Mechanisms of spontaneous current generation in an inhomogeneous *d*-wave superconductor

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A boundary between two *d*-wave superconductors or an *s*-wave and a *d*-wave superconductor generally breaks time-reversal symmetry and can generate spontaneous currents due to proximity effect. On the other hand, surfaces and interfaces in *d*-wave superconductors can produce localized current-carrying states by supporting the $\mathcal{T}$-breaking combination of dominant and subdominant order parameters. We investigate spontaneous currents in the presence of both mechanisms and show that at low temperatures, counterintuitively, the subdominant coupling *decreases* the amplitude of the spontaneous current due to the proximity effect. Superscreening of spontaneous currents is demonstrated to be present in any ideal d-d (but not s-d) junction and surface with $d+id'$ order parameter symmetry. We show that this superscreening is the result of contributions from the local magnetic moment of the condensate to the spontaneous current.

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The time-reversal symmetry ($\mathcal{T}$) breaking on surfaces and interfaces of superconductors with *d*-wave orbital pairing has been intensively investigated in the last years both in theory and experiment.[1–8] Several mechanisms of $\mathcal{T}$ breaking have been proposed, which fall in two categories: appearance of the subdominant order parameter and proximity effect.[2,3]

In the first case the surface or interface suppresses the dominant order parameter [$d_{x^2-y^2}$ in Y-Ba-Cu-O (Ref. 4)]. If the pairing interaction in other channels is nonzero, the subdominant order parameter will be formed below the corresponding, smaller critical temperature T_{c2}.[9] The combination of the two order parameters with complex coefficients breaks the $\mathcal{T}$ symmetry[1] and leads to spontaneous surface currents and magnetic fluxes. Usually $d_{x^2-y^2}\pm is$ or $d_{x^2-y^2}\pm id_{xy}$ combinations are predicted. Recent observations of zero-bias peak splitting in surface tunneling experiments[5] and spontaneous fractional flux [$(0.1–0.2)\Phi_0$] near the ''green phase'' inclusions in Y-Ba-Cu-O films[6] agree with this picture.

The other possibility arises in a junction between two *d*-wave superconductors with different orientations of the order parameter.[7] In this case the two order parameters necessary to form a $\mathcal{T}$-breaking state, $d_{1,2}$, are supplied by the bulk superconductors. The equilibrium phase difference across the boundary, ϕ_0, is generally neither 0 nor π, and therefore the states with $d_1+e^{\pm i\phi_0}d_2$ orderings are degenerate and may support spontaneous currents. The same mechanism applies in case of a boundary between an *s*- and a *d*-wave superconductor.[8]

In order to investigate the interplay of both mechanisms, in this paper we consider d-d and s-d interfaces as well as (110) surfaces of a *d*-wave superconductor. We will see that generally the spontaneous currents due to the proximity effect are suppressed by the existence of the subdominant order parameter. There is also an important distinction between the d-d and s-d cases: In the former case the superconductor may have local orbital and magnetic moments, contributing to the nondissipative current. In the latter case such a contribution is absent. Our results indicate that in an ideal d-d junction (i.e., a junction with perfect transparency and no roughness), all of the spontaneous current can be attributed to this ''molecular current'' mechanism. We also show that this effect leads to a ''superscreening'' of spontaneous currents in d-d junctions (i.e., to the existence of countercurrents independent of the Meissner effect).

We use the standard approach based on quasiclassical Eilenberger equations for Green's functions integrated over energy,[10]

$$\mathbf{v}_F\cdot\nabla\hat{G}_\omega+[\omega\hat{\tau}_3+\hat{\Delta},\hat{G}_\omega]=0, \tag{1}$$

where ω is the Matsubara frequency and

$$\hat{G}_\omega(\mathbf{v}_F,\mathbf{r})=\begin{pmatrix} g_\omega & f_\omega \\ f_\omega^\dagger & -g_\omega \end{pmatrix},\qquad \hat{\Delta}(\mathbf{v}_F,\mathbf{r})=\begin{pmatrix} 0 & \Delta \\ \Delta^\dagger & 0 \end{pmatrix}.$$

