Computer Physics Communications 142 (2001) 391–395

Computer Physics Communications

www.elsevier.com/locate/cpc

# Computing microscopic structures of inhomogeneities in superconductors

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**Abstract**

We present an efficient computational method to solve selfconsistently the Bogoliubov–de Gennes equations of weak coupling superconductivity. As a function of system size, the scaling of the CPU time required by the scheme is shown to be preferable compared to the methods commonly used. Also, the scheme allows taking into account nonlocal pairing interactions without additional computational cost. The favourable scaling behavior enables computation of microscopic electronic structures for ranges of physical parameter values previously inaccessible. © 2001 Elsevier Science B.V. All rights reserved.

*PACS:* 74.25.Jb; 74.80.-g; 02.70.Bf

*Keywords:* Superconductivity; Bogoliubov–de Gennes equations; Finite-difference methods

## 1. Introduction

Problems with spatially or temporally dependent pair potentials are the most interesting and challenging ones in the theory of weak coupling (BCS) superconductivity. In addition to fundamental questions concerning the electronic structure near surfaces and in the intermediate and mixed states in type I and type II superconductors, respectively, such problems include, for example, the effects of impurities, vortex motion and energy dissipation processes, vortex pinning, the electromagnetic response of superconductors, and in general relaxation and fluctuation effects. However, as the BCS formalism of superconductivity is analytically solvable for homogeneous systems, it poses serious computational difficulties for systems lacking translational invariance.

The Bogoliubov–de Gennes (BdG) formalism [1], a fully microscopic wavefunction formulation of the BCS theory, is a natural and reliable framework to model inhomogeneous superconductivity [2]. Its quasiclassical approximations have proven to be efficient, but their validity is limited to sufficiently long length and time scales. The applicability of quasiclassical theories is especially questionable for high-temperature superconducting materials with coherence lengths of the order of atomic distances. Also, atomic scale inhomogeneities in conventional superconductors are typically associated with rapid Friedel oscillations in the pair potential, a phenomenon that can be properly described only within a fully microscopic theory, such as the BdG formalism.

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PII: S0010-4655(01)00368-X

## 2. Bogoliubov–de Gennes formalism

The Bogoliubov–de Gennes equations consist of Schrödinger-type coupled eigenvalue equations

$$\widehat{H}_e(\mathbf{r})u_n(\mathbf{r}) + \int \mathrm{d}\mathbf{r}'\, \Delta(\mathbf{r},\mathbf{r}')v_n(\mathbf{r}') = E_n u_n(\mathbf{r}),$$
$$-\widehat{H}_e^*(\mathbf{r})v_n(\mathbf{r}) + \int \mathrm{d}\mathbf{r}'\, \Delta^*(\mathbf{r},\mathbf{r}')u_n(\mathbf{r}') = E_n v_n(\mathbf{r}) \quad (1)$$

determining the quasiparticle excitation energies $E_n$ and the corresponding electron- and hole-like amplitudes $u_n(\mathbf{r})$, $v_n(\mathbf{r})$. Above, $\widehat{H}_e(\mathbf{r})$ denotes the single-electron Hamiltonian

$$\widehat{H}_e(\mathbf{r}) = -\frac{\hbar^2}{2m}D(\mathbf{r})^2 + U_0(\mathbf{r}) - E_\mathrm{F};$$
$$D(\mathbf{r}) \equiv \nabla - \frac{\mathrm{ie}}{\hbar c}\mathbf{A}(\mathbf{r}) \quad (2)$$

with $\mathbf{A}(\mathbf{r})$ the magnetic field vector potential, $U_0(\mathbf{r})$ an external (for example, lattice) potential and $E_\mathrm{F}$ the Fermi energy. The quasiparticle equations are coupled via convolutions of the amplitudes with the superconducting pairing amplitude $\Delta(\mathbf{r},\mathbf{r}')$. In addition to the quasiparticle eigenequations, the formalism consists of selfconsistency conditions

$$\Delta(\mathbf{r},\mathbf{r}') = V(\mathbf{r},\mathbf{r}')\sum_n \big[v_n^*(\mathbf{r})u_n(\mathbf{r}') + v_n^*(\mathbf{r}')u_n(\mathbf{r})\big] \times\big[1-2f(E_n)\big],$$

$$\mathbf{j}(\mathbf{r}) = \frac{\mathrm{e}\hbar}{m}\sum_n \mathrm{Im}\big\{f(E_n)u_n^*(\mathbf{r})D(\mathbf{r})u_n(\mathbf{r}) + \big[1-f(E_n)\big]v_n(\mathbf{r})D(\mathbf{r})v_n^*(\mathbf{r})\big\} \quad (3)$$

relating the pair potential $\Delta(\mathbf{r},\mathbf{r}')$ and the current density $\mathbf{j}(\mathbf{r})$ to the quasiparticle eigensolutions. Above, $f(E_n) = (\mathrm{e}^{E_n/k_\mathrm{B}T}+1)^{-1}$ denotes the temperature-dependent Fermi distribution function, and the summations extend over all positive-energy quasiparticle solutions of Eqs. (1) below a cut-off energy. The selfconsistent solutions of Eqs. (1)–(3), together with Maxwell's equations relating the current density $\mathbf{j}(\mathbf{r})$ and the vector potential $\mathbf{A}(\mathbf{r})$, determine the electronic structure and the excitation spectrum of a superconductor for given external potential, magnetic field, and temperature.

