Efficient Numerical Approach to Inhomogeneous Superconductivity: The Chebyshev-Bogoliubov–de Gennes Method

L. Covaci,[1,2] F. M. Peeters,[1] and M. Berciu[2]

[1]Department Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium
[2]Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z1

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We propose a highly efficient numerical method to describe inhomogeneous superconductivity by using the kernel polynomial method in order to calculate the Green's functions of a superconductor. Broken translational invariance of any type (impurities, surfaces, or magnetic fields) can be easily incorporated. We show that limitations due to system size can be easily circumvented and therefore this method opens the way for the study of scenarios and/or geometries that were unaccessible before. The proposed method is highly efficient and amenable to large scale parallel computation. Although we only use it in the context of superconductivity, it is applicable to other inhomogeneous mean-field theories.

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In the past decades the mean-field description of inhomogeneous superconductivity through the Bogoliubov–de Gennes (BdG) equations has been highly successful in uncovering novel phenomena. Because in the presence of broken translational invariance one needs to use a real space formulation, the numerical simulation becomes computationally involved. While alternative approaches to inhomogeneous superconductivity like quasiclassical approximations or Ginzburg-Landau methods exist, the need for a fully quantum-mechanical approach has become imperative. This is manifest in questions regarding high-T_c superconductors for which the superconducting coherence length is of the order of the Fermi wavelength, or in questions regarding nanoscale superconductivity for which the superconducting coherence length is comparable to the system size.

The BdG equations have been extensively used in a multitude of situations where translational symmetry is broken. Examples include the description of quasiparticles in s-wave or d-wave vortices [1–3], self-consistent calculation of order parameters and local density of states (LDOS) near surfaces and interfaces [4–9], self-consistent description of magnetic and nonmagnetic impurities in superconductors [10–12], calculation of dc Josephson currents through weak links [5,6], uncovering of the effect of electron confinement on superconductivity [13], etc.

Throughout these studies several methods of solving the BdG equations have been employed. After a discretization of the mean-field Hamiltonian one can use the straightforward approach of diagonalizing exactly the resulting Hamiltonian. Although exact diagonalization can in principle treat any inhomogeneous situation, it has severe limitations on the size of the discretization grid. There exist several ways of circumventing these limitations if the translational symmetry is recovered either by considering surfaces and interfaces or highly symmetric geometries (cylindrical or square). Supercell methods are also used in order to increase the energy resolution of calculated local densities of states.

A completely different approach is based on approximating the Green's functions. In this case the eigenenergies will appear as poles of the Green's function while the wave-function amplitudes will appear as weights of the poles. One such method is the recursive method based on the Lanczos procedure [9,14]. The approach we use here is similar in spirit but has many benefits when compared to the recursive Lanczos method. We will show how the Green's function can be efficiently expanded in series of Chebyshev polynomials. This Letter is organized as follows: first we will introduce a general model Hamiltonian which is typically used for describing inhomogeneous superconductors. We will next present the Chebyshev-Bogoliubov–de Gennes (CBdG) method and show, by an example, how this method can be implemented.

The Bogoliubov–de Gennes equations are mean-field coupled equations which describe the behavior of electrons and holes in superconductors. If we consider second quantization and work within the Nambu spinor formalism, a general Hamiltonian describing superconductivity can be written as follows:

$$\mathcal{H} = \sum_{\langle i,j \rangle} (c_{i\uparrow}^{\dagger} c_{i\downarrow}) \hat{\mathcal{H}}_{ij} \begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow}^{\dagger} \end{pmatrix}, \tag{1}$$

where $\hat{\mathcal{H}}_{ij}$ is a 2×2 matrix,

$$\hat{\mathcal{H}}_{ij} = \begin{pmatrix} \epsilon_i - \mu & \Delta_i \\ \Delta_i^{\star} & -\epsilon_i + \mu \end{pmatrix} \delta_{ij} + \begin{pmatrix} -t_{ij} & \Delta_{ij} \\ \Delta_{ij}^{\star} & t_{ij}^{\star} \end{pmatrix} (1 - \delta_{ij}). \tag{2}$$

ϵ_i describes an on-site potential due to impurities, μ is the chemical potential, t_{ij} describes hopping between nearest neighbor sites, while Δ_i (Δ_{ij}) are the on-site (nearest-neighbor) superconducting order parameters. The effect

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of a magnetic field is contained in the complex order parameters through the usual Peierls phases $t_{ij} = |t_{ij}| \exp(i\frac{\pi}{\phi_0}\int_i^j A_{ij}dl)$, where A_{ij} is the vector potential and $\phi_0 = h/2e$ is the flux quantum.

