Magnetic flux periodicity in mesoscopic *d*-wave symmetric and asymmetric superconducting loops

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The magnetic flux dependence of energy and supercurrent in mesoscopic d-wave symmetric and asymmetric superconducting loops is investigated by numerically solving the Bogoliubov-de Gennes equations self-consistently. For square loops, we find an hc/e-flux periodicity in energy and supercurrent and demonstrate that the flux periodicity is sensitive to the hole size and the superconducting pairing strength as well as temperature. The $hc/2e$-periodic behavior can be restored almost entirely when we displace the central hole sufficiently out of the center of the sample. In rectangular loops, the discrete current-carrying low-energy spectrum can exist for an odd winding number of the order parameter.

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I. INTRODUCTION

According to the Bardeen-Cooper-Schrieffer theory of superconductivity,[1] the electronic condensate is formed by Cooper pairs, which carry twice the elementary charge. The quantization of magnetic flux in units of $hc/2e$ in multiply connected superconducting geometries is considered as an inevitable consequence of electronic pairing in conventional[2–6] and high-temperature[7] superconductors. Other related phenomena include the $hc/2e$ periodicity of the Little-Parks critical-temperature oscillations with magnetic flux of a superconducting cylinder[8] and the $hc/2e$ flux quantization of Abrikosov vortices.[9]

The requirement of the single valuedness of the superconducting wave function in the presence of a supercurrent implies the periodicity in $hc/2e$. Fundamentally, an important additional condition, which has to be satisfied to ensure the periodicity, is the degeneracy in energy[4–6] of the two distinct classes of supercurrent carrying states. However, this degeneracy can be lifted for discrete systems, and this problem has been investigated recently for a mesoscopic d-wave loop[10] at low temperatures, where the breaking of the $hc/2e$ periodicity, associated with discrete current-carrying low-energy states, was predicted. In fact, for nodal superconductors, such as d-wave superconductors, and s-wave superconductors with small gaps or states in the energy gap, the ground-state energy is generically hc/e periodic. Based on different models, recent studies have shown this effect in mesoscopic conventional[11–13] and d-wave[14–16] superconducting rings or hollow cylinders. In particular, the crossover from hc/e to $hc/2e$ current oscillations in rings of s-wave superconductors has been predicted.[17,18] However, it has remained unaddressed how the magnetic flux periodicity manifests and evolves for d-wave superconducting loops. Moreover, for mesoscopic asymmetric rings of conventional superconductors, the Little-Parks effect and flux-induced vortex states have been found theoretically[19,20] and experimentally.[21] Therefore, one may expect that interesting phenomena related to magnetic flux periodicity in asymmetric d-wave loops may be present.

In the present work, we systematically investigate the energy and supercurrent in mesoscopic d-wave symmetric and asymmetric superconducting loops by solving the Bogoliubov-de Gennes (BdG) equations[22] in a self-consistent manner. This approach has been used before for the investigation of the vortex structure and impurity effects in macroscopic d-wave superconducting systems.[23–26] Our numerical analysis concerns the flux periodicity in symmetric and asymmetric d-wave mesoscopic loops as a function of the hole size and the superconducting pairing strength as well as temperature. We also discuss the periodic oscillation pattern in the case when the hole is displaced from the center of the square loop. Finally, we show the dependence of the discrete current-carrying low-energy states for different winding numbers of the order parameter in rectangular loops.

The paper is organized as follows: in Sec. II, we present our theoretical formalism. The evolution of the energy and supercurrent with magnetic flux for symmetric and asymmetric d-wave loops is discussed in Secs. III and IV, respectively. Our results are summarized in Sec. V.

II. THEORETICAL APPROACH

To investigate the flux periodicity in mesoscopic loops of d-wave superconductors, we start with the pairing Hamiltonian by assuming nearest-neighbor attraction V for d-wave superconducting (DSC) paring

$$H = -\sum_{\langle \mathbf{ij}\rangle,\sigma} t_{\mathbf{ij}} \exp(i\varphi_{\mathbf{ij}}) c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + \sum_{\mathbf{i},\sigma} (-\mu) c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{i}\sigma} + \sum_{\langle \mathbf{ij}\rangle} (\Delta_{\mathbf{ij}} c^{\dagger}_{\mathbf{i}\uparrow} c^{\dagger}_{\mathbf{j}\downarrow} + \Delta^{*}_{\mathbf{ij}} c_{\mathbf{j}\downarrow} c_{\mathbf{i}\uparrow}), \tag{1}$$