## 3. Computational challenges

Calculation of the properties of many-particle systems from first-principles microscopic quantum theories is in general an extremely difficult task. In computational treatments of the Bogoliubov–de Gennes formalism, these difficulties are manifested in the large number of quasiparticle eigensolutions needed for the summations of the selfconsistency equations. Typically, for system sizes of the order of a few superconducting coherence lengths $\xi$, the number of quasiparticle eigensolutions required ranges from approximately $10^4$ up to $10^6$ in order to satisfy even moderate accuracy criteria. The computational effort can be partly reduced by using semiclassical approximations for excitations exceeding a given energy level [3], but in order to reach high accuracy, the number of eigenstates requiring exact treatment remains large.

Furthermore, numerical solving of the eigenvalue Eq. (1) is rather difficult due to two widely separated energy scales in the problem: for conventional low-temperature superconductors the Fermi energy $E_\mathrm{F}$ exceeds the gap energy $\Delta$ in general by at least two orders of magnitude. Fig. 1 displays quasiparticle am-

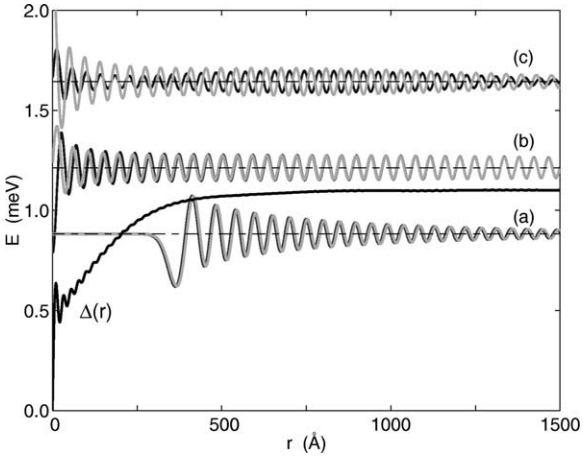


Fig. 1. Three selfconsistently computed quasiparticle solutions and the magnitude of the pairing amplitude $\Delta$ of an axisymmetric vortex containing one flux quantum. The quasiparticle amplitudes $u(r)$ and $v(r)$, where $r$ is the distance from the vortex axis, are denoted with the blue and the red curves, respectively, at the corresponding eigenenergies. The materials parameters have been chosen to correspond to $NbSe_2$ ($T_c \approx 7.2$ K) at the temperature $T = 0.01$ K. Note the mixing of the Fermi wavelength and the coherence length scales in the pairing amplitude in the quantum limit temperatures.

plitudes of three quasiparticle eigenstates in the vicinity of an isolated axisymmetric vortex line enclosing one magnetic field flux quantum. The materials parameter values correspond to $NbSe_2$, a typical low-temperature superconductor with $T_c = 7.2$ K. The two energy scales of the system are manifested in two well-separated length scales in the quasiparticle wavefunctions: the rapid oscillations at the Fermi wavelength are related to the Fermi energy $E_F$, whereas the modulational oscillation with approximate wavelength $\xi$ corresponds to the gap energy. Especially, the quasiparticle wavefunctions oscillate rapidly in typical computational domains with diameters dictated by the coherence length scale. Consequently, in order to reach even moderate accuracy for the quasiparticle eigenstates, the discretization of Eq. (1) has to be dense, thus implying heavy computational cost. It is to be noted that an exact, elementary separation of these energy scales for example by a factorized Ansatz is not possible due to the requirement of selfconsistency: as seen in Fig. 1, at ultralow temperatures the pairing amplitude often displays oscillations corresponding to both energy scales, mixed in a way which crucially depends on the selfconsistency of the solution.

Due to the above-mentioned difficulties, combined with the requirement of selfconsistency which necessitates use of iterative methods, solving of problems which do not possess any continuous spatial symmetries is nowadays practically impossible. The rapid development of supercomputers has recently facilitated first calculations for effectively two-dimensional problems (i.e. possessing one continuous symmetry) [4,5], but even for effectively 1D problems one is still restricted to use computational domains with diameters of just a few coherence lengths.