The quantity of interest is the 2×2 Green's function, which is defined as

$$\bar{G}_{ij}(\omega) = \langle \mathrm{vac}| \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow}^\dagger \end{pmatrix} \hat{G}(\omega) (c_{j\uparrow}^\dagger c_{j\downarrow}) |\mathrm{vac}\rangle, \quad (3)$$

where $\hat{G}(\omega + i\eta) = [\omega + i\eta - \mathcal{H}]^{-1}$ and $|\mathrm{vac}\rangle$ is the vacuum. The diagonal and off-diagonal components are the normal and anomalous Green's functions:

$$\bar{G}_{ij}^{11}(\omega) = \langle c_{i\uparrow}|\hat{G}(\omega)|c_{j\uparrow}^\dagger\rangle \quad (4)$$

$$\bar{G}_{ij}^{12}(\omega) = \langle c_{i\downarrow}^\dagger|\hat{G}(\omega)|c_{j\uparrow}^\dagger\rangle^*, \quad (5)$$

where $|c_{i\uparrow}^\dagger\rangle = c_{i\uparrow}^\dagger|\mathrm{vac}\rangle$ creates a spin-up electron and $|c_{i\downarrow}\rangle = c_{i\downarrow}|\mathrm{vac}\rangle$ destroys a spin-down electron. For finite temperatures the expectation value also contains a thermal average.

As mentioned before, the Green's function can be approximated by using a Lanczos procedure to invert the Hamiltonian [9,14]. This method has proven to be efficient mostly in the homogeneous case or when the Lanczos procedure can be easily extrapolated. The need of extrapolation is of utmost importance because, due to numerical roundoff errors, the Lanczos procedure becomes unstable due to loss of orthogonality. Reorthogonalization schemes exist, but the method becomes less and less efficient.

We therefore propose another approach to approximate the Green's function. Our method is based on the kernel polynomial method [15] which expands the single particle Green's function into a series of Chebyshev polynomials.

In order to be able to expand the Green's function, one first needs to rescale the Hamiltonian such that its spectrum is contained in the $[-1, 1]$ interval. We therefore have to work with the rescaled Hamiltonian $\tilde{\mathcal{H}} = (\mathcal{H} - \mathbb{1}b)/a$ and rescaled energies $\tilde{E} = (E - b)/a$, $\tilde{\omega} = (\omega - b)/a$, where $a = (E_{\max} - E_{\min})/(2 - \eta)$ and $b = (E_{\max} + E_{\min})/2$, where $\eta > 0$ is a small number. It is not essential to have accurate bounds on the spectrum; thus a quick Lanczos procedure to find $E_{\max}$ and $E_{\min}$ can be used.

Following Ref. [15] both the real and imaginary parts of the Green's function can be approximated by Chebyshev polynomials. The components of the full Green's function can be written as

$$\bar{G}_{ij}^{11(12)}(\tilde{\omega}) = \frac{-2i}{\sqrt{1-\omega^2}} \sum_{n=0}^{\infty} a_n^{11(12)}(i,j) e^{-in \arccos(\tilde{\omega})}, \quad (6)$$

with

$$a_n^{11}(i,j) = \langle c_{i\uparrow}|T_n(\mathcal{H})|c_{j\uparrow}^\dagger\rangle/(1 + \delta_{0,n}), \quad (7)$$

$$a_n^{12}(i,j) = \langle c_{i\downarrow}^\dagger|T_n(\mathcal{H})|c_{j\uparrow}^\dagger\rangle/(1 + \delta_{0,n}), \quad (8)$$

where $T_n(x) = \cos[n \arccos(x)]$ are the Chebyshev polynomials of first kind and they obey the known recursive relation $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$.