where $t_{\mathbf{ij}}=t$ are the nearest-neighbor hopping integral. $c_{\mathbf{i}\sigma}(c^{\dagger}_{\mathbf{i}\sigma})$ are destruction (creation) operators for electron of spin σ, $n_{\mathbf{i}\sigma}=c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{i}\sigma}$ is the number operator, and μ is the chemical potential determining the averaged electron density. The Peierls phase factor is given by $\varphi_{\mathbf{ij}}=2\pi/\Phi_0\int_{r_{\mathbf{i}}}^{r_{\mathbf{j}}}\mathbf{A}(\mathbf{r})\cdot d\mathbf{r}$ with the superconducting flux quantum $\Phi_0=hc/e$. We choose a vector potential of the form $\mathbf{A}(\mathbf{r})=(y,-x,0)\Phi/[2\pi(x^2+y^2)]$, yielding a flux threading the hole with no magnetic field penetrating the superconductor, where $\phi=(e/hc)\Phi$ measures the flux in units of hc/e. The DSC order has the following definition: $\Delta_{\mathbf{ij}}=V\langle c_{\mathbf{i}\uparrow}c_{\mathbf{j}\downarrow}-c_{\mathbf{i}\downarrow}c_{\mathbf{j}\uparrow}\rangle/2$. Using the Bogoliubov transformation, $c_{\mathbf{i}\sigma}=\sum_n[u^n_{\mathbf{i}\sigma}\gamma_{n\sigma}-\sigma v^{n*}_{\mathbf{i}\sigma}\gamma^\dagger_{n\bar{\sigma}}]$, the Hamiltonian in Eq. (1) can be diagonalized by solving the resulting BdG equations self-consistently,

$$\sum_{\mathbf{j}}^{N}\begin{pmatrix}\mathcal{H}_{\mathbf{ij}\sigma} & \Delta_{\mathbf{ij}}\\ \Delta^*_{\mathbf{ij}} & -\mathcal{H}^*_{\mathbf{ij}\bar{\sigma}}\end{pmatrix}\begin{pmatrix}u^n_{\mathbf{j}\sigma}\\ v^n_{\mathbf{j}\bar{\sigma}}\end{pmatrix}=E_n\begin{pmatrix}u^n_{\mathbf{i}\sigma}\\ v^n_{\mathbf{i}\bar{\sigma}}\end{pmatrix}, \tag{2}$$

where $\mathcal{H}_{\mathbf{ij}\sigma}=-t_{\mathbf{ij}}-\mu\delta_{\mathbf{ij}}$. With the open boundary conditions (for which the wave function vanishes on the inner and outer boundaries of the loop) we can get the eigenvalues $\{E_n\}$ with eigenvectors $\{\mathrm{u}^n,\mathrm{v}^n\}$. The order parameter $\Delta_{\mathbf{ij}}$ is calculated self-consistently from

$$\Delta_{\mathbf{ij}}=\sum_n\frac{V}{4}(\mathbf{u}^n_{\mathbf{i}}\mathbf{v}^{n*}_{\mathbf{j}}+\mathbf{v}^{n*}_{\mathbf{i}}\mathbf{u}^n_{\mathbf{j}})\tanh\left(\frac{E_n}{2k_BT}\right). \tag{3}$$

Since the order parameter has to be single valued, the phase difference when circulating the hole once must be $2\pi q$, where q is the winding number. The current density J_{ij} from lattice site i to j is

$$J_{\mathbf{ij}}=-4\frac{et}{\hbar c}\sum_n\mathrm{Im}(\{\mathbf{u}^n_{\mathbf{j}}\mathbf{u}^{n*}_{\mathbf{i}}f(E_n)+\mathbf{v}^{n*}_{\mathbf{j}}\mathbf{v}^n_{\mathbf{i}}[1-f(E_n)]\}\exp(i\varphi_{\mathbf{ij}})), \tag{4}$$

where $f(E)=(e^{E/k_BT}+1)^{-1}$ is the Fermi-Dirac distribution function.

Throughout this work, the distance is measured in units of the lattice constant a, and the energy is scaled to t. In the numerical calculations, we take $k_B=a=t=1$ for simplicity.

