Size effects of critical temperatures and order parameter distributions under four-fold symmetry of nano-structured superconductors

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Abstract. We investigate size and shape dependences of critical temperatures $T_c$'s and order parameter distributions for nano-structured superconductors. We use the finite element method to solve the Gor'kov equations. We find that order parameter distributions hold four-fold symmetry for square superconductors. It is different from order parameter distributions of rectangular superconductors, which have two-fold symmetry. We show that the difference comes from symmetry of the superconductor and degeneracy of states of Cooper pairs, by investigating size dependences of order parameter distributions and those of eigen-energies of quasi-particles.

1. Introduction
Bulk superconducting material has own critical temperature $T_c$. However, $T_c$ for a nano-structured superconductor depends on size and shape of the superconductor. Parmenter showed that $T_c$ increases monotonically with decreasing size of a cubic superconductor, using the BCS theory [1]. Experimentally Nishizaki showed that the high pressure torsion [2-3] makes many fine grains in bulks of Nb, and enhances $T_c$, because these fine grains become nano-structured superconductors [4]. $T_c$ for the nano-structured superconductor depends on surface modes of phonon spectrum [5] and quantum size effects on electrons [6-9]. We study the quantum size effects for nano-structured superconductors, by solving Gor’kov equations. We use the finite element method (FEM) [10] to incorporate effects of shapes of superconductors and real space order parameter distributions into numerical calculations. In previous study, we obtained size dependences of $T_c$, eigen-energies and order parameter distributions [11] for rectangular and square superconductors. Then we found that $T_c$ shows saw-tooth behaviour as a function of size. Also we found $T_c$’s for rectangular superconductors ($L \times 2L$; $L$ is a length of a shorter side of the system) are higher than those of square superconductors. In this paper we discuss size effects on $T_c$, eigen-energies, and order parameter distributions for square plates. We show differences between square plates and rectangular plates.

2. Methods
We use the Gor’kov equations and a self-consistent equation, and the FEM to determine $T_c$, eigen-energies and order parameter distributions.
The Matsubara frequency. We approximate it up to the first order. Then the self-consistent equation becomes

\[ \Delta^*(x) = -\frac{g}{\hbar \beta} \sum_{\omega_n} e^{-i\omega_n \hbar} F^e(x, x', \omega_n) \]

Where, \( \mathcal{G} \) is the Green’s function, \( F \) is the anomalous Green’s function, \( \Delta \) is a order parameter, \( E \) is the cut-off energy of the BCS theory and \( \omega_n = (2n+1)k_B T / \hbar \) is the Matsubara frequency. We expand Green’s functions and the order parameter using area coordinates \( \{ N^i \} \)

\[ \mathcal{G}(x, x', \omega_n) = \sum_{e, e'} \sum_{i, j} \mathcal{G}_{i j}^{e e'}(\omega_n) N^i(x) N^{j'}(x') \]
\[ F(x, x', \omega_n) = \sum_{e, e'} \sum_{i, j} \mathcal{F}_{i j}^{e e'}(\omega_n) N^i(x) N^{j'}(x') \]
\[ \Delta(x) = \sum_{e, i} \Delta_i^e N^i(x) \]

where subscripts and superscripts are node numbers and element numbers, respectively.

\[ \sum_{\gamma \delta} \left[ \left( i\hbar \omega_n + \mu \right) I^e_{\gamma \delta} - \hbar^2 / 2m \sum_a \sum K^{\alpha \gamma}_{\delta \beta} \mathcal{G}_{i j}^{e e'}(\omega_n) + \sum_{\gamma} \sum_{\beta} I_{i j}^{\gamma \delta} \Delta_i^e \mathcal{G}_{i j}^{e e'}(\omega_n) \right] I^{e'}_{\gamma \delta} = \hbar \delta_{e e'} I^e_{\gamma \delta}, \]
\[ \sum_{\gamma \delta} \left[ -i\hbar \omega_n (\mu + \hbar^2 / 2m \sum_a \sum K^{\alpha \gamma}_{\delta \beta} \mathcal{F}_{i j}^{e e'}(\omega_n) - \sum_{\gamma} \sum_{\beta} I_{i j}^{\gamma \delta} \Delta_i^e \mathcal{F}_{i j}^{e e'}(\omega_n) \right] I^{e'}_{\gamma \delta} = 0, \]
\[ \sum_{\beta} \Delta_i^e I^{e}_{\beta \gamma} = \frac{g}{\hbar \beta} \sum_{\omega_n} \sum_{\gamma \delta} e^{-i\omega_n \hbar} \sum_{\alpha} \mathcal{F}_{i j}^{e e'}(\omega_n) I^{e}_{\alpha \beta}, \]

where

\[ I^e_{\gamma \delta} = \int N^i(x) N^j(x) dx \]
\[ K^{\alpha \gamma}_{\delta \beta} = \int \frac{\partial N^i(x)}{\partial x^\alpha} \frac{\partial N^j(x)}{\partial x^\beta} dx. \]