Here $\hat{G}_\omega$ is the matrix Green's function and Δ is the superconducting order parameter. They both are functions of Fermi velocity $\mathbf{v}_F$ and position $\mathbf{r}$. We also need to satisfy the normalization condition $g_\omega=\sqrt{1-f_\omega f_\omega^\dagger}$. In general, Δ depends on the direction of the vector $\mathbf{v}_F$ and is determined by the self-consistency equation

$$\Delta(\mathbf{v}_F,\mathbf{r})=2\pi N(0)T\sum_{\omega>0}\langle V_{\mathbf{v}_F\mathbf{v}_F'}f_\omega(\mathbf{v}_F',\mathbf{r})\rangle_\theta, \tag{2}$$

where $V_{\mathbf{v}_F\mathbf{v}_F'}$ is the interaction potential. In our calculations we will consider two dimensions (2D); $N(0)=m/2\pi$ is 2D density of states and $\langle\cdots\rangle_\theta=\int_0^{2\pi}d\theta/2\pi\cdots$ is the averaging over directions of the 2D vector $\mathbf{v}_F=(v_F\cos\theta, v_F\sin\theta)$. Generally, it is possible to obtain a mixture of different symmetries of the order parameter, $\Delta(\theta)=\Delta_{x^2-y^2}(\theta)+\Delta_{xy}(\theta)+\Delta_s$, where $\Delta_{x^2-y^2}(\theta)=\Delta_1\cos 2\theta$, $\Delta_{xy}(\theta)=\Delta_2\sin 2\theta$, and Δ_s are the $d_{x^2-y^2}$, d_{xy}, and *s*-wave components of the order parameter, respectively. The corresponding interaction potential $V_{\theta\theta'}=V_{d1}\cos 2\theta\cos 2\theta'+V_{d2}\sin 2\theta\sin 2\theta'+V_s$ must be substituted in the self-consistency equation (2) for the order parameter in each channel. The current density $\mathbf{j}(\mathbf{r})$ is found from the solution of the matrix equation (1) as

$$\mathbf{j}(\mathbf{r})=-4\pi ieN(0)T\sum_{\omega>0}\langle \mathbf{v}_F g_\omega(\mathbf{v}_F,\mathbf{r})\rangle_\theta . \tag{3}$$

Here we consider three cases: (i) the boundary between two semi-infinite d-wave superconductors with crystallographic orientations with respect to the boundary given by angles χ_l and χ_r (''d-d interface''), (ii) boundary between an s-wave and a d-wave superconductor with 45° orientation (''45° s-d interface''), and (iii) (110) surface of a d-wave superconductor. In all three cases it is possible to have a time-reversal symmetry-breaking ground state. The direction and magnitude of the spontaneous current depend on the relative phases of the order parameters.

Assuming constant order parameters on both sides of an ideal interface, one can obtain an analytical (non-self-consistent) expression for the current density:

$$\mathbf{j}(x)=4\pi eN(0)T\sin\phi \times\sum_{\omega>0}\left\langle \frac{\mathbf{v}_F\Delta_l\Delta_r\,\mathrm{sign}(\cos\theta)}{\Omega_l\Omega_r+\omega^2+\Delta_l\Delta_r\cos\phi}e^{-2|x|\Omega_r/|v_F\cos\theta|}\right\rangle_\theta , \tag{4}$$

where l (r) labels left (right) side of the interface, and $\Omega_i=\sqrt{\omega^2+|\Delta_i|^2}$. This expression is valid for arbitrary symmetry of the order parameters $\Delta_{l,r}$. For a d-d interface we have $\Delta_l=\Delta_0(T)\cos 2(\theta-\chi_l)$ and $\Delta_r=\Delta_0(T)\cos 2(\theta-\chi_r)$, where $\Delta_0(T)$ depends on the superconducting coupling and temperature.