III. SYMMETRIC *d*-WAVE LOOPS

First, we consider a symmetric square d-wave loop as schematically shown in the inset of Fig. 1 with a size of $N_x\times N_y=40\times40$ and a centered hole of size $N_{xx}\times N_{yy}=12\times12$. The results of the self-consistent calculations for the eigenenergies below the Fermi energy $E_F=0$ in the gap region are shown in Fig. 1 and the total energy and the total supercurrent (in units of $J_0=et/\hbar c$) at $T=0$ are plotted in Fig. 2 (black solid lines) for chosen pair interaction $V=0.6$. Clearly, two distinct regimes of condensate states with an even and an odd winding number q of the order parameter are found, and the circulating supercurrent oscillates as a function of the magnetic flux with an observable period of $\Phi_0=hc/e$ (which is consistent with the results of Ref. 10). In what follows, we only discuss the flux values between 0 and $hc/2e$, because all quantities for the flux values from $hc/2e$ to hc/e are (anti)symmetric with respect to the flux interval between 0 and $hc/2e$.

The reconstruction of the condensate is the origin of the hc/e periodicity in the ground-state energy and the supercurrent. Some well-separated discrete states close to E_F are present in the regime with $q=0$ due to the nodal character of the order parameter, and the states further away from E_F provide most of the condensation energy (see Fig. 1). Therefore, the main contribution to the supercurrent arises from the occupied levels closest to E_F, since the contributions

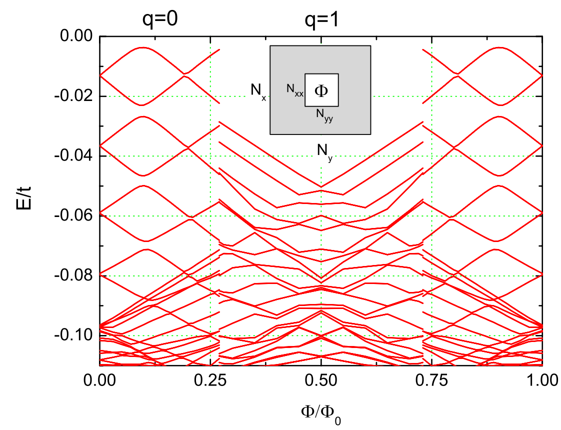

FIG. 1. (Color online) The eigenenergies in the gap region are shown for a square 40×40 loop with a centered 12×12 hole as a function of flux Φ in units of $\Phi_0=hc/e$. The superconducting condensate consists of the states below $E_F=0$ (red lines). The pair interaction is $V=0.6$, and the temperature $T=0$. q is the winding number of the order parameter, and there is a clear difference between condensate states with $q=0$ and $q=1$. The inset shows schematically a two-dimensional square loop with a system size of $N_x\times N_y$ lattice sites and a hole of $N_{xx}\times N_{yy}$ lattice sites, which is threaded by a magnetic flux Φ in the hole.

from the lower-lying states tend to cancel in adjacent pairs.[10] As the highest occupied state shifts with increasing flux to higher energies, the magnitude of supercurrent in the square loop first increases for small flux, then decreases when the level with an orbital moment opposite to the applied magnetic field starts to dominate. As a consequence, a zigzaglike feature of flux-dependent current shows up in the $q=0$ sector [see the black solid line in Fig. 2(b)]. Figure 3 displays the current distribution for the highest occupied level for two different flux values. Comparing both contour plots, we see clearly the effect of the transition in the current-carrying state leading to opposite directions of current.

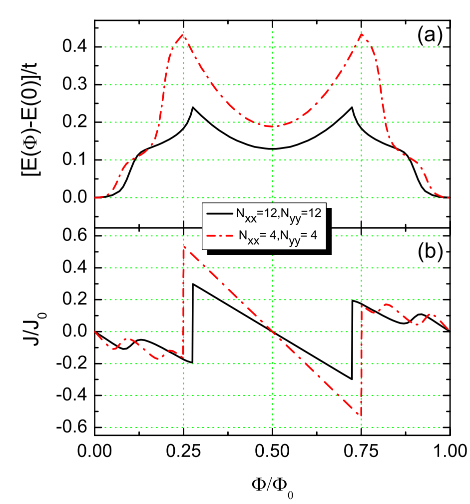

FIG. 2. (Color online) Total energy (a) and total supercurrent (b) for two square 40×40 loops with a centered hole of 12×12 (black solid lines) and 4×4 (red dash-dotted lines) as a function of magnetic flux. The calculation is performed with $V=0.6$ and $T=0$.