The most important part of the calculation has now shifted to the calculation of the expansion coefficients $a_n^{\alpha\beta}(i,j)$. Fortunately, due to the recurrence relation between Chebyshev polynomials, these moments can be obtained efficiently through a recursive procedure. If we define $|j_n\rangle = T_n(\mathcal{H})|c_{j\uparrow}^\dagger\rangle$, then after using the recursive property of Chebyshev polynomials we can write

$$|j_{n+1}\rangle = 2\mathcal{H}|j_n\rangle - |j_{n-1}\rangle, \quad (9)$$

where $|j_0\rangle = |c_{j\uparrow}^\dagger\rangle$ and $|j_1\rangle = \mathcal{H}|c_{j\uparrow}^\dagger\rangle$. At each iteration step $a_n^{1\alpha}(i,j) = \langle\alpha|j_n\rangle$, where $\langle 1| = \langle c_{i\uparrow}|$ and $\langle 2| = \langle c_{i\downarrow}^\dagger|$. It is important to note at this point that in the recursion defined by Eq. (9) the most expensive computation is a sparse matrix-vector multiplication. Moreover, the Hamiltonian matrix does not have to be stored since it always has the same form, thus allowing for simple rules for the multiplication. Another great benefit of this method is the possibility of obtaining in a single iteration all the normal and anomalous Green's functions, $\bar{G}_{ij}^{1\alpha}(\tilde{\omega})$, for all $\{i\}$ and $\{\alpha\}$ when the starting vector is $|c_{j\uparrow}^\dagger\rangle$. As explained in Ref. [15], because we can only keep a finite number of terms in the expansion, one needs to convolute the approximated function with kernel polynomials in order to remedy the effect of Gibbs oscillations. This is imperative when approximating Green's functions because of their discontinuous nature; the imaginary part is a summation over delta functions. We will use the Lorentz kernel [15], since it allows for the manipulation of a Lorentzian broadened delta function. The expansion has the same form, but the coefficients have to be multiplied by factors defined by the Lorentz kernel:

$$\tilde{a}_n^{\alpha\beta}(i,j) = a_n^{\alpha\beta}(i,j) \frac{\sinh[\lambda(1 - \frac{n}{N})]}{\sinh(\lambda)}, \quad (10)$$

where N is the total number of terms in the expansion and λ is a real number. If we write the Lorentzian approximation as $\delta(x) = 1/\pi \lim_{\epsilon\to 0} \epsilon/(x^2 + \epsilon^2)$, there is a direct relation between the broadening ϵ and λ: $\epsilon = \lambda/N$. This allows for a good control over the broadening of the Green's function's features, whether used artificially at zero temperature or naturally at finite temperature. As we will show later, in certain situations where interference between parts of the considered system is important, one needs a large number of coefficients in order to accurately obtain the Green's function. In that case the only way to keep the broadening constant is by changing λ accordingly.

Once the Green's functions are known, it is straightforward to calculate physically relevant quantities. The local density of states can be calculated as

$$N^{\uparrow(\downarrow)}(E,i) = -\frac{1}{\pi} \mathrm{Im}\bar{G}_{ii}^{11(22)}(E). \quad (11)$$

The electron density is

$$n_i = \int_{-\infty}^{\infty} [N^{\uparrow}(E,i) + N^{\downarrow}(E,i)] f(E) dE. \quad (12)$$

The order parameter, $\Delta_{ij} = U_{ij}\langle c_{i\uparrow} c_{j\downarrow}\rangle$ is

$$\Delta_{ij} = iU_{ij} \int_{-E_c}^{E_c} \bar{G}_{ij}^{12}(E)[1 - 2f(E)] dE, \quad (13)$$

where E_c is a cutoff energy (Debye energy for conventional superconductors or the bandwidth for cuprates). The current density between grid points i and j is

$$J_{ij}^{\uparrow(\downarrow)} = \frac{-1}{\pi} \int \mathrm{Im}[it_{ij}\bar{G}_{ij}^{11(22)}(E) - it_{ij}^{\star}\bar{G}_{ij}^{11(22)\star}(E)] f(E) dE. \quad (14)$$

One of the great benefits of this method is that the Green's function is calculated separately for each grid point, thus allowing for a trivial parallel implementation. An iteration can be started on a separate CPU for each grid point with a given order parameter profile. Next, the order parameter for that grid point is updated in the Hamiltonian in order to achieve self-consistency. The convergence of the self-consistent procedure is stable, and even more it is more efficient than a similar procedure for the exact diagonalization method. Because information about each grid point is obtained sequentially, updating the order parameters after each recurrence will provide information to the next grid point (preferably nearest neighbor). In addition, grid points near or around inhomogeneities (impurities, surfaces, or vortex cores) can be sampled with higher frequency improving the convergence and thus reducing the computational effort considerably. The present method is general and it can be applied not only to any mean-field Hamiltonian but also to more complex band structures, multiband superconductivity, and even to three-dimensional systems. Of course in these cases the number of operations increases, but the calculation can be done even on a desktop computer since the Hamiltonian is sparse.