In the following, we present an efficient computational method for solving the BdG equations for effectively 1D systems. The method is compared with previously used schemes, and its computational cost as a function of the system size is shown to be excellent, thus enabling consideration of problems previously inaccessible.

## 4. Comparison of computational methods

The most commonly used methods for solving the Bogoliubov–de Gennes eigenvalue Eq. (1) for effectively one-dimensional systems are shooting methods [6] and eigenfunction expansion methods [7–10].

### 4.1. Shooting methods

Shooting methods are particularly well suited for solving 1D boundary value problems when the corresponding initial value problem does not have very rapidly growing solutions — such solutions are usually related to high sensitivity of the problem on the initial values, thus hampering shooting algorithms. When applicable, shooting algorithms are effective in yielding solutions with high accuracy. However, they are not optimal for searching selfconsistent solutions of the BdG equations. First of all, computation of the large number of eigensolutions needed in a reliable way is rather complicated to realize by using such methods — especially the dense (quasi)continuum part of the spectrum above the gap energy is cumbersome to compute. Furthermore, due to the large Fermi energy scale in the problem, the equations have rapidly growing exponential solutions, which cause numerical instabilities when shooting methods are applied.

### 4.2. Eigenfunction expansion methods

In the eigenfunction expansion methods (EEM), the eigenvalue problem of Eq. (1) is discretized by approximating the solutions with projections to a finite-dimensional subspace spanned by a chosen set of basis functions:

$$u_n(r) \simeq \sum_{j=1}^{N} a_{nj}\phi_j(r),$$
$$v_n(r) \simeq \sum_{j=1}^{N} b_{nj}\phi_j(r). \tag{4}$$

The basis functions $\{\phi_j\}_{j=1}^{N}$ are typically selected to be an orthogonal set of the lowest $N$ eigensolutions in the case $\mathbf{A}(\mathbf{r}) \equiv 0$; $\Delta(\mathbf{r}) \equiv 0$, which usually is analytically solvable. The discretization transforms Eq. (1) to an eigenvalue problem of a $2N \times 2N$ coefficient matrix [7]. In order to attain given accuracy criteria for the solutions, the number of degrees of freedom $N$ has to scale in proportion to the linear dimension $L$ of the system; typically $N \gtrsim 10M$, where $M$ is the number of solutions required [11]. As the computation of the

individual coefficient matrix elements involves numerical integration over the length $L$, the computational cost of the method in terms of CPU time $\tau$ is seen to scale as $\tau \sim L^3$ with respect to the system size.

### 4.3. Finite-difference discretization

Instead of the above-mentioned schemes, we have used a computational method based on real-space discretization for solving the Bogoliubov–de Gennes equations [12–14]. For convenience, we use evenly spaced grids and approximate the derivatives with high-order central difference formulas [15]. For an $N$-point lattice, this discretization converts Eq. (1) to a $2N \times 2N$ matrix eigenvalue problem. The structure of this coefficient matrix differs, however, essentially from the forms given by general eigenfunction expansion methods: For an $n$-point central difference scheme and a local pairing interaction, each of the finite-difference equations couples only $n$ nearest lattice points, which yields a narrow-banded coefficient matrix with bandwidth $2n-1$. Furthermore, the range of the pairing interaction is in general only of the order of the Fermi wavelength, such that the off-diagonal integral terms in Eqs. (1) can be discretized in a way which does not essentially broaden the bandwidth. Although in general the number of degrees of freedom $N$ for the real-space discretization has to be larger than for eigenfunction expansion methods in order for the solutions to satisfy same accuracy criteria, the narrow-bandedness of the matrix is a definite advantage in terms of memory storage and CPU time requirements for large system sizes.

We use an iterative Lanczos method implemented in the ARPACK subroutine libraries [16] to solve the discretized eigenvalue problem. The algorithm utilizes the sparcity of the matrix by storing only the band elements, thus yielding a memory storage requirement which scales linearly with $N$. This is highly advantageous in comparison to the EEM with storage requirement scaling as $\sim N^2$. Furthermore, the scaling of the computational cost required to diagonalize the narrow-banded matrices is much more favourable than for the full matrices of the EEM. Fig. 2 displays the CPU time $\tau$ as a function of $N$ for various numbers of required eigensolutions $M$. The tests were carried out on a Compaq AlphaServer GS140 supercomputer using 5-point discretization