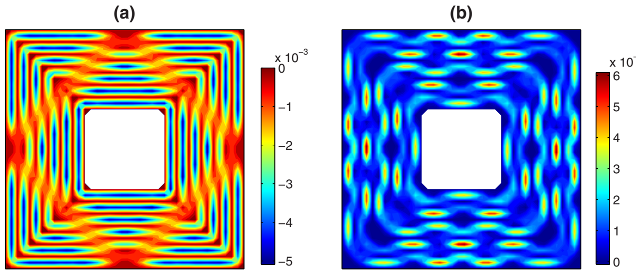

FIG. 3. (Color online) Contour plot of the current distribution for the occupied state closest to $E_F=0$ in a square 40×40 loop with a centered 12×12 hole when $\Phi=0.184hc/e$ (a) and $\Phi=0.195hc/e$ (b).

Remarkably, an abrupt change in levels takes place for a flux value near $hc/4e$, and the condensate state enters the regime with $q=1$, that is, the condensate reconstructs. This reconstruction results from the motion of the center of mass of the Cooper pair, and each pair's center of mass angular momentum is increased by $\hbar$. A considerable empty spectral gap appears in the $q=1$ sector (see Fig. 1), and an alternation of the diamagnetic and paramagnetic response is generated. Notice that there is a small offset in the position of the transition with respect to the flux value $hc/4e$ when changing $q=0$ to $q=1$. For a small superconducting annulus, Vakaryuk[13] recently suggested that the internal energy of the center of mass state leads to this shift. In addition, Fig. 2 (the red dash-dotted lines) and Fig. 4 depict, respectively, the flux periodicity of the energy and supercurrent for a smaller hole of size $N_{xx}\times N_{yy}=4\times4$ and the corresponding energy spectrum. In Fig. 4, we notice a clear large jump in the energy spectrum at $\Phi=hc/4e$ when q changes from $q=0$ to $q=1$. This reconstruction of the condensation energy breaks the $\Phi_0/2$ periodicity in the supercurrent. Furthermore, a more pronounced zigzag oscillation occurs in the $q=0$ sector as a consequence of the Φ derivative of the energy of the highest occupied state.

For a different *d*-wave pairing interation V, the corresponding evolution of the total energy and supercurrent with magnetic flux is plotted in Fig. 5. We find that with increasing V the system evolves toward a state where the supercurrent exhibits $\Phi_0/2$ periodicity. The total energy still reaches a local minimum at $\Phi=hc/2e$ for an enlarged gap regime [$V=1.2$ (red dash-dotted lines)] and the value of this minimum approaches the energy value for $\Phi=0$. Simultaneously, the flux value of the $q\rightarrow q+1$ jump shifts gradually toward $hc/4e$, and the current peaks become more symmetric about the $J=0$ axis. With further increasing V [=2.4 (blue dashed lines)], the system almost shows a $\Phi_0/2$-periodic behavior. We note that the total energy and the supercurrent are not exactly $\Phi_0/2$ periodic due to the energy difference of the $q=0$ and $q=1$ states in finite systems. In addition, the flux dependence of the energy and supercurrent for $V=1.2$ and different temperatures below the critical temperature T_c is displayed in Fig. 6. For a nonzero temperature $T=0.01$ (red dash-dotted lines), one can see that the flux value of the q jump is close to $\Phi=hc/4e$, which leads to an almost $\Phi_0/2$ periodicity of the supercurrent. Note that the Φ_0 periodic behavior of the corresponding total energy is still clearly visible in Fig. 6(a). For a larger temperature $T=0.28$ (blue dashed line), the difference in energy between $\Phi=0$ and $\Phi_0/2$ becomes very small.

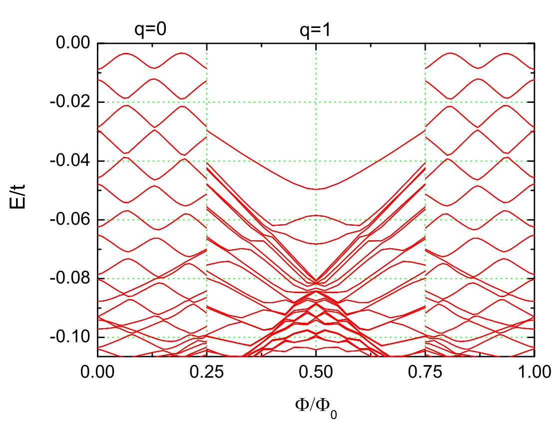

FIG. 4. (Color online) The eigenenergies in the gap region are shown for a square 40×40 loop with a centered 4×4 hole as a function of magnetic flux. Other parameter values are the same as those in Fig. 1.