We perform our numerical calculations using the Schopohl-Maki parametrization of the Green's functions,[11]

$$g=\frac{1-aa^\dagger}{1+aa^\dagger},\quad f=\frac{2a}{1+aa^\dagger},\quad f^\dagger=\frac{2a^\dagger}{1+aa^\dagger},$$

which transforms Eq. (1) into

$$\mathbf{v}_F\cdot\nabla a=2\omega a-\Delta^* a^2+\Delta, \tag{5}$$

$$-\mathbf{v}_F\cdot\nabla a^\dagger=2\omega a^\dagger-\Delta a^{\dagger 2}+\Delta^*. \tag{6}$$

For positive v_x, Eq. (5) [Eq. (6)] is stable if the boundary condition at $x\to-\infty$ $[+\infty]$ is chosen. The opposite is true for negative v_x. We use the solutions in a homogeneous system, $a=\Delta/(\omega+\Omega)$ and $a^\dagger=\Delta^*/(\omega+\Omega)$, as boundary conditions at $\pm\infty$. The values of a ($a^\dagger$) at all other points on the trajectory are then easily found. The self-consistency is introduced through iterations, assuming a constant order parameter in either half of the junction for the first iteration.

Figure 1(a) shows the spatial distribution of the spontaneous current in ideal d-d and s-d junctions. The left superconductor is a d-wave superconductor with 45° crystal orientation with respect to the boundary. The right side is either an s-wave or a d-wave superconductor aligned with the boundary. The current distribution is qualitatively different in s-d and d-d junctions. In the d-d case, the current density

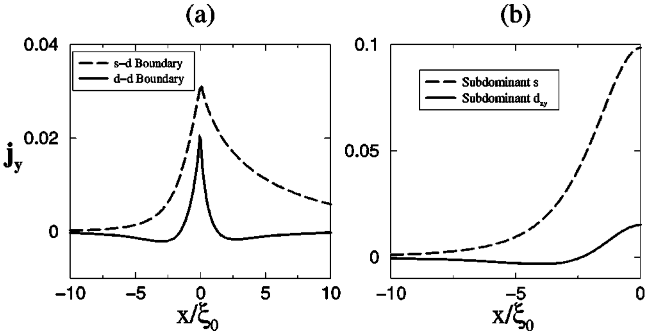

FIG. 1. (a) Spontaneous current for ideal d-d and s-d junctions. The boundary is located at $x=0$. Calculations are done at $t\equiv T/T_c=0.05$, with $T_{c2}=0.05T_c$ for the d-d case and $T_{cs}=0.1T_c$ and $T_{c2}=0.05T_c$ for the s-d junction. (b) Spontaneous current at the (110) surface of a d-wave superconductor at $t=0.05$ with $T_{c2}=T_{cs}=0.1T_c$ for both s or d_{xy} subdominant order parameters.

is at maximum in a layer of width of about coherence length, $\xi_0=v_F/\pi\Delta$, along the boundary; there also exists a counterflow, spread over about $10\xi_0$ on either side of the boundary. The total current in the y direction is zero within the numerical accuracy, on the right and left sides of the junction, *independently*. This effect can be called ''superscreening,'' since the resulting magnetic field of the spontaneous current is canceled on the scale of $\sim 10\xi_0 \ll \lambda_L,\lambda_J$, the London and Josephson magnetic penetration depths. Note that this has nothing to do with the Meissner screening; it appears without taking into account the vector potential of the magnetic field of the current (and makes it unnecessary).[12] On the contrary, in the s-d junction the counterflows are absent (unless the Meissner effect is taken into account[8]).

The same situation takes place near the surface, *if* the subdominant pairing is present. Figure 1(b) shows the current distribution at the (110) surface of a d-wave superconductor. If d_{xy} is the leading subdominant order parameter, the form of the current distribution is similar to the one in the d-d boundary. The superscreening is absent if the subdominant order parameter is s wave.

The superscreening effect can be obtained analytically from the non-self-consistent expression (4) in case of a 0°–45° junction. The nullification of the total current results from integrating the spontaneous current,

$$\int_0^\infty dx\, j_y(x)\propto\left\langle \frac{\Delta_l\Delta_r\sin\theta\,\mathrm{sign}(\cos\theta)}{\Omega_l\Omega_r+\omega^2+\Delta_l\Delta_r\cos\phi}\,\frac{v_F|\cos\theta|}{\Omega_r}\right\rangle_\theta \sin\phi,$$

which is zero after angle averaging. Our numerical calculations, however, show that in ideal boundary junctions the total current is zero (within the numerical accuracy) even after self-consistent calculations and at all other misorientation angles [see Fig. 2(a)].

