Generalized Bogolubov-de Gennes theory for nanoscale superconductors

B. Deloof\textsuperscript{1,2}, V. V. Moshchalkov\textsuperscript{2}, L. F. Chibotaru\textsuperscript{1}

\textsuperscript{1} INPAC - Institute of Nanoscale Physics and Chemistry and Theory of Nanomaterials Group, Departement of Chemistry, KU Leuven, Celestijnenlaan 200 F, B-3001 Leuven, Belgium
\textsuperscript{2} INPAC - Institute of Nanoscale Physics and Chemistry and Nanoscale Superconductivity and Magnetism Group, Departement of Physics and Astronomy, KU Leuven, Celestijnenlaan 200 D, B-3001 Leuven, Belgium

Abstract. The generalized Bogolubov-de Gennes (BdG) theory, including explicitly the Zeeman energy of electrons, is developed for nanoscale superconductors. To this end the system of four BdG equations is derived, corresponding to four coherent functions (instead of two in conventional BdG theory), two for electron-like excitations and two for hole-like excitations. These equations are transformed into matrix equations by using the basis set of particle-in-the-box problem and solved self-consistently with the equation for the order parameter and the chemical potential. The proposed microscopic approach is suitable for the study of unconventional vortex states and the appearance of FFLO phase in thin nanoscale superconductors.

The impressive progress in the fabrication and characterization of superconducting nanostructures achieved in the last years \cite{1} calls for more accurate description of their superconducting properties. The first theoretical descriptions of vortex states in mesoscopic superconductors have been done within the phenomenological Ginzburg-Landau theory \cite{2, 3, 4, 5}. This theory is formally exact close to the superconducting-normal phase boundary only \cite{6} and for the space variations of superconducting order parameter $\Delta(\vec{r})$ not exceeding the superconducting coherence length $\xi_0$. The last condition is hardly fulfilled for mesoscopic superconductors and not fulfilled in most nanoscale superconductors. For the latter the application of a microscopic theory becomes indispensable. The most simple way to do so is to employ the Bogolubov-de Gennes (BdG) theory \cite{6}.

The BdG theory \cite{6} is an extension of Bardeen-Cooper-Schrieffer (BCS) theory over superconductors with arbitrary electronic potentials and placed in arbitrary magnetic fields. Since both these potentials generally lift the translational symmetry, the BCS coherence factors $u_{\vec{k}}$ and $v_{\vec{k}}$, characterizing the strength of superconducting pairing of electrons in the Bloch states $\psi_{\vec{k}}(\vec{r})\ket{\uparrow}$ and $\psi_{-\vec{k}}(\vec{r})\ket{\downarrow}$, are replaced by coherence functions $u_n(\vec{r})$ and $v_n(\vec{r})$, describing the pairing of electrons in the non-translational time-reversed orbital states $\psi_n(\vec{r})\ket{\uparrow}$ and $\psi^*_n(\vec{r})\ket{\downarrow}$, $|\alpha\rangle$ denotes the spin states. These coherence functions are found from the BdG equations \cite{6}:

\begin{align}
\epsilon u(\vec{r}) &= \left[\mathcal{H}_e + U(\vec{r}) - \mu\right] u(\vec{r}) + \Delta(\vec{r}) v(\vec{r}), \\
\epsilon v(\vec{r}) &= -\left[\mathcal{H}_e^* + U(\vec{r}) - \mu\right] v(\vec{r}) + \Delta^*(\vec{r}) u(\vec{r}),
\end{align}

where

\begin{equation}
\mathcal{H}_e = -\frac{1}{2m} \left(-i\hbar \nabla - e\vec{A}\right)^2 + U_0(\vec{r})
\end{equation}
is a general one-electron Hamiltonian with $U_0(\vec{r})$ containing translational and non-translational contributions; $\vec{A}$ is the vector potential corresponding to applied magnetic field, $\vec{H} = \nabla \times \vec{A}$; $\mu$ is the chemical potential found from the equation:

$$N = 2 \int \sum_n \left[ f(\epsilon_n) |u_n(\vec{r})|^2 + (1 - f(\epsilon_n)) |v_n(\vec{r})|^2 \right],$$