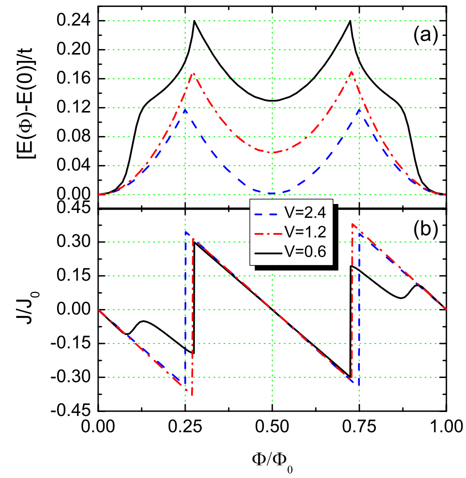

FIG. 5. (Color online) Total energy (a) and total supercurrent (b) for a square 40×40 loops with a centered 12×12 hole and pair interaction $V=0.6$ (black solid line), $V=1.2$ (red dash-dotted line), and $V=2.4$ (blue dashed line) as a function of magnetic flux for $T=0$.

IV. ASYMMETRIC *d*-WAVE LOOPS

In this section, we describe the case of asymmetric *d*-wave loops with the same superconducting surface area as the one in the inset of Fig. 1 and choose the parameter values: $V=0.6$ and $T=0$. In Ref. 20, asymmetric superconducting rings of finite width were investigated for low magnetic fields. It was found that the energy region where metastable states exist decreases with increasing the off-centered distance of the hole. Beyond a critical shift in the hole, the ring continuously transits between different flux states with a continuous energy as function of the magnetic field. Figure 7 shows the evolution of the total energy and supercurrent with magnetic flux for different displacements δN_x of the hole

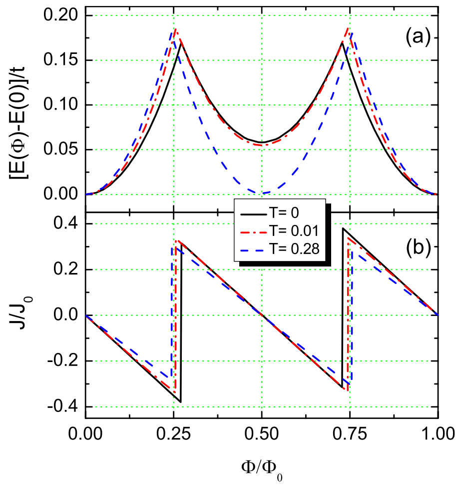

FIG. 6. (Color online) Total energy (a) and total supercurrent (b) for a square 40×40 loop with a centered 12×12 hole and temperature $T=0$ (black solid lines), $T=0.01$ (red dash-dotted lines), and $T=0.28$ (blue dashed lines) as a function of magnetic flux for $V=1.2$.

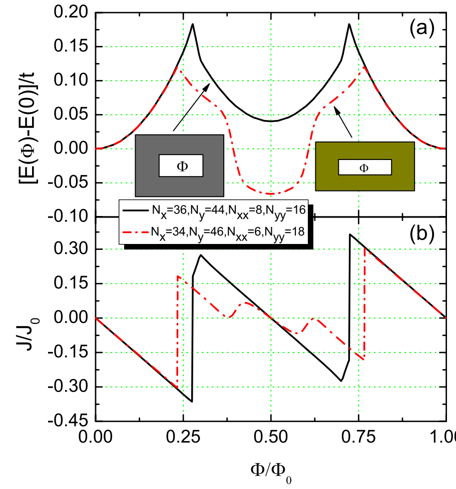

FIG. 8. (Color online) Total energy (a) and total supercurrent (b) for two rectangular loops with $N_x\times N_y=36\times44$, $N_{xx}\times N_{yy}=8\times16$ (black solid lines) and $N_x\times N_y=34\times46$, $N_{xx}\times N_{yy}=6\times18$ (red dash-dotted lines) as a function of magnetic flux. The parameter values are $V=0.6$ and $T=0$. The left and right insets in (a) show a schematic drawing of the two rectangular loops.

