physica status solidi

www.interscience.wiley.com

reprints

www.pss-rrl.com

www.pss-c.com

www.pss-b.com

www.pss-a.com

WILEY-VCH

REPRINT

Phys. Status Solidi B **246**, No. 5, 985–988 (2009) / **DOI** 10.1002/pssb.200881552

physica status solidi b
www.pss-b.com
basic solid state physics

Electron pair current through the correlated quantum dot

T. Domański*and A. Donabidowicz

Institute of Physics, M. Curie-Skłodowska University, 20-031 Lublin, Poland

Received 31 August 2008, revised 18 January 2009, accepted 19 January 2009
Published online 3 April 2009

PACS 72.15.Qm, 73.23.–b, 73.63.Kv

* Corresponding author: e-mail doman@kft.umcs.lublin.pl, Phone: +48 81 537 62 35, Fax: +48 81 537 61 91

We study the charge current transmitted through the correlated quantum dot characterized by a finite magnitude of the Coulomb interaction $|U|$. At low temperatures the correlations can lead to a formation of the spin (for $U > 0$) or charge (for $U < 0$) Kondo states which qualitatively affect the transport properties. We explore the influence of charge Kondo effect on the electron pair tunneling introducing the auxiliary two-channel model accounting for the fluctuations between the empty and doubly occupied states on QD.

1 Introduction Electronic transport through the correlated quantum dots (QDs) has recently attracted a considerable interest both from a point of view of fundamental research as well as practical applications [1]. Both these aspects are possible because of a large degree of flexibility for adjusting a coupling of QD to the external leads and a controlled positioning of the quantized QD levels by the gate voltage.

Among the most interesting achievements, there has been obtained an equivalent of the many-body Kondo effect [2] earlier known in the solid state physics [3]. At sufficiently low temperatures $T < T_K$ (where T_K denotes the, so called, Kondo temperature) the spin of QD combines a singlet state with the spins of itinerant electrons from the leads. In consequence the QD spectrum develops a narrow resonance at the chemical potential which enhances the low bias conductance up to the perfect unitary limit value $2e^2/h$ [2]. On a microscopic level the underlying Kondo physics arises from effective an antiferromagnetic interaction between the QD and mobile electrons as envisaged by Schrieffer and Wolf within the perturbative canonical transformation [4].

Recently several authors [5,6] have pointed out that molecular quantum dots affected by the bosonic degrees of freedom such as e.g. phonons could show up (besides the side-band structure) signatures of the charge Kondo effect. This phenomenon has been previously theoretically predicted for the heavy fermion compounds [7] and it might occur when the bipolaronic shift lowers the charging energy to a negative value $U < 0$. The essential physics involved in the charge Kondo effect relies on a neutralization of the electron pair charge at the negative U center (in the present context on QD) by electrons (or holes) from the adjacent leads. Due to a preferred double occupancy of QD there is activated a mechanism of the electron pair tunneling which manifests the qualitative features of charge Kondo effect in the differential conductance [6,8] and in the thermopower [9].

In what follows we propose a phenomenological two-channel model which allows for a simple description of charge tunneling under the circumstances when the empty $|0\rangle$ and doubly occupied $|\uparrow\downarrow\rangle$ states are degenerate (being the necesary condition for realization of the charge Kondo effect [5–7]). We discuss some preliminary results obtained for the QD spectral function and the differential conductance in the symmetric case using an approximate treatment for the on-dot correlations.