In order to determine \( T_c \), we set temperature \( T \) tends to \( T_c \). Then we replace the Green’s function by the normal metal Green’s function. We expand the anomalous Green’s function in power series of the order parameter. We approximate it up to the first order. Then the self-consistent equation becomes

\[ \sum_i \left[ I^e_{\gamma \delta} - \frac{g}{\hbar \beta} \sum_{\omega_n} \sum_{\gamma \delta} \sum_{i j} \left( D^{-1}\right)^{\gamma}_{\delta} I^{e}_{\gamma \delta} \left( C^{-1}\right)^{\gamma}_{\delta} I^{e}_{\gamma \delta} \right] \Delta_i^e = 0. \]
The secular equation for equation (10) becomes

\[
\det \left[ I^e_{ij} - \frac{g}{\beta} \sum_k e^{-\omega_n \beta} \sum_{\lambda_k} (D^{-1})^\lambda_{i\lambda_k} I^e_{\lambda_k i} \left\{ (G^{-1})^\lambda_{j\lambda_k} I^e_{\lambda_k j} \right\} \right] = 0. \tag{11}
\]

Here, \( T_c \) is the maximum \( T \) that satisfies equation (11). Here

\[
C_{\alpha_i} = \left\{ i\hbar \omega_n + \mu + \frac{i\omega_n \hbar}{2\hbar} \right\} I^e_{\alpha_i} - \frac{\hbar^2}{2m} \sum_{\alpha} K^{\text{coa}}_{\alpha_i \alpha_i}
\]

\[
D_{\alpha_i} = \left\{ -i\hbar \omega_n + \mu - \frac{i\omega_n \hbar}{2\hbar} \right\} I^e_{\alpha_i} - \frac{\hbar^2}{2m} \sum_{\alpha} K^{\text{coa}}_{\alpha_i \alpha_i}. \tag{12}
\]

In addition, the chemical potential \( \mu \) is determined by the equation as follows,

\[
N(T,V,\mu) = \sum_{\omega_n} \int d^3x \text{tr} G(\omega_n, x). \tag{14}
\]

### 3. Results and Discussions

We consider superconducting square \((L \times L)\) and rectangular \((L \times 3L)\) plates. We impose boundary conditions that wave functions of electrons are zero at edges of plates. Therefore order parameters become zero at edges of these plates. We set that \( k_F \xi = 3.0 \), and \( \Delta_0 / E_c = 0.2 \), and densities of electrons and interaction constants \( g \) are fixed. Figure 1 shows models of the square and rectangular nano-structured superconductors for the FEM. Figure 2 shows size dependences of \( T_c \)'s for superconducting square and rectangular plates. Here, we compare size dependences of \( T_c \)'s between superconducting plates with same areas. From this result, we can see that smaller superconductors show higher \( T_c \), \( T_c \) has saw-tooth behavior as a function of size, and the square superconductor shows smaller \( T_c \) comparing with the rectangular superconductor. These results are similar to our previous study [11].

Figure 3 shows size dependences of \( T_c \) and eigen-energies from the chemical potential \( \xi_k = \varepsilon_k - \mu \). Figure 4 shows order parameter distributions at the sizes of the superconductors (a)-(f) in figure 3. From these results, we can see that drops of \( T_c \) and changes of order parameter distributions occur when one of eigen-energies becomes larger than \( E_c \), as we discussed in previous study [11]. For example, from (a) to (b) in figure 3 (A), drop of \( T_c \) occurs, eigen-energy becomes larger than the cut off energy in figure 3 (B) and order parameter distribution changes from (a) to (b) in figure 4. Next we see changes of order parameter distributions. Figure 5 (a-b) shows a difference between figure 4 (a) and figure 4 (b), figure 5 (b-c) shows a difference between figure 4 (b) and figure 4 (c), and so on. Differences in figures 5 (a-b), 5 (c-d) and 5 (e-f) show distributions of Cooper pairs, which cease to contribute to superconductivity. Differences in figures 5 (b-c) and 5 (d-e) are negligible comparing with other differences in figure 5. This is because these two distribution differences represent concentration of Cooper pairs around center of the superconductor.