from the center of the square loop. With increasing δN_x, the relative total energy as well as the energy difference between the $q=0$ and $q=1$ states reduces, and the deviation from a $\Phi_0/2$-periodic behavior becomes smaller. For some critical displacement the energies at $\Phi=0$ and at $\Phi=\Phi_0/2$ are basically same, then the system looks to have $\Phi_0/2$ periodicity (blue dashed lines). This signifies that a larger displacement of the hole leads to a smaller reconstruction of the energy spectrum of the condensate for different q values.

To understand better the influence of asymmetry on the magnetic flux periodicity, we considered rectangular loops with the same arm width as the square one depicted in the inset of Fig. 1. The evolution of the total energy and supercurrent with magnetic flux for the two different rectangular loops is displayed in Fig. 8. The black solid lines are for the sample [left inset in Fig. 8(a)] with $N_x\times N_y=36\times44$ and $N_{xx}\times N_{yy}=8\times16$, and the red dash-dotted lines for the sample [right inset in Fig. 8(a)] with $N_x\times N_y=34\times46$ and $N_{xx}\times N_{yy}=6\times18$. We find a Φ_0-periodic behavior of the total energy and supercurrent for both loops. Interestingly, the zigzag feature of the supercurrent as function of the flux shows up in the $q=1$ sector for a sufficiently large ratio of length to height N_y/N_x of the rectangular loop [see the dash-dotted line in Fig. 8(b)]. In Fig. 9, the eigenenergies below E_F in the gap region corresponding to the two samples in Fig. 8 are shown. We find a strong transformation of the energy spectrum with increasing N_y/N_x. As a result of the reconstruction of the condensate and the flux-driven change in the quasiparticle subgap states in both cases we find a Φ_0 periodicity. For a small asymmetric ratio [see Fig. 9(a)], the empty energy gap in the $q=1$ regime in Fig. 1 decreases and becomes smaller than that in the $q=0$ regime. Moreover, the highest occupied states show a linear behavior in Φ. By contrast, for a larger asymmetric ratio [see Fig. 9(b)], there exists a large empty energy gap for $q=0$, and well-separated

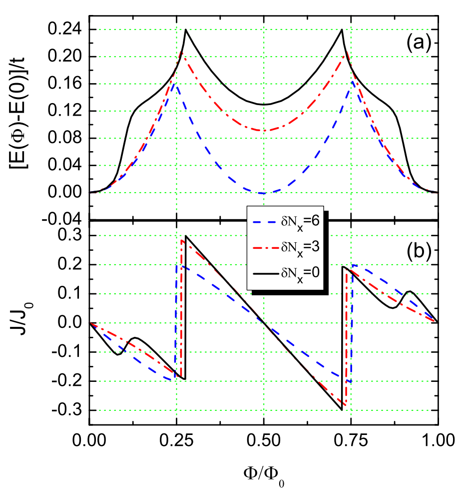

FIG. 7. (Color online) Total energy (a) and total supercurrent (b) for different asymmetric square 40×40 loops with a hole of 12×12 unit cells as a function of magnetic flux. The parameter values are $V=0.6$ and $T=0$. The off-centered distance of the hole is $\delta N_x=0$ (black solid lines), $\delta N_x=3$ (red dash-dotted lines), and $\delta N_x=6$ (blue dashed lines).

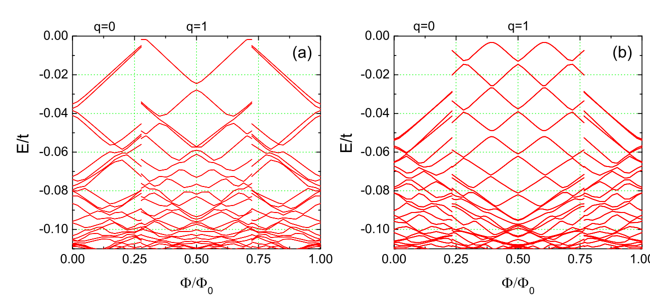

FIG. 9. (Color online) The eigenenergies in the gap region are shown for a rectangular loop with (a) $N_x\times N_y=36\times44$, $N_{xx}\times N_{yy}=8\times16$ and (b) $N_x\times N_y=34\times46$, $N_{xx}\times N_{yy}=6\times18$ as a function of flux. The other parameter values are the same as those in Fig. 1.

discrete low-energy states appear in the $q=1$ regime, where a zigzag character in the flux-dependent supercurrent is obtained. Note that a discrete current-carrying low-energy spectrum can exist only for even winding numbers q of the order parameter in d-wave square loops.