2 The spin versus charge Kondo effects For a description of charge tunneling through the single level correlated quantum dot we use the Anderson model [3]

$$\hat{H} = \sum_{\mathbf{k},\beta,\sigma} \xi_{\mathbf{k}\beta} \hat{c}^{\dagger}_{\mathbf{k}\beta\sigma} \hat{c}_{\mathbf{k}\beta\sigma} + \sum_{\mathbf{k},\beta,\sigma} \left(V_{\mathbf{k}\beta} \hat{d}^{\dagger}_{\sigma} \hat{c}_{\mathbf{k}\beta\sigma} + V^{*}_{\mathbf{k}\beta} \hat{c}^{\dagger}_{\mathbf{k}\beta\sigma} \hat{d}_{\sigma} \right) + \hat{H}_{\rm QD}, \tag{1}$$

$$\hat{H}_{\rm QD} = \sum_{\sigma} \varepsilon_d \, \hat{d}^{\dagger}_{\sigma} \hat{d}_{\sigma} + U \, \hat{d}^{\dagger}_{\uparrow} \hat{d}_{\uparrow} \, \hat{d}^{\dagger}_{\downarrow} \hat{d}_{\downarrow}. \tag{2}$$

Operators $\hat{c}^{(\dagger)}_{\mathbf{k}\beta\sigma}$ correspond to annihilation (creation) of electrons in the left $\beta=L$ or right h.s. $\beta=R$ lead. The energies $\xi_{\mathbf{k}\beta\sigma}=\epsilon_{\mathbf{k}\sigma}-\mu_\beta$ are measured with respect to the chemical potentials which under nonequilibrium conditions can be shifted by an applied bias V through $\mu_L-\mu_R=eV$. The other terms containing $V^{(*)}_{\mathbf{k}\beta}$ describe hybridization of the QD to external leads. As usually in (2) $\hat{d}^{(\dagger)}_\sigma$ denote the annihilation (creation) of electron at the QD energy level ε_d and U is the on-dot Coulomb potential.

Let us first start by focusing on a widely studied case of the repulsive charging energy $U>0$. Conditions necesarry for a formation of the Kondo effect can be explained using a perturbative treatment for the hybridization term $\hat{H}_{hyb} = \sum_{\mathbf{k},\beta,\sigma}[V_{\mathbf{k}\beta}\hat{d}^\dagger_\sigma\hat{c}_{\mathbf{k}\beta\sigma}+h.c.]$. Unitary transformation $\hat{\tilde{H}}=e^{\hat{A}}\hat{H}e^{-\hat{A}}$ with the antihermitean generating operator $\hat{A}=\hat{\mathcal{A}}-\hat{\mathcal{A}}^\dagger$ where $\hat{\mathcal{A}}=\sum_{\mathbf{k},\beta,\sigma}\frac{V_{\mathbf{k}\beta}}{\varepsilon_d-\xi_{\mathbf{k}\beta}}\left[\frac{U}{\varepsilon_d+U-\xi_{\mathbf{k}\beta}}\hat{d}^\dagger_{-\sigma}\hat{d}_{-\sigma}-1\right]\hat{c}^\dagger_{\mathbf{k}\beta\sigma}\hat{d}_\sigma$ eliminates $\hat{H}_{hyb}$ up to the quadratic terms [4]. Since for $U>0$ the double occupancy of QD is energetically expensive we can restrict to a subspace of the singly occupied states when transformed Hamiltonian reduces to the spin Kondo model [4]

$$\hat{\tilde{H}}^{\text{Kondo}}_{\text{spin}} = \sum_{\mathbf{k},\beta,\sigma}\xi_{\mathbf{k}\beta}\hat{c}^+_{\mathbf{k}\beta\sigma}\hat{c}_{\mathbf{k}\beta\sigma} - \sum_{\mathbf{k},\mathbf{q},\beta,\beta'} J^{\beta,\beta'}_{\mathbf{k},\mathbf{q}}\ \hat{\mathbf{S}}_d\cdot\hat{\mathbf{S}}_{\mathbf{k}\beta,\mathbf{q}\beta'}. \tag{3}$$