where $n$ numbers the quasiparticle eigenstates of (1) and $f(\epsilon_n)$ is the Fermi-Dirac distribution of quasiparticles. The functions $U(\vec{r})$ and $\Delta(\vec{r})$ are Hartree-Fock and pairing potentials [6]:

$$U(\vec{r}) = -V \sum_n \left[ f(\epsilon_n) |u_n(\vec{r})|^2 + (1 - 2f(\epsilon_n)) |v_n(\vec{r})|^2 \right],$$

$$\Delta(\vec{r}) = V \sum_n (1 - 2f(\epsilon_n)) v_n^*(\vec{r}) u_n(\vec{r}),$$

where $V (> 0)$ is the pairing constant and the sum in the second equation runs over all states with the energy located within the Debye window $[-h\omega_D, h\omega_D]$ around the chemical potential. The equations (1) are solved self-consistently with (3,4). This microscopic theory has been applied to mesoscopic superconductors [7, 8, 9] in the particle-in-the-box model for the electronic levels ($U_0(\vec{r})=$const in the sample). It was found, in particular, that the Hartree-Fock potential $U(\vec{r})$ has little effect on the results of calculations [8].

Contrary to mesoscopic samples, in nanoscale superconductors with sizes of (tens of) nanometers, the entry of the first vortex is expected for applied fields of several Teslas. In this case the Zeeman energy, which depends on the projection of the electron spin ($\sigma$) on the direction of the field, cannot be neglected and should be included in the electronic Hamiltonian:

$$\mathcal{H}_{\sigma} = -\frac{1}{2m^*} \left( -i\hbar \nabla - e\vec{A} \right)^2 + \mu_B \sigma H,$$

where $m^*$ is the effective electron effective mass, $\mu_B$ is the Bohr magneton, $H$ is the homogeneous applied magnetic field and it was supposed $U_0(\vec{r})=0$. Taking into account that spin $g$ factor is 2, $\sigma$ equals to 1 for spin up and $-1$ for spin down. Due to the spin dependence of (5), the energies of quasiparticles and coherence functions are expected to be spin-dependent too. The corresponding generalized BdG equations are found in a similar way as the conventional ones [6] and result in four equations for the coherence factors:

$$\epsilon_\uparrow u_\uparrow(\vec{r}) = [\mathcal{H}_{\uparrow} - \mu] u_\uparrow(\vec{r}) + \Delta(\vec{r}) v_\uparrow(\vec{r})$$

$$\epsilon_\uparrow v_\uparrow(\vec{r}) = -[\mathcal{H}_{\uparrow} - \mu] v_\uparrow(\vec{r}) + \Delta^*(\vec{r}) u_\uparrow(\vec{r})$$

and

$$\epsilon_\downarrow u_\downarrow(\vec{r}) = [\mathcal{H}_{\downarrow} - \mu] u_\downarrow(\vec{r}) + \Delta(\vec{r}) v_\downarrow(\vec{r})$$

$$\epsilon_\downarrow v_\downarrow(\vec{r}) = -[\mathcal{H}_{\downarrow} - \mu] v_\downarrow(\vec{r}) + \Delta^*(\vec{r}) u_\downarrow(\vec{r})$$

where $U(\vec{r})$ has been neglected due to reasons given above. The pair potential is obtained in the form:

$$\Delta(\vec{r}) = +V \sum_\nu \left[ -f_{\nu,\uparrow} v_{\nu,\uparrow}^*(\vec{r}) u_{\nu,\downarrow}(\vec{r}) + (1 - f_{\nu,\downarrow}) v_{\nu,\downarrow}^*(\vec{r}) u_{\nu,\uparrow}(\vec{r}) \right],$$

where $f_{\nu,\sigma} = 1/(e^{\beta(\epsilon_{\nu,\sigma} - \mu)} + 1)$ is the Fermi function for quasiparticles of spin $\sigma$ ($\beta = 1/(k_B T)$) and the chemical potential is found from the equation:

$$N = \int \sum_{\nu,\sigma} \left[ f_{\nu,\sigma} |u_{\nu,\sigma}(\vec{r})|^2 + (1 - f_{\nu,\sigma}) |v_{\nu,\sigma}(\vec{r})|^2 \right],$$
With knowledge of $\Delta(\vec{r})$ the two sets of equations, (6) and (7), can be solved separately. They respectively correspond to the pairing of an electron-like quasiparticle with spin up and a hole-like quasiparticle with spin down ($\uparrow, \downarrow$), and the pairing of an electron-like quasiparticle with spin down and a hole-like quasiparticle with spin up ($\downarrow, \uparrow$). The self-consistent solutions of Eqs. (6,7,8,9) are used to calculate the free energy of the condensate:

$$F = \sum_{\nu,\sigma} \left[ \epsilon_{\nu,\sigma} f_{\nu,\sigma} - \epsilon_{\nu,\sigma} \int |v_{\nu,\sigma}(\vec{r})|^2 d^3\vec{r} \right]$$

$$- 2k_B T \sum_{\nu,\sigma} [f_{\nu,\sigma} \ln f_{\nu,\sigma} + (1 - f_{\nu,\sigma}) \ln (1 - f_{\nu,\sigma})]$$

$$+ \int |\Delta(\vec{r})|^2 V d^3\vec{r},$$

Note that in all equations the magnetic field is always an applied one, because one can neglect the effect of screening currents for thin nanoscale superconductors. This exempt us from the necessity to solve an additional Maxwell equation for the vector potential and to add the energy of the field to the total free energy (10).

In order to assess the difference of conventional and generalized BdG theory in application to nanosuperconductors, we consider further a thin superconducting square in homogeneous perpendicular magnetic field. As an example, we investigated a sample with size $a = 15\,nm$, effective mass of two electron masses, a coupling constant of $105\,meV$ and a bulk Fermi level of $39\,meV$. The Debye window is taken at $[-32.315, +32.315]\,meV$ around the Fermi level. For the sample of size $a = 15\,nm$ the corresponding Fermi level should then be taken at $44.3\,meV$ which can be calculated by requiring unchanged electron density with respect to the bulk value [11] These parameters give $\xi_0 = 0.2a$ (calculated with the BCS expression $\xi_0 = \hbar\omega_f/\pi\Delta(0)$) and a bulk value for the pair potential of $\Delta(0) = 0.2\hbar\omega_D$. They are obtained by starting from parameters that closely reproduce the properties of a superconductor like NbSe$_2$ and slightly increasing the effective mass and coupling constant in order to reduce computational effort by reducing the system’s size needed to obtain vortex entry in the sample.

The BdG equations have been solved by the basis set decomposition method [5]. To this end the coherence factors entering the above equations have been decomposed in the basis of the eigenstates of the particle in a square box problem. Integrating these equations after electronic coordinates yields matrix form of equations (1-4) and (6-9) with respect to decomposition coefficients for each of four coherent factors, which are then solved self-consistently. Besides, the convergence of calculation results with respect to the size of the basis set was also achieved. Fig. 1 shows the difference between the free energy of superconducting and normal state as a function of applied magnetic field at $T = 0K$. We can observe non-negligible differences in the free energy plots obtained by conventional and generalized BdG theory, which confirms the necessity to apply the latter for nanoscale samples. In agreement with the expectations, the differences in the predictions of generalized and conventional BdG approaches increase with the strength of applied magnetic field.

The developed microscopic approach can be applied for the study of nanosuperconductors in strong magnetic field. This concerns, first of all, the investigation of vortex-antivortex patterns in superconducting nanosamples [11]. Secondly, the high critical magnetic field and the low orbital contribution to depairing, making these systems Pauli-limited superconductors, allow for the realization of Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase [12, 13] at sufficiently high magnetic fields. Indeed, for Zeeman energy of the order of superconducting gap, the superconducting order parameter is expected to be non-homogeneous even in the Meissner state. This inhomogeneity is a fingerprint of the FFLO phase which can be detected in STM experiments for sufficiently clean superconductors.
Figure 1. (Colour online) Free energy difference $\Delta F$ as a function of applied magnetic field expressed in units of flux quanta $\Phi_0$ at $T = 0K$. Different curves correspond to different total winding numbers $L$. The upper curves are the solution obtained by generalized BdG theory, Eqs. (6) and (7), and the lower curves are corresponding conventional solutions, Eqs. (1). The curves obtained by generalized BdG theory are reversed (lower) only for $L = 3$.

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