V. CONCLUSIONS

We have investigated the flux dependence of the energy and the supercurrent in symmetric and asymmetric d-wave superconducting loops by numerically solving the BdG equations self-consistently. We found an hc/e-periodic energy and supercurrent due to the reconstruction of the condensate and the flux-driven change in the quasiparticle low-energy states in mesoscopic systems. For square loops, the flux periodicity is sensitive to the hole size and the superconducting pairing strength as well as temperature; the breaking of $hc/2e$ periodicity can be weakened with increasing either pairing strength or temperature. In addition, for an asymmetric square loop, the $hc/2e$-periodic behavior can be restored almost completely for sufficiently large displacement of the hole from the center of the sample. Interestingly, in rectangular loops discrete current-carrying low-energy states can exist for odd winding numbers q of the order parameter.

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[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[2] R. Doll and M. Nabauer, Phys. Rev. Lett. **7**, 51 (1961).
[3] B. S. Deaver and W. M. Fairband, Phys. Rev. Lett. **7**, 43 (1961).
[4] N. Byers and C. N. Yang, Phys. Rev. Lett. **7**, 46 (1961).
[5] L. Onsager, Phys. Rev. Lett. **7**, 50 (1961).
[6] W. Brenig, Phys. Rev. Lett. **7**, 337 (1961).
[7] C. E. Gough, M. S. Colclough, E. M. Forgan, R. G. Jordan, M. Keene, C. M. Muirhead, A. I. M. Rae, N. Thomas, J. S. Abell, and S. Sutton, Nature (London) **326**, 855 (1987).
[8] W. A. Little and R. D. Parks, Phys. Rev. Lett. **9**, 9 (1962).
[9] A. A. Abrikosov, Sov. Phys. JETP **5**, 1174 (1957).
[10] F. Loder, A. P. Kampf, T. Kopp, J. Mannhart, C. W. Schneider, and Y. S. Barash, Nat. Phys. **4**, 112 (2008).
[11] K. Czajka, M. M. Maska, M. Mierzejewski, and Z. Sledz, Phys. Rev. B **72**, 035320 (2005).
[12] T.-C. Wei and P. M. Goldbart, Phys. Rev. B **77**, 224512 (2008).
[13] V. Vakaryuk, Phys. Rev. Lett. **101**, 167002 (2008).
[14] Y. S. Barash, Phys. Rev. Lett. **100**, 177003 (2008).
[15] V. Juričić, I. F. Herbut, and Z. Tešanović, Phys. Rev. Lett. **100**, 187006 (2008).
[16] J.-X. Zhu, arXiv:0806.1084v2 (unpublished).
[17] J.-X. Zhu and Z. D. Wang, Phys. Rev. B **50**, 7207 (1994).
[18] F. Loder, A. P. Kampf, and T. Kopp, Phys. Rev. B **78**, 174526 (2008).
[19] J. Berger and J. Rubinstein, Phys. Rev. Lett. **75**, 320 (1995); Phys. Rev. B **56**, 5124 (1997); **59**, 8896 (1999).
[20] D. Y. Vodolazov, B. J. Baelus, and F. M. Peeters, Phys. Rev. B **66**, 054531 (2002).
[21] A. Kanda, B. J. Baelus, D. Y. Vodolazov, J. Berger, R. Furugen, Y. Ootuka, and F. M. Peeters, Phys. Rev. B **76**, 094519 (2007).
[22] P. G. de Gennes, *Superconductivity of Metals and Alloys* (Addison-Wesley, New York, 1994).
[23] Y. Wang and A. H. MacDonald, Phys. Rev. B **52**, R3876 (1995).
[24] J.-X. Zhu, I. Martin, and A. R. Bishop, Phys. Rev. Lett. **89**, 067003 (2002).
[25] Y. Chen and C. S. Ting, Phys. Rev. Lett. **92**, 077203 (2004).
[26] G. Q. Zha, H. W. Zhao, and S. P. Zhou, Phys. Rev. B **76**, 132503 (2007).