The QD spin operator $\hat{\mathbf{S}}_d$ can be conveniently expressed through $\hat{S}^+_d=\hat{d}^\dagger_\uparrow\hat{d}_\downarrow$, $\hat{S}^-_d=\hat{d}^\dagger_\downarrow\hat{d}_\uparrow$, and $\hat{S}^z_d=\frac{1}{2}(\hat{d}^\dagger_\uparrow\hat{d}_\uparrow-\hat{d}^\dagger_\downarrow\hat{d}_\downarrow)$ and similarly $\hat{S}^+_{\mathbf{k}\beta,\mathbf{q}\beta'}=\hat{c}^\dagger_{\mathbf{k}\beta\uparrow}\hat{c}_{\mathbf{q}\beta\downarrow}$ etc. Near the Fermi surface the effective coupling $J^{\beta,\beta'}_{\mathbf{k},\mathbf{q}}$ simplifies to [4] $J^{\beta,\beta'}_{\mathbf{k}_F,\mathbf{k}_F}=\frac{U}{\varepsilon_d(\varepsilon_d+U)}\ V_{\mathbf{k}_F\beta}V^*_{\mathbf{k}_F\beta'}$. In the regime of antiferromagnetic coupling $J^{\beta,\beta'}_{\mathbf{k}_F,\mathbf{k}_F}<0$ and at sufficiently low temperatures $T<T_K$ the magnetic moment of QD is perfectly screened by spins of the itinerant electrons. For typical QDs the value of Kondo temperature $T_K\simeq\frac{\sqrt{U\Gamma}}{2}\exp\left\{\frac{\pi\varepsilon_d(\varepsilon_d+U)}{U\Gamma}\right\}$ (where $\Gamma\simeq 2\pi\sum_\beta|V_{\mathbf{k}_F\beta}|^2\rho_\beta(\varepsilon_F)$ is the electrodes' density of states at the Fermi level) is of the order of hundreds mK. Appearance of such resulting Kondo resonance pinned at the electrodes' chemical potentials leads to enhancement of the zero bias conductance which has been confirmed experimentally [2].

Formally in the negative U model the canonical transformation can be done in the same way. However, since the empty and doubly occupied QD states are energetically more favorable therefore one has to focus mainly on the terms describing pair tunneling [6]

$$\sum_{\mathbf{k},\mathbf{q},\beta,\sigma,\sigma'}\left(J^{\beta,\beta'}_{\mathbf{k},\mathbf{q}}\ \hat{d}^\dagger_\sigma\hat{d}^\dagger_{-\sigma}\hat{c}_{\mathbf{k}\beta-\sigma'}\hat{c}_{\mathbf{q}\beta'\sigma'}+\text{h.c.}\right).$$

Taraphder and Coleman [7] have shown that in the symmetric case $\varepsilon_d+U/2=0$ (here assuming also $V=0$) the attractive $U<0$ model becomes exactly isomorphic to its repulsive $U>0$ counterpart (2) under the following particle–hole (p–h) transformation $\hat{d}^\dagger_\downarrow\to-\hat{d}_{-\downarrow}$, $\hat{c}^\dagger_{\mathbf{k}\beta\downarrow}\to\hat{c}_{-\mathbf{k}\beta\downarrow}$. Outside the symmetric situation the p–h transformation still renders the structure of (2) with an additional Zeeman field $B^z=2\varepsilon_d+U$ (see Ref. [6] for details). One can then express the effective Hamiltonian [4] operating on the relevant empty and doubly occupied QD states by

$$\hat{\tilde{H}}^{\text{Kondo}}_{\text{charge}} = \sum_{\mathbf{k},\beta,\sigma}\xi_{\mathbf{k}\beta}\hat{c}^+_{\mathbf{k}\beta\sigma}\hat{c}_{\mathbf{k}\beta\sigma} + 2\sum_{\mathbf{k},\mathbf{q},\beta,\beta'} J^{\beta,\beta'}_{\mathbf{k},\mathbf{q}}\ \hat{\boldsymbol{\mathcal{T}}}_d\cdot\hat{\boldsymbol{\mathcal{T}}}_{\mathbf{k}\beta,\mathbf{q}\beta'}+\hat{\mathcal{T}}^z_d\ B^z \tag{4}$$