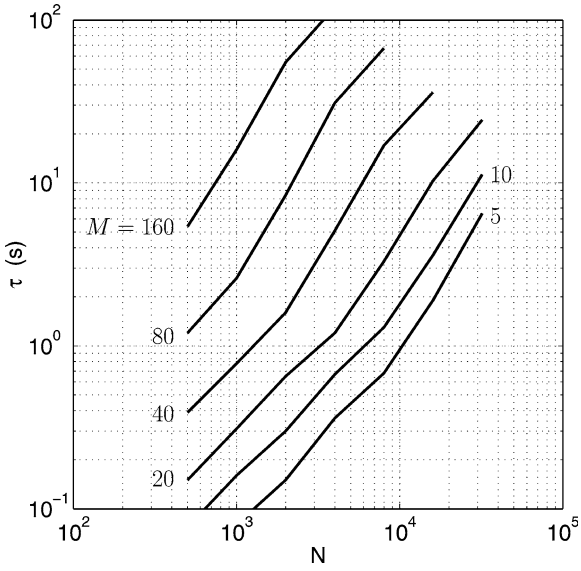


Fig. 2. CPU time required for the computation of the $M$ lowest eigenstates using the real-space discretization with $N$ grid points. These indicative tests have been performed on a Compaq AlphaServer GS140 computer, using five-point central difference formulas and the Lanczos method implemented in the ARPACK subroutine libraries.

and ARPACK's Lanczos algorithm. The data is only indicative, owing to the fact that the parameters for the Lanczos method were not optimized for each $(N, M)$ combination, and the total load of the system was not invariant for all the test runs. However, it is seen that the CPU time scales in the range investigated approximately as $\tau \sim N^{1.5}$, which is much more favourable than scaling of algorithms diagonalizing full matrices.

To fulfill a given accuracy requirement, $N$ has to scale linearly with the system size $L$. On the other hand, also the density of the quasiparticle states is proportional to $L$ (when the system size is modified only in the dimension corresponding to the computational domain). As a function of the number of required solutions $M$, the CPU time required by the ARPACK routines grows faster than linearly for $M \gtrsim 40$, but this can be reduced to a linear dependence by splitting the computation. Altogether, the computational time is seen to scale as a function of the system size as $\tau \sim L^{2.5}$, which for large systems is definitely advantageous compared to the EEM with $\tau \sim L^3$.

## 5. Discussion

We have developed an efficient computational method based on real-space discretization to solve the Bogoliubov–de Gennes equations in effectively one-dimensional geometries. Compared to the other methods commonly used for the same problem, the real-space discretization combined with a fast band-matrix solver is shown to be superior in efficiency in the limit of large system sizes. An additional advantage of the method is that nonlocal electron pairing interactions can be taken into account without essentially increasing the computational cost. In the future, possibilities to extend similar ideas to effectively two-dimensional systems are to be investigated.

## Acknowledgements

This research is supported by the Academy of Finland Grant “Theoretical Materials Physics”. The Academy of Finland is acknowledged for supporting SMMV within the Graduate School in Technical Physics. CSC – Scientific Computing Ltd. is thanked for computer resources.

## References

[1] P.G. de Gennes, Superconductivity of Metals and Alloys, Addison-Wesley, Reading, MA, 1989.

[2] I. Kosztin, Š. Kos, M. Stone, A. Leggett, Phys. Rev. B 58 (1998) 9365–9384.

[3] J. Reidl, A. Csordás, R. Graham, P. Szépfalusy, Phys. Rev. A 59 (1999) 3816–3822.

[4] M. Franz, Z. Tešanović, Phys. Rev. Lett. 80 (1998) 4763–4766.

[5] K. Yasui, T. Kita, Phys. Rev. Lett. 83 (1999) 4168–4171.

[6] J.D. Shore, M. Huang, A.T. Dorsey, J.P. Sethna, Phys. Rev. Lett. 62 (1989) 3089–3092.

[7] F. Gygi, M. Schlüter, Phys. Rev. B 43 (1991) 7609–7621.

[8] N. Hayashi, T. Isoshima, M. Ichioka, K. Machida, Phys. Rev. Lett. 80 (1998) 2921–2924.

[9] T. Isoshima, K. Machida, J. Phys. Soc. Jpn. 66 (1997) 3502–3511.

[10] F.V. De Blasio, Ø. Elgarøy, Phys. Rev. Lett. 82 (1999) 1815–1818.

[11] For computationally 1D systems, the eigenvalue equations are solved separately for each combination of quantum numbers corresponding to momenta in the directions of the continuous symmetries.

[12] S.M.M. Virtanen, M.M. Salomaa, Phys. Rev. B 60 (1999) 14 581–14 584.

[13] S.M.M. Virtanen, M.M. Salomaa, Physica B 284–288 (2000) 741–742.

[14] S.M.M. Virtanen, M.M. Salomaa, J. Phys.: Condens. Matter. 12 (2000) L147–L153.

[15] For problems in which the pairing amplitude satisfies certain additional symmetries, the symmetric and evenly spaced discretization combined with suitable rescaling of the equations yields an eigenvalue problem of a *symmetric* matrix, which is computationally more convenient than that of nonsymmetric matrices.

[16] We use software available from the ARPACK Home Page at Comp. and Appl. Math. Dept., Rice Univ., http://www.caam.rice.edu/software/ARPACK/.