As mentioned earlier the closest in efficiency with the Chebyshev method is the Lanczos recursion technique. While there are similarities between the methods, for the purposes of calculating Green's functions and order parameters in inhomogeneous situations the Chebyshev expansion method is more efficient on many different issues. Similarity between the methods comes from the fact that recursive procedures can be applied in both cases with the most expensive computation being a sparse matrix-vector multiplication. However, the Lanczos procedure becomes unstable because of loss of orthogonality between the generated basis vectors, while the Chebyshev expansion is stable with its moments decaying exponentially above a given number of iterations (this is usually set by the desired broadening, $N > \lambda/\epsilon$). Another benefit of using CBdG is the fact that off-diagonal elements (e.g., correlations between nearest neighbors) of all the neighbors of site $|i\rangle$ are obtained from only one iteration. This is not possible within the Lanczos procedure since only diagonal matrix elements can be calculated; instead, if one wants to calculate $G_{ij}(\omega)$, separate iterations have to be started for $|i\rangle + |j\rangle$ and $|i\rangle - |j\rangle$ for each neighbor grid point $|j\rangle$. Yet another benefit comes from the fact that the Chebyshev expansion [Eq. (6)] is in fact a Fourier expansion with a change of variable, and thus any integration of the Green's functions components over energy variables can be treated as a Fourier transform and the integral can be evaluated by using an efficient fast Fourier transform. Lastly, the Chebyshev procedure allows for easy coupling to baths [16] which are also described by Chebyshev expansions. We show elsewhere that this allows for easy calculation of transport properties of inhomogeneous mesoscopic superconductors.

As an example we will show how the LDOS depends on the number of Chebyshev coefficients. We consider first a planar system composed of a normal metal of length $L_x^N = 380a$ and an s-wave superconductor of length $L_x^S = 20a$ while $L_y = 500a$. In Fig. 1(a) we plot the LDOS at the surface of the normal metal region. Choosing $\Delta = 0.1t$ such that $\xi \approx 7a$, we observe in the LDOS the appearance of Andreev bound states below the superconducting gap. In Fig. 1(b) we plot the moments of the Chebyshev expansion for three iteration sequences. Here we choose a constant broadening $\epsilon = 0.001t$, thus the coefficient $\lambda = \epsilon N$ will modify the Chebyshev moments for each sequence. We observe an oscillatory behavior of the Chebyshev moments which is given by the interference of quasiparticles scattering off the normal-metal–superconducting and normal-metal–vacuum interfaces. Note that the Chebyshev iteration is equivalent to a propagation of a quasiparticle defined by the starting vector $|i\rangle$. Interestingly, the LDOS is not converged within

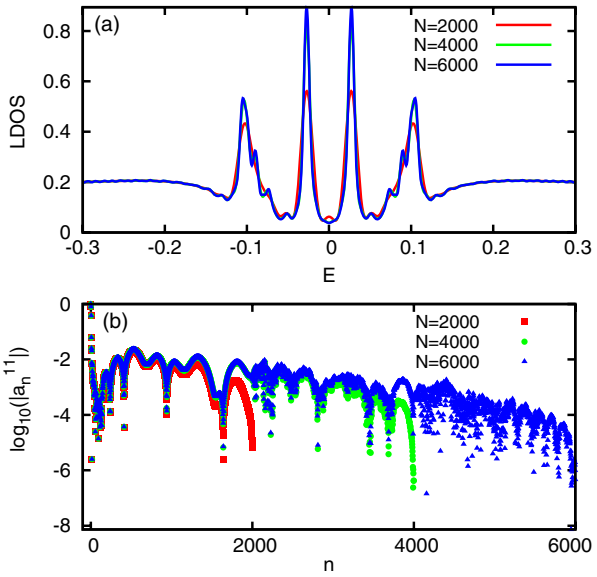

FIG. 1 (color online). LDOS and a_n^{11} at the surface of a planar s-wave superconductor–normal-metal system. The parameters are $\Delta_{s\ \mathrm{wave}} = 0.1t$, $L_x^S/a = 380$, $L_x^N/a = 20$, and $L_y/a = 500$.