To understand the situation, let us recall that in a system with local magnetic moment density $\mathbf{m}(\mathbf{r})$ the ''molecular currents'' flow with density $\mathbf{j}(\mathbf{r})=c\nabla\times\mathbf{m}(\mathbf{r})$. In a superconductor with order parameter $d_{x^2-y^2}+e^{i\phi_0}d_{xy}$ the local orbital and magnetic moment density

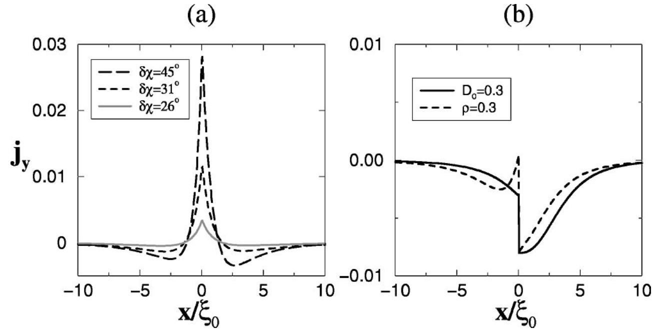

FIG. 2. (a) Spontaneous currents for ideal ($0°-\delta\chi$) junctions with different misorientation angles $\delta\chi$. (b) Spontaneous current at imperfect (0°–45°) junctions. Solid line: junction with transparency $D_0=0.3$. Dashed line: junction with roughness $\rho=0.3$. All calculations are done at $t=0.1$.

$$\mathbf{m}(\mathbf{r})\propto\hat{\mathbf{z}}\int_0^{2\pi}\frac{d\theta}{2\pi}[\Delta_1(x)\cos 2\theta+\Delta_2(x)e^{-i\phi_0}\sin 2\theta]$$
$$\times\frac{1}{i}\frac{\partial}{\partial\theta}[\Delta_1(x)\cos 2\theta+\Delta_2(x)e^{i\phi_0}\sin 2\theta]$$
$$=2\Delta_1(x)\Delta_2(x)\hat{\mathbf{z}}\sin\phi_0 .$$

The contribution to the spontaneous current is thus $\mathbf{j}(\mathbf{r})\propto\nabla\times\mathbf{m}(\mathbf{r})\|\hat{\mathbf{y}}$. Notice that the same expression is obtained from the Ginzburg-Landau equations[13] ($\mathbf{j}\propto\nabla\times[\hat{z}\,\mathrm{Im}\,d_1(\mathbf{r})d_2(\mathbf{r})^*]$). The total current in the y direction due to this mechanism is $I_{\text{total}}\propto\int_\Omega d\mathbf{S}\cdot\nabla\times\mathbf{m}=\oint_{\partial\Omega}d\mathbf{l}\cdot\mathbf{m}=0$, where Ω is a cross section perpendicular to the junction from $x=-\infty$ to ∞ and $\partial\Omega$ is its boundary. The latter integral is obviously zero because $d\mathbf{l}\cdot\mathbf{m}=0$ ($\mathbf{m}\|\hat{\mathbf{z}}$) everywhere except where the contour closes ($x=\pm\infty$), but there $\mathbf{m}=0$. This is certainly not the case in s-d junctions (cf. Fig. 1). (Of course, since the Meissner currents must be taken into account in this case, the results presented in Fig. 1 are valid only for distances much less than the London penetration depth.)

We also calculate the spontaneous current for an imperfect boundary, i.e., a boundary with arbitrary transparency $0<D_0<1$ and also with finite roughness ρ. We use Zaitsev's boundary condition[14,15] to incorporate the finite-transparency effect. For surface roughness we assume a thin layer with scattering centers at the junction.[16] We take the mean free path l and the layer thickness d to zero while keeping $\rho\equiv d/l$ finite. The details of the calculations will be given in a separate publication. Here we only present the results of our calculation for asymmetric (0°–45°) d-d junction in Fig. 2(b). As is clearly seen, the spontaneous current now does not necessarily have a counterflow (at small ρ or $D_0\approx 1$ there will be some counterflow), and exact superscreening no longer takes place. They are now carried merely by Andreev bound states at the interface, the same as in s-d or SND (Ref. 8) junctions.