where $\hat{\mathcal{T}}^+_d=\hat{d}^\dagger_\uparrow\hat{d}^\dagger_\downarrow$, $\hat{\mathcal{T}}^-_d=\hat{d}_\downarrow\hat{d}_\uparrow$, and $\hat{\mathcal{T}}^z_d=\frac{1}{2}(\hat{d}^\dagger_\uparrow\hat{d}_\uparrow+\hat{d}^\dagger_\downarrow\hat{d}_\downarrow-1)$ [7]. Using this pseudospin representation the spin Kondo effect can be directly translated into the charge Kondo effect of the model (4) taking place near the degeneracy point $\varepsilon_d+U/2\sim 0$. Its consequences on the pair tunneling conductance have been partly examined in Refs. [5,6].

3 Two-channel model To consider the situation when the empty and doubly occupied states of QD are nearly degenerate we introduce the following auxiliary model

$$\hat{H}_{\text{QD}} = \sum_\sigma E_d\ \hat{d}^\dagger_\sigma\hat{d}_\sigma + g\left(\hat{b}^\dagger\ \hat{d}_\downarrow\hat{d}_\uparrow+\hat{d}^\dagger_\uparrow\hat{d}^\dagger_\downarrow\ \hat{b}\right)+E_{\text{pair}}\ \hat{b}^\dagger\hat{b}. \tag{5}$$

Whenever the electron pair happens to arrive on the d-QD we let it be stored on the side-coupled buffer described by the operators $\hat{b}^{(\dagger)}$. They obey the hard-core boson relations [11] so that at most only one electron pair can be allocated on this side-coupled b-QD. Similar lattice version of this model has been proposed in the solid state physics to account for the bipolaron superfluidity in the crossover between the adiabatic and antiadiabatic regimes [11].

Loosely speaking the correspondence between (5) and the negative $U<0$ Hamiltonian (2) holds via substitutions $g=U$, $E_{\text{pair}}=2\varepsilon_d+U$. This relation can be further supported analytically in the Lagrangian language after performing the Hubbard-Stratonovich transformation which eliminates $U\hat{d}^\dagger_\uparrow\hat{d}_\uparrow\hat{d}^\dagger_\downarrow\hat{d}_\downarrow$ through the additional bosonic fields, here denoted by $\hat{b}^{(\dagger)}$.

We will show that the two-channel QD described by (5) is able to capture the charge Kondo effect [7] known for the negative U Anderson model [12] near the symmetric situation. The underlying mechanism is driven by supressing the quantum fluctuations between the empty and doubly occupied states. Within the phenomenological model (5) such fluctuations are present even in the case of isolated

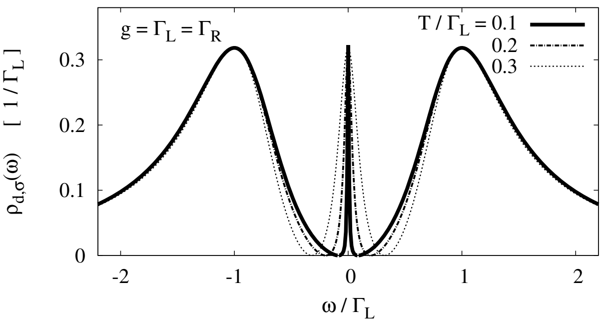

Figure 1 Spectral function of the molecular quantum dot for the equilibrium situation ($V=0$) in the symmetric case $E_{\rm pair}=0$, $E_d=0$ for several temperatures. We used $g=\Gamma_\beta$ assuming the wide-band limit $\Gamma_\beta=0.001D$, where D denotes the conduction electron bandwidth.