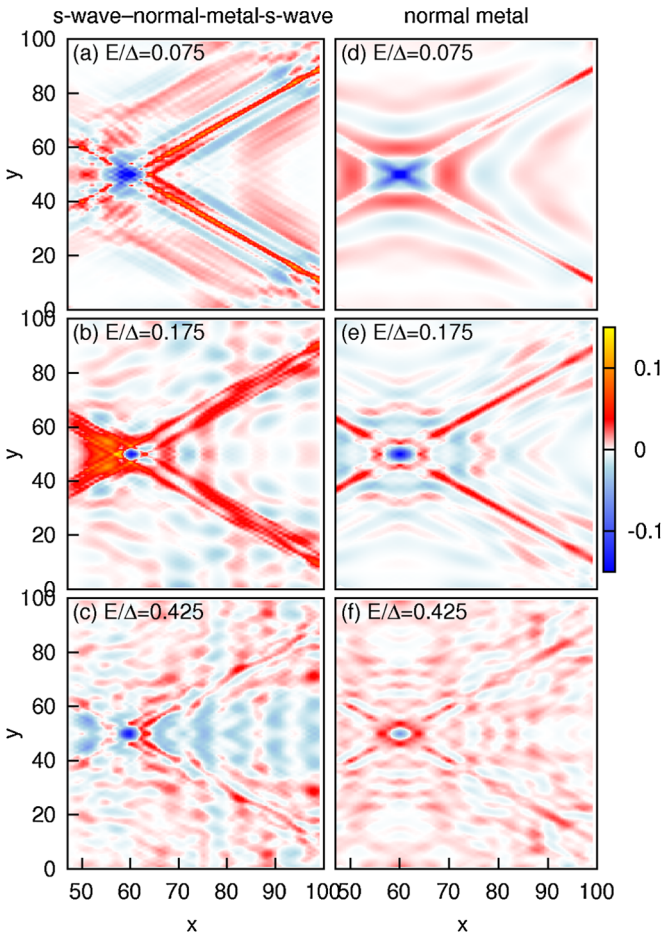

FIG. 2 (color online). Local density of states map around an impurity in a normal metal for various energies. For (a)–(c) the normal metal is sandwiched between two s-wave superconducting regions located at $x < 50a$ and $x > 100a$, respectively, while for (d)–(f) the whole system is normal. The LDOS for the corresponding clean systems (no impurity) is subtracted in both cases, for clarity.

ϵ for $N < 2000$, instead a larger number of moments is needed. It is exactly for these types of systems that a stable method is essential. When interference between quasiparticles scattered of distant regions of the system is important, an accurate solution requires a large number of moments. The recursion method based on the Lanczos method is inefficient in these situations.

To further illustrate the power of the method we show in Fig. 2 the LDOS for a s-wave SC–normal-metal–s-wave SC of size $(50a–50a–50a) \times 100a$ in the presence of a nonmagnetic impurity in the normal region $V_i = V \exp[-(\mathbf{r}_i - \mathbf{r}_{i0})^2/a]$ with $V = 2t$ and $r_{i0} = (60a, 50a)$. The left-hand panels show the LDOS around the impurity for various subgap energies while the right-hand panels show the LDOS for a homogeneous normal system plus the impurity. Modifications of the LDOS induced by the impurity are seen in both cases, but for the s-wave–normal-metal–s-wave system extra states are induced by the interference of quasiparticles undergoing Andreev reflection at the superconductor–normal-metal interface and specular reflection at the impurity site. Andreev states of the clean multilayer system are destroyed by the impurity, but new states appear due to impurity scattering.

In conclusion, we have introduced and demonstrated a new method of solving the mean-field self-consistent BdG equations by expanding the Nambu Green's functions in terms of Chebyshev polynomials. Because the method is stable the results are arbitrarily accurate since the accuracy is given by the number of moments kept in the expansion. The most expensive numerical operation is a sparse matrix-vector multiplication, thus allowing for large sized systems to be solved with little memory requirements. Moreover, since each grid point is calculated separately, the method is amenable to trivial parallel implementations. The present method can be easily expanded to consider spin-orbit interactions, complex band structures, multiband superconductivity, multidimensional systems, and other inhomogeneous mean-field Hamiltonians.

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