[1] In what follows we will present a method for generating approximate wave functions for these equations. First, we will present a general technique for constructing approximate solutions for any inhomogeneous problem. We will then apply the method to the problem of the quasiparticle states in the neighborhood of a vortex core which has recently been experimentally probed using scanning tunneling microscopy.[2] These authors detected a zero-bias anomaly (peak in the local density of states at $E=0$) when probing the vortex core ($r=0$ region). Theoretical discussions of this problem were given first by Overhauser and Damien[3] using a semiempirical self-energy approach and then by Shore *et al.*[4] and Gygi and Schluter[5] using a numerical method for solving the BdeG equations. Related theoretical work has been done by Klien.[6] The most recent work of Gygi and Schluter[7] has explained the hexagonal symmetry reported in Ref. 2(b). They constructed approximate Bloch states due to the crystal lattice (or vortex lattice) using their numerical solution of the BdeG equations. In this paper we derive a complete set of bound and scattering states for the BdeG equations using methods based on the Andreev approximation.[8] We then compare our wave functions with those of Refs. (4) and (5) and find excellent agreement using only two adjustable parameters.

We begin the treatment with a brief exposition of the Andreev approximation which will be used to generate the proposed approximate wave functions. Much work has been done for one-dimensional inhomogeneities using this method. This SN, SI, and superconductor–normal-metal–superconductor (SNS) interfaces have been treated by various authors.[9] We will first give a general derivation of the Andreev approximation and then look specifically at the SNS junction for the pair potential $\Delta(z,T)=\Delta_\infty(T)\tanh|(z/\xi)|$. This problem will provide a basis for our treatment of the vortex problem in cylindrical coordinates where $\Delta(r,T)=\Delta_\infty(T)\tanh(r/\xi)$ is the usual first guess.

The principal idea behind the Andreev approximation is to separate out the rapidly and slowly varying parts of the wave function. Thus the normal part of the quasiparticle wave function varies over a distance $z \sim \lambda_F$, the Fermi wavelength, while the superconducting part varies over a characteristic distance $z \sim \xi$, the coherence length. The validity of the Andreev approximation is based on the condition $\lambda_F/\xi \ll 1$. We believe that using variational trial functions based on this approximation will optimize what is a relatively simple approach to inhomogeneous superconductors by choosing the wave-function parameters so as to minimize the BdeG energy functional as well as optimize self-consistency.

Our starting point will be the BdeG equations in the form

$$\{\boldsymbol{\sigma}_z H_N + \boldsymbol{\sigma}_x \Delta - E_n \boldsymbol{l}\}\boldsymbol{\psi} = 0 \tag{1}$$

where $\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y, \boldsymbol{\sigma}_z$, are Pauli spin matrices, H_N is a normal conductor Hamiltonian, $\boldsymbol{\psi}$ is the spinor of quasiparticle amplitudes u and v, Δ is the pair potential connected to the u and v by the self-consistency condition $\Delta = V\sum u_n v_n^*(1-2f_n)$, V is the effective electron interaction, $f=(e^{\beta E n}+1)^{-1}$ is the Fermi function, with E_n measured relative to E_F, and $\beta \equiv 1/kT$.

We restrict our present treatment to the case where $H_N = (-\hbar^2/2m)\nabla^2$, i.e., the effective one-body potential felt by the normal electrons has been approximated by a constant and subsumed into the Fermi energy E_F in the usual way. We now proceed to define, as well as separate, the rapidly and slowly varying parts of $\boldsymbol{\psi}$. Let $u=\phi_1 f_1$, $v=\phi_2 f_2$, where $\boldsymbol{\sigma}_z H_N \boldsymbol{\phi} = \epsilon \boldsymbol{\phi}$ and the spinor $\boldsymbol{\phi} = \binom{\phi_1}{\phi_2}$, comprise the normal conductor's quasiparticle states that vary on the scale of the Fermi wavelength. The spinor $\mathbf{f} = \binom{f_1}{f_2}$ represents the superconductor quasiparticle states that vary on the scale of the coherence length ξ. Inserting this form into Eq. (1) we find

$$-\frac{\hbar^2}{2m}\{2\nabla\phi_1\cdot\nabla f_1 + \phi_1\nabla^2 f_1\} - (E-\epsilon)\phi_1 f_1 + \Delta\phi_2 f_2 = 0\ ,$$
$$\frac{\hbar^2}{2m}\{2\nabla\phi_2\cdot\nabla f_2 + \phi_2\nabla^2 f_2\} - (E+\epsilon)\phi_2 f_2 + \Delta\phi_1 f_1 = 0\ . \tag{2}$$