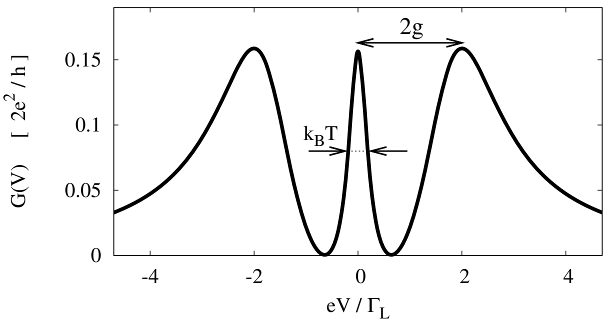

Figure 2 The differential conductance $G(V)$ as a function of bias voltage V for the symmetric case with $T=0.2g$ and $g=\Gamma_L$. Width of the central (superradiance) peak is proportional to temperature whereas the zero bias value $G(0)$ still remains constant (temperature-independent) [6].

molecular quantum dot i.e. for $V_{\mathbf{k}\beta}=0$. Out of 8 possible configurations being a product of the fermionic states $|0>$, $|\uparrow>$, $|\downarrow>$, $|\uparrow\downarrow>$ and the hard-core bosonic ones $|0)$, $|1)$ two of them $\uparrow\downarrow>\otimes|0)$ and $|0>\otimes|1)$ get mixed due to the Andreev-like interaction. A complete set of the eigenstates can be obtained using the transformation [13]

$$|B>=\sin(\varphi)\;|0>\otimes|1)\;+\;\cos(\varphi)\;|\uparrow\downarrow>\otimes|0), \qquad (6)$$

$$|A>=\cos(\varphi)\;|0>\otimes|1)\;-\;\sin(\varphi)\;|\uparrow\downarrow>\otimes|0) \qquad (7)$$

with $\tan(2\varphi)=2g/\,(2E_d-E_{\rm pair})$.

For such limit $V_{\mathbf{k}\beta}\to 0$ the Green's function $\mathcal{G}_d(\omega)=\langle\langle\hat{d}_\sigma;\hat{d}_\sigma^\dagger\rangle\rangle_\omega$ acquires the three pole structure [13]

$$\mathcal{G}_d^{V_{\mathbf{k}\beta}=0}(\omega)=\frac{\mathcal{Z}}{\omega-E_d}+(1-\mathcal{Z})\left[\frac{u^2}{\omega-E_+}+\frac{v^2}{\omega-E_-}\right] \qquad (8)$$

where

$$v^2,u^2=\frac{1}{2}\left(1\mp\frac{1}{\gamma}\right), \qquad (9)$$

$$E_-,E_+=\frac{1}{2}\left[E_{\rm pair}\mp(2E_d-E_{\rm pair})\gamma\right] \qquad (10)$$

with $\gamma^2=1+4g^2/(2E_d-E_{\rm pair})^2$ and

$$\mathcal{Z}=\left(1+e^{-E_d/k_BT}+e^{-(E_d+E_{\rm pair})/k_BT}+e^{-(2E_d+E_{\rm pair})/k_BT}\right)\Big/\left(1+2e^{-E_d/k_BT}+e^{-(E_d+E_-)/k_BT}+e^{-(E_d+E_+)/k_BT}+2e^{-(E_d+E_{\rm pair})/k_BT}+e^{-(2E_d+E_{\rm pair})/k_BT}\right).$$

Spectral weight $\mathcal{Z}$ of the single particle level is gradually depleted for a decreasing temperature and its amount is transferred to the bonding E_- and antibonding E_+ levels.