Although near realistic surfaces and interfaces with d-d ordering the superscreening is not complete, the magnetic fields created by the spontaneous currents are nevertheless suppressed on very short distances. This can be practically important for attempting to build a "quiet" qubit based on such junctions.[17]

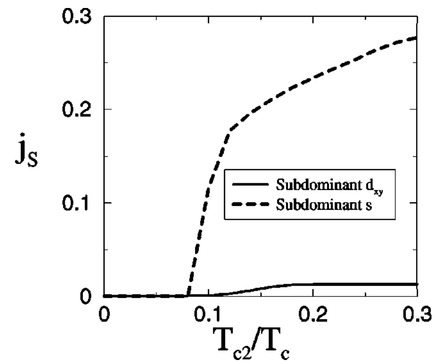

FIG. 3. The effect of subdominant interaction on the spontaneous current j_S [$\equiv j_y(x=0)$] at the surface of a d-wave superconductor. A second-order phase transition happens at $T_{c2}=T=0.1T_c$.

Figure 3 presents the spontaneous current as a function of the subdominant critical temperature T_{c2} at the (110) surface of a d-wave suprconductor. One notices that the spontaneous current vanishes when $T_{c2}<T$. In fact, at temperatures below $T=T_{c2}$ the subdominant order parameter starts to appear at the surface through a second-order phase transition. Spontaneous symmetry breaking and generation of the spontaneous current are the consequences of the emergence of this second-order parameter. The symmetry of the subdominant order parameter is dictated by whichever channel (s or d_{xy}) has a stronger interaction potential.

In the d-d and s-d interfaces, on the other hand, the subdominant order parameter is induced by the proximity to a different superconductor. One important difference is that unlike the surface case, at the d-d or s-d interfaces the presence of the subdominant order parameter is not necessary for generation of spontaneous current. From Eqs. (3) and (1) we see that it is the Green's function (the pairing *amplitude*), not the order parameter (pairing *potential*), which determines the current. In fact, the presence of a subdominant order parameter does not always increase the spontaneous current. At low temperatures, it actually *decreases* the spontaneous current.[18] This counterintuitive effect is displayed in Fig. 4 in

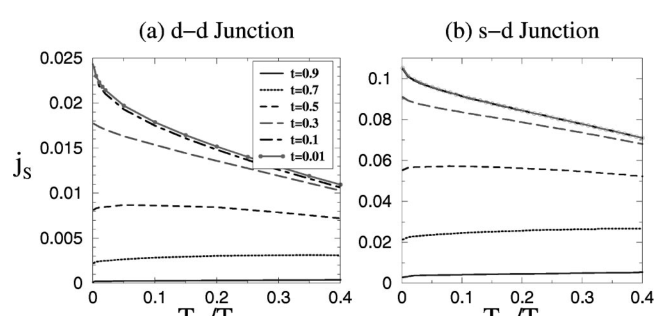

FIG. 4. Suppression of spontaneous current by subdominant order parameter. (a) A d-d grain boundary. (b) An s-d interface. In the s-d case, we have taken the same T_c for both sides and also $T_{cs}=T_{c2}$.

which the spontaneous current is plotted as a function of T_{c2}. The temperature used in the calculations is $t=0.1$ and we take the same T_c for both *d*- and *s*-wave superconductors. Increasing T_{c2} increases the interaction in the subdominant channel and therefore the magnitude of the subdominant order parameter. The spontaneous current on the other hand decreases with increasing T_{c2}. The situation is the same for both d-d and s-d interfaces.

The decrease of the spontaneous currents when there is interaction in the subdominant channel may seem paradoxical. Nevertheless, it is easy to understand in the DND model of $\mathcal{T}$-breaking junctions[8,19] (Fig. 5). First consider the case without subdominant order parameters. The spontaneous currents in this model flow exclusively within the normal layer and are carried by ''zero'' and ''π'' Andreev bound states, which connect the lobes of the *d*-wave order parameter with the same and opposite signs, respectively: in equilibrium there is no net current across the boundary. Now let us assume that the subdominant order parameters are present. Due to continuity, they must have the same phase as the dominant order parameter on the other side (Fig. 5). Therefore now we will have two extra sets of current-carrying Andreev states, the ones linking the *subdominant* order parameters, and it is obvious that the spontaneous currents they carry will always flow opposite to the currents carried by the ''dominant-dominant'' states.