Now we can define what we mean by rapid and slow variations. Note that $|\nabla f_1|\sim\xi^{-1}$, $|\nabla f_2|\sim\xi^{-1}$, while $|\nabla\phi_1|\sim\lambda_F^{-1}$ and $|\nabla\phi_2|\sim\lambda_F^{-1}$. Therefore, since $\lambda_F\ll\xi$, we may safely ignore the $\nabla^2 f_1$ and $\nabla^2 f_2$ terms compared to the $\nabla\phi_1\cdot\nabla f_1$ and $\nabla\phi_2\cdot\nabla f_2$ terms.[10] Equation (2) now becomes the Andreev approximation in its most general form,

$$\begin{aligned} &-\frac{\hbar^2}{m}\left[\frac{\nabla\phi_1}{\phi_1}\right]\cdot\nabla f_1-(E-\epsilon)f_1+\Delta\left[\frac{\phi_2}{\phi_1}\right]f_2=0\ ,\\ &\frac{\hbar^2}{m}\left[\frac{\nabla\phi_2}{\phi_2}\right]\cdot\nabla f_1-(E+\epsilon)f_1+\Delta\left[\frac{\phi_2}{\phi_1}\right]f_1=0\ . \end{aligned}\tag{3}$$

These *first-order* equations govern the quasiparticle motion when $\lambda_F\ll\xi$. We suggest in this report that using the solutions to Eq. (3) as trial functions with various variational parameters will relax the $\lambda_F\ll\xi$ restriction and thereby optimize the Andreev method. Another virtue of this approach is to generate convenient and effective sets of basis functions to use in inhomogeneous superconductor problems.

If the superconducting part of the wave function varies in only one dimension, Eqs. (3) become particularly simple. Letting z be the requisite variable and assuming that f_1 and f_2 depend only z, then $\phi_1=\phi_2=\exp(ik_F\cdot\mathbf{r})$, $v_F=\hbar k_F/m$, and $\epsilon=\epsilon_F=0$,

$$\begin{aligned} &-i\hbar v_{F_z}\frac{df_1}{dz}-Ef_1+\Delta f_2=0\ ,\\ &i\hbar v_{F_z}\frac{df_2}{dz}-Ef_2+\Delta f_1=0\ . \end{aligned}\tag{4}$$

These equations can be exactly uncoupled and subsequently solved as shown by Bar-Sagi and Kuper.[9(b)–9(d)] They used $\Delta(z,T)=\Delta_\infty(T)\tanh\alpha z$ for $z>0$ to represent the SI interface and α was chosen to approximately satisfy self-consistency for $T\simeq T_c$. Thus they used $\alpha(T)=\sqrt{2}/\xi_0(T)$, where $\xi_0(T)=\hbar v_F/\Delta_\infty(T)$ is essentially the BCS coherence length. The solutions to Eq. (4) are given by associated Legendre functions in terms of the variable $y=\tanh(\alpha z)$ and the results are

$$\begin{bmatrix} f_1\\ f_2\end{bmatrix}\propto\begin{bmatrix} P_n^{\pm m}(y)-i\left[\dfrac{n+m}{n-m}\right]^{1/2}P_{-n}^{\pm m}(y)\\ P_n^{\pm m}(y)+i\left[\dfrac{n+m}{n-m}\right]^{1/2}P_{-n}^{\pm m}(y)\end{bmatrix}\ ,\tag{5}$$

where $n=\Delta_\infty/\hbar v_{FZ}\alpha$ and $m=n(1-E^2/\Delta^2)^{1/2}$. We note that both bound states, $m^2<0$, and scattering states, $m^2>0$, are included in Eq. (5). The one-dimensional solutions are useful in their own right for a variety of interface problems.[10] In particular the solutions for $\Delta(z)=\Delta_\infty|\tanh(\alpha z)|$ have interesting bound states for SNS problems. Specifically we make note of two particularly simple solutions of the BdeG equations. For $E=0$ we easily find that $f=A\binom{1}{i}\mathrm{sech}^n(\alpha z)$, where $A^{-1}=(\|f_1\|^2+\|f_2\|^2)^{1/2}$. Also for $E=\Delta_\infty$ we find that $f=A\binom{1}{i}[\tanh(\alpha z)+i]$.