In figure 6 and figure 7, we show order parameter distributions and changes of order parameter distributions for the rectangular superconductor, as in figures 4 and 5 for the square superconducting plate. We can see that all of changes of order parameter distributions for the rectangular superconductor in figure 7 has well-ordered peaks. However, changes of order parameter distributions for the square plate in figures 5 (a-b) and 5 (c-d) don’t have such simple structures. These differences come from symmetries of superconductors. Since the rectangular superconductor has two-fold
symmetry, all of order parameter distributions and changes of order parameter distributions have two-fold symmetry. Also superconducting electron states, with same number of peaks in rectangular superconductor, have different eigen-energies when numbers of the peaks along shorter side and longer side are opposite. However, for the square superconductor, such electron states degenerate. Figure 8 (a) shows sum of differences of order parameter distributions in figures 7 (a-b) and 7 (e-f). Figure 8 (b) is a deformation of figure 8 (a) with aspect ratio 1:1. From comparing figure 8 (b) and figure 5 (c-d), we can see that they have same structure. This result shows that two Cooper pair states, with same number of peaks of which number of peaks along shorter side and longer side are opposite, degenerate for the square superconductor because of its four fold-symmetry. Therefore, we can see that the number of cusps of $T_c$ as a function of size of superconductor depends on the symmetry of superconductor. In addition, we expect more symmetric superconductor shows less cusps of $T_c$, because of degeneracy of Cooper pair states.

![Figure 1](image1.png)  
**Figure 1.** The systems of square and rectangular ($L \times 3L$) nano-structured superconducting plates for the FEM

![Figure 2](image2.png)  
**Figure 2.** Size dependence of $T_c$ for square (1) ($S=1$) and rectangular ($L \times 3L$) (2) ($S=3$) nano-structured superconductor with same area. Here $\xi$ is the coherence length at $T=0$.

![Figure 3](image3.png)  
**Figure 3.** Size dependence of $T_c$ (A) and eigen-energies (B) for a square superconductor and size dependence of $T_c$ (C) and eigen-energies (D) for a rectangular ($L \times 3L$) superconductor where $\xi$ is the coherence length at $T=0$. 


Figure 4. Distributions of amplitudes of order parameter $\Delta_0$, for a nano-square superconductor. Where (a)-(f) correspond to the (a)-(f) in figure 3 (A). ($L/\xi = 0.4050$ (a), 0.4040 (b), 0.3920 (c), 0.3915 (d), 0.3815 (e) and 0.3810(f)).

Figure 5. Differences of order parameter distributions, for nano-square superconductor. Figure (a-b), (b-c), (c-d), (d-e) and (e-f) show differences of order parameter distributions between figure 4 (a) and (b), figure 4 (b) and (c) and so on.
Figure 6. Distributions of amplitudes of order parameter $\Delta_0$, for a nano-rectangular $(L \times 3L)$ superconductor. Where (a)-(f) correspond to the (a)-(f) in figure 3 (C). ($L / \xi = 0.3820$ (a), 0.3810 (b), 0.3570 (c), 0.3560 (d), 0.3540 (e), and 0.3530 (f)).

Figure 7. Difference of order parameter distributions for the nano-rectangular $(L \times 3L)$ superconductor. Figure (a-b), (b-c), (c-d), (d-e) and (e-f) show differences of order parameter distributions between figure 6 (a) and (b), figure 6 (b) and (c) and so on.
Figure 8. Sum of differences of order parameter distributions figure 6 (a-b) and figure 6 (e-f), for the nano-rectangular \((L \times 3L)\) superconductor (a). (b) is a deformation of (a) with aspect ratio 1:1.

4. Summary
We have obtained \(T_c\), eigen-energies, and order parameter distributions for superconducting square plates, by solving the Gor’kov equations with the FEM numerically. We have found that characteristic structure of order parameter distributions and changes of order parameter distributions for the superconducting square plate, which are different from those for the rectangular superconductor. These differences come from difference of symmetries of systems, because all of order parameter distributions and changes of order parameter distributions for square and rectangular superconductors have four and two-fold symmetry, respectively. In addition, we have shown that Cooper pair states in square superconductor are degenerate because of the four-fold symmetry.

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