In conclusion, we have investigated the spontaneous currents near the surface and d-d and s-d boundaries in *d*-wave superconductors. We obtained the contributions to the spontaneous currents due to the proximity effect and due to the subdominant order parameter generation, and found that at interfaces the latter generally decreases the magnitude of the effect. In d-d junctions, we separated the contribution from the local orbital and magnetic moment of the condensate; this contribution dominates spontaneous currents in ideal d-d junctions, which explains the superscreening of the spontaneous currents in such systems.

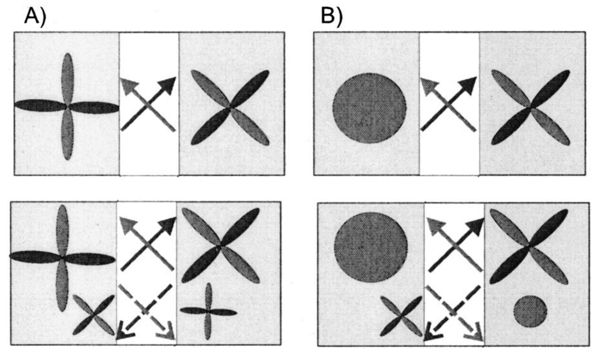

FIG. 5. The DND and SND model of a $\mathcal{T}$-breaking junction. (a) DND junction. The normal region contains current-carrying Andreev bound states (arrows); in equilibrium the net current across the boundary is zero, while the spontaneous currents flow along the normal layer (above). If the subdominant order parameter is present, the additional set of Andreev levels in equilibrium carries spontaneous current in the opposite direction (below). The model gives the same predictions for the SND case (b).

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[1] M. Sigrist, Prog. Theor. Phys. **99**, 899 (1998).
[2] M. Fogelström and S.-K. Yip, Phys. Rev. B **57**, R14 060 (1998).
[3] T. Löfwander, V.S. Shumeiko, and G. Wendin, Phys. Rev. B **67**, R14 653 (2000).
[4] I. Iguchi *et al.*, Phys. Rev. B **62**, R6131 (2000).
[5] M. Covington *et al.*, Phys. Rev. Lett. **79**, 277 (1997); L.H. Greene *et al.*, Physica B **280**, 159 (2000).
[6] F. Tafuri and J.R. Kirtley, Phys. Rev. B **62**, 13 934 (2000).
[7] S. Yip, J. Low Temp. Phys. **91**, 203 (1993); T.P. Devereaux and P. Fulde, Phys. Rev. B **47**, 14 638 (1993); Y. Tanaka, Phys. Rev. Lett. **72**, 3871 (1994).
[8] A. Huck, A. van Otterlo, and M. Sigrist, Phys. Rev. B **56**, 14 163 (1997).
[9] E.M. Lifshits and L.P. Pitaevskii, *Statistical Physics* (Pergamon, Oxford, 1980), Sec. 54, p. 2.
[10] G. Eilenberger, Z. Phys. **214**, 195 (1968).
[11] N. Schopohl and K. Maki, Phys. Rev. B **52**, 490 (1995); N. Schopohl, cond-mat/9804064 (unpublished).
[12] A similar distribution of spontaneous current density on (110) surfaces and interfaces of *d* superconductors was obtained in Ref. 2 [Fig. 4(a)].
[13] D.B. Bailey, M. Sigrist, and R.B. Laughlin, Phys. Rev. B **55**, 15 239 (1997).
[14] A.V. Zaitsev, Zh. Eksp. Teor. Fiz. [Sov. Phys. JETP **59**, 1015 (1984)].
[15] S.-K. Yip, J. Low Temp. Phys. **109**, 547 (1997).
[16] A.N. Omelyanchouk, R. deBruyn Ouboter, and C.J. Muller, Low Temp. Phys. **20**, 398 (1994); A.A. Golubov and M.Yu. Kupriyanov, Pis'ma Zh. Eksp. Teor. Fiz. **69**, 247 (1999) [JETP Lett. **69**, 268 (1999)].
[17] L.B. Ioffe *et al.*, Nature (London) **398**, 679 (1999).
[18] Subdominant pairing potential also suppresses the Josephson current. See Y. Tanaka and S. Kashiwaya, Phys. Rev. B **58**, 2948 (1998).
[19] A.M. Zagoskin, J. Phys.: Condens. Matter **9**, L419 (1997).