To get some insight into the many-body physics we employ a simple approximation based on the following self-energy

$$\mathcal{G}_d(\omega)^{-1}=\mathcal{G}_d^{V_{\mathbf{k}\beta}=0}(\omega)^{-1}-\sum_{\mathbf{k},\beta}\frac{|V_{\mathbf{k}\beta}|^2}{\omega-\xi_{\mathbf{k}\beta}}. \qquad (11)$$

In Figure 1 we show the spectral function $\rho_{d,\sigma}(\omega)=-\frac{1}{\pi}{\rm Im}\mathcal{G}_d(\omega+i0^+)$ for the symmetric case $E_{\rm pair}=0$, $E_d=0$ when $u^2=0.5=v^2$ and $E_+=g$, $E_-=-g$. We notice the three-peak structure where the middle one is sensitive to temperature due to transfer of its spectral weight $\mathcal{Z}$. Let us emphasize that this is a behavior typical for the Dicke effect known in quantum optics where the narrow/broad energy features correspond to the states weakly/strongly coupled to the electromagnetic field and they contribute the subradiant/superradiant emission lines [14]. Recently a similar concept of the Kondo-Dicke effect has been proposed in mesoscopic physics for a set of three vertically coupled quantum dots [15]. Our proposal (5) formally belongs to the same class of models. Some details concerning its relation to the Dicke effect has been already in pointed out in the review paper [14].

For the present context it is important to mention that the particular value of the spectral function $\rho_{d,\sigma}(\omega=0)$ is fixed (temperature-independent). This property has an impact on the low-voltage differential conductance of the charge current.

4 Transport properties External bias V applied between the electrodes induces the charge and energy transport through the interface. We calculate the charge current $I(V)=-e\frac{d}{dt}\langle\hat{N}_L\rangle$ following the standard procedure [1] which leads to the following Landauer-type formula [10]

$$I(V)=\frac{2e}{h}\int_{-\infty}^{\infty}d\omega[f(\omega-\mu_L)-f(\omega-\mu_R)]\;T(\omega), \qquad (12)$$

where $f(\omega) = [1 + \exp(\omega)/k_B T]^{-1}$. The transmission coefficient $T(\omega)$ depends on the spectral function

$$T(\omega) = \sum_\sigma \frac{\Gamma_L(\omega)\Gamma_R(\omega)}{\Gamma_L(\omega) + \Gamma_R(\omega)}\, \rho_{d,\sigma}(\omega)s \tag{13}$$

where the hybridization couplings are defined by $\Gamma_\beta(\omega) = 2\pi \sum_{\mathbf{k}} |V_{\mathbf{k}\beta}|^2 \delta(\omega - \varepsilon_{\mathbf{k}\beta})$. In particular, at low temperatures the zero bias conductance

$$G(V=0) = \frac{2e^2}{h} \int_{-\infty}^{\infty} d\omega \left[-\frac{df(\omega)}{d\omega} \right] T(\omega)$$

simplifies to

$$\lim_{T\to 0} G(0) = \frac{2e^2}{h} \frac{\Gamma_L(0)\Gamma_R(0)}{\Gamma_L(0) + \Gamma_R(0)} \sum_\sigma \rho_{d,\sigma}(0). \tag{14}$$

Such result along with the behavior presented in Figure 1 explains why the value of low temperature conductance $G(0)$ is pinned at a constant value. However, right outside the zero bias the differential conductance drops off as is illustrated in Figure 2. Width of the narrow conductance peak around the its zero bias value is proportional to temperature in agreement with the previous study [6].

5 Summary We have studied the charge transport through a correlated quantum dot with an effective negative value of the Coulomb interaction $U < 0$. To account for the quantum fluctuations between the empty and doubly occupied states we have introduced the phenomenological model with QD dot coupled to an additional electron pair buffer via the Andreev-type interaction. Focusing on the symmetric case, when the Kondo effect can arise in the pseudospin charge channel [7], we have examined its influence on the spectral function and the differential conductance. For both these quantities we have found the narrow peak whose height is constant whereas its width is proportional to temperature. This resembles the properties of the Dicke effect [14] which has been recently independently reported for a configuration composed of three vertically coupled quantum dots [15]. It might be of some interest to proceed an analysis of here proposed model outside the symmetric case and to adopt some more sophisticated self-consistent