We now proceed to construct a variational trial function for the single vortex. The coordinate system appropriate to the vortex problem is cylindrical and it will be more convenient to work directly with the radial equation when invoking the Andreev approximation.[11]

Using essentially the notation of Gygi and Schluter[5] we have

$$\begin{aligned} &\tilde{U}_{\mu n k_z}=e^{ik_z z}e^{-i\mu\theta}U_{\mu n k_z}\ ,\\ &\tilde{V}_{\mu n k_z}=e^{ik_z z}e^{i\mu\theta}V_{\mu n k_z}\ , \end{aligned}\tag{6}$$

where n is a radial quantum number and μ is half an odd integer. The functions $U_{\mu n k_z}=r^{1/2}u_{\mu n k_z}$ and $V_{\mu n k_z}=r^{1/2}v_{\mu n k_z}$ satisfy the equations

$$\begin{aligned} &\left\{-\frac{d^2}{dr^2}+\left[\frac{(\mu-\frac{1}{2})^2+\frac{1}{4}}{r^2}-\frac{2m}{\hbar^2}E_{\mu n k_z}\right]\right\}U_{\mu n k_z}\\ &\qquad\qquad+\frac{2m}{\hbar^2}\Delta V_{\mu n k_z}=0\ ,\\ &\left\{-\frac{d^2}{dr^2}+\left[\frac{(\mu+\frac{1}{2})^2+\frac{1}{4}}{r^2}+\frac{2m}{\hbar^2}E_{\mu n k_z}\right]\right\}V_{\mu n k_z}\\ &\qquad\qquad-\frac{2m}{\hbar^2}\Delta U_{\mu n k_z}=0\ . \end{aligned}\tag{7}$$

We now apply the same argument that led to Eqs. (4). Letting $U=\phi_1 f_1, V=\phi_2 f_2$, the normal conductor functions ϕ_1 and ϕ_2 now satisfy

$$\begin{aligned} &\left\{\frac{d^2}{dr^2}+\frac{(\mu_-^2+\frac{1}{4})}{r^2}-\frac{2m}{\hbar^2}E_{\mu k_z}\right\}\phi_1(r)=0\ ,\\ &\left\{\frac{d^2}{dr^2}+\frac{(\mu_+^2+\frac{1}{4})}{r^2}-\frac{2m}{\hbar^2}E_{\mu k_z}\right\}\phi_2(r)=0\ , \end{aligned}\tag{8}$$

where $\mu_-\equiv\mu-\frac{1}{2}$ and $\mu_+\equiv\mu+\frac{1}{2}$. The solutions to Eq. (8) are Bessel functions times $r^{-1/2}$.

The superconductor functions f_1 and f_2 satisfy the first-order equation with notation now suppressed;

$$\begin{aligned} &-\frac{\hbar^2}{m}\frac{1}{\phi_1}\frac{d\phi_1(r)}{dr}\frac{df_1}{dr}+\Delta(r)\frac{\phi_2(r)}{\phi_1(r)}f_2(r)=Ef_1(r)\ ,\\ &\frac{\hbar^2}{m}\frac{1}{\phi_2}\frac{d\phi_2(r)}{dr}\frac{df_2}{dr}+\Delta(r)\frac{\phi_1(r)}{\phi_2(r)}f_1(r)=Ef_2y(r)\ , \end{aligned}\tag{9}$$

and $E=E_{\mu n k_z}$ and depends on μ through ϕ_1 and ϕ_2. These equations can now be uncoupled in a straightforward way which would lead to a complicated set of second-order equations for $f_1(r)$ and $f_2(r)$. Instead we proceed more simply as well as consistently and evaluate the functions ϕ_1 and ϕ_2 in Eq. (9) using their asymptotic forms. This can be justified as follows: $\phi(r/\lambda_F)=\phi((\xi/\lambda_F)(r/\xi))$ and since r/ξ is the appropriate variable for Eq. (9) and $\xi/\lambda_F\gg1$ then we can use the asymptotic forms of $\phi_{1,2}$. In the simplest case Eqs. (9) become

$$-i\hbar v_{11}\frac{df_1(r)}{dr}-Ef_1(r)+\Delta(r)f_2(r)=0\ ,$$
$$i\hbar v_{11}\frac{df_2(r)}{dr}-Ef_2(r)+\Delta(r)f_1(r)=0\ . \tag{10}$$

We can now identify the parameters of Eq. (10) with those of Refs. 9(b) and 9(c). This allows us to make use of those solutions for f_1 and f_2. We have

$$f_1(r)=A_1\left[P_n^{\pm m}(y)-i\left[\frac{n+m}{n-m}\right]P_{-n}^{\pm m}(y)\right]\ ,$$
$$f_2(r)=A_2\left[P_n^{\pm m}(y)+i\left[\frac{n+m}{n-m}\right]P_{-n}^{\pm m}(y)\right]\ , \tag{11}$$

where now $y\equiv\tanh(\alpha r)$, $n\equiv\Delta_\infty/\hbar v_{11}\alpha$. We suggest that these functions will provide a useful set of trial functions for variational solution of the vortex problem. We note in this connection that only the parameters α and v_{11} appear in Eq. (11) as possible variational parameters. However, a linear variational calculation involving all of the basis functions $P_{\pm n}^{\pm m}$ allows for a complete solution of the problem.

In this connection it must be recognized that the BdeG operator $\sigma_z H_N+\sigma_x\Delta$ is not positive definite and therefore the appropriate functional to be used in a variational calculation is $\langle(\sigma_z H_N+\sigma_x\Delta)^2\rangle$. This was first pointed out by de Gennes.[1] In general, of course, one must minimize the free-energy functional subject to self-consistency.

The previous discussion serves a primarily heuristic purpose. In a future work,[10] we present a more careful analysis. Following the work of Bardeen *et al.*,[12] we invoke the functional form of Caroli and co-workers,[1(b)] $f=gH^{(1),(2)}(k_{11}r)+$c.c. with asymptotic form

$$H_\mu^{(1),(2)}\sim\exp\left[\pm i\int_{r_\mu}^{r}dr'\beta(r')\right]/(r^2-r_\mu^2)^{1/4}\ ,$$

where $\beta(r)\equiv(k_{11}/r)(r^2-r_\mu^2)^{1/2}$ and $r_\mu=\mu/k_{11}$ is the classical turning point. Using this method the equation for g becomes

$$-i\hbar v_{11}\frac{(r^2-r_\mu^2)^{1/2}}{r}\sigma_z\frac{d}{dr}g+\Delta\sigma_x g=Eg\ . \tag{12}$$

In terms of the new independent variable $x\equiv\xi^{-1}(r^2-r_\mu^2)^{1/2}$ we obtain

$$-2i\sigma_z\frac{dg}{dx}+\frac{\Delta(x)}{\Delta_\infty}\sigma_x g=\frac{E}{\Delta_\infty}g\ . \tag{13}$$

Equation (13) can now be identified with our preceding equations [(4) or (10)]. Thus, using $y\equiv\tanh\alpha x$, which goes to tanh $(\alpha r/\xi)$ for $r\gg r_\mu$, we have

$$\Delta(x)=\Delta_\infty\tanh\alpha(\xi^2x^2+r_\mu^2)^{1/2}$$
$$=\begin{cases}\Delta_\infty\tanh\alpha r_\mu\ , & x\to 0\\ \Delta_\infty\tanh\alpha\xi x\ , & x\to\infty\ .\end{cases} \tag{14}$$

The wave functions of Eq. (11) are valid for $x\to\infty$ but can be used approximately by joining them at $x=0$.

The boundary condition analysis of Ref. 12 now applies; g is real at $r=r_\mu$, or $x=0$, in order to ensure that f goes into an ordinary Bessel function. This condition in turn requires that $(m+n)$ be zero or an integer. It can be shown[10] that the optimum value of E is given by $E_\mu^2=\Delta^2(r_\mu)$. We note that this remarkably simple formula for the bound-state energy, namely

$$E_\mu=\pm\Delta(r_\mu)\ ,\quad r_\mu=\mu/k_{11}\ ,\quad \mu=\pm\tfrac{1}{2}\ ,\ \pm\tfrac{3}{2},\ldots \tag{15}$$

is independent of the form $\Delta(r)=\Delta_c\tanh(\alpha r)$.

In the simplest case of $m=-n$ the wave functions are $P_n^n=\mathrm{sech}^n(y)$. Since our main interest in the present work is to establish feasibility of the trial solutions to the vortex problem, we will use an empirical procedure for determining the variational parameters embodied in the preceding equations. A beginning estimate of α is taken from Refs. 9(b) and 9(c) on the one-dimensional BdeG solutions and v_F is the same as that used in Refs. 4 and 5. In Fig. 1 we compare our variational functions and ener-

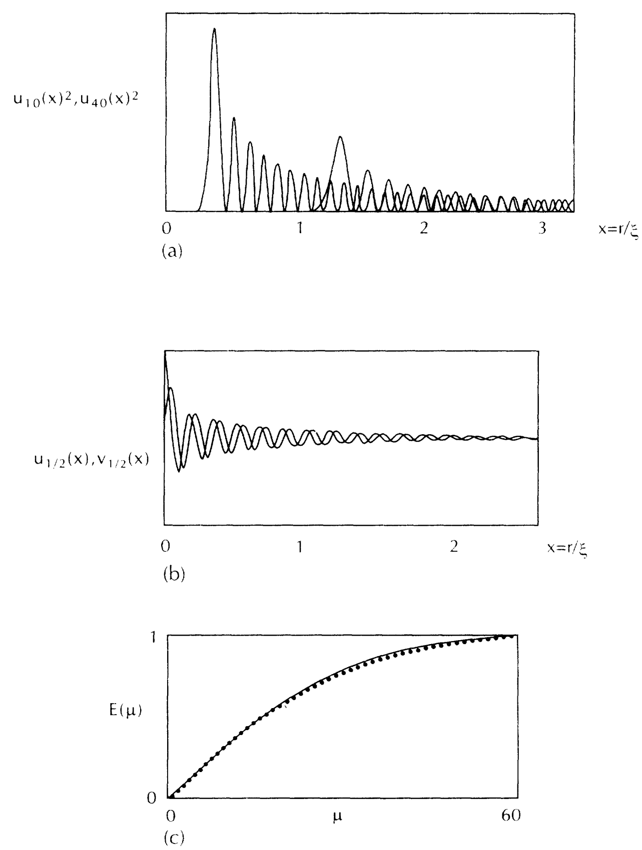

FIG. 1. (a) The density $|U_\mu|^2=|J_{\mu+1/2}(K_{Fr})|^2$. These curves replicate to within graphical accuracy the corresponding plots in Ref. 4. For these large values of μ the P_n^m part of the wave function is essentially unity. (b) The functions $U_{1/2}=J_0(k_F r)\mathrm{sech}(r/\xi)$ and $V_{1/2}=J_1(k_F r)\mathrm{sech}(r/\xi)$. These curves replicate to within graphical accuracy the corresponding plots in Ref. 5. (c) $E_\mu=\Delta(\mu/k_{11})$. Solid curve is $\Delta(r_\mu)$ courtesy of M. Schluter. Open circles are exact E_μ courtesy of J. Shore and M. Schluter.

gies to those calculated numerically in Refs. 4 and 5. The agreement is excellent to the graphical accuracy reported in Refs. 4 and 5.

In summary we have presented a method for generating approximate wave functions for BdeG equations. Special solutions for the SNS junction are used to study the vortex problem. These solutions should be useful for a variety of studies of the vortex state.

[1](a) P. G. de Gennes, *Superconductivity of Metals and Alloys* (Benjamin, New York, 1966); (b) C. Caroli, P. G. de Gennes, and J. Matricon, Phys. Lett. **9**, 307 (1964); C. Caroli and J. Matricon, Phys. Kondens. Mater. **3**, 380 (1965).

[2](a) H. F. Hess, R. B. Robinson, R. C. Dynes, J. M. Valles, Jr., and J. V. Waszzak, Phys. Rev. Lett. **62**, 214 (1989); (b) H. F. Hess, R. B. Robinson, and J. V. Narzzak, *ibid.* **64**, 2711 (1990).

[3]A. W. Overhauser and L. L. Damien, Phys. Rev. Lett. **62**, 169 (1989).

[4]J. D. Shore, M. Huang, A. T. Dorsey, and J. P. Sethna, Phys. Rev. Lett. **62**, 3089 (1989).

[5]F. Gygi and M. Schluter, Phys. Rev. B **41**, 833 (1990).

[6]U. Klein, Phys. Rev. B **41**, 4819 (1990).

[7]F. Gygi and M. Schluter, Phys. Rev. Lett. **65**, 1820 (1990).

[8]J. F. Andreev, Zh. Eksp. Teor. Fiz. **46**, 1823 (1964) [Sov. Phys.—JETP **19**, 1228 (1964)]. See also W. L. McMillan, Phys. Rev. **175**, 559 (1968), and references therein.

[9]For example, (a) J. Bardeen and J. Johnson, Phys. Rev. B **5**, 72 (1972); (b) J. Bar-Sagi and C. G. Kuper, Phys. Rev. Lett. **28**, 1556 (1972); (c) W. L. Clinton, Phys. Rev. B **8**, 1962 (1973); (d) D. Y. Chen and C. R. Hu, J. Low Temp. Phys. **25**, 43 (1976); (e) H. Alberle and R. Kummel, Phys. Rev. Lett. **57**, 3206 (1986).

[10]This argument can be couched in more rigorous terms using perturbation theory. This will be done in a more detailed publication.

[11]It appears that an option here is to partition the phase factor $e^{i\theta}\equiv e^{ia\theta}e^{ib\theta}$ with $a+b=1$, between the functions ϕ and g.

[12]J. Bardeen, R. Kummel, A. E. Jacobs, and L. Tewordt, Phys. Rev. **187**, 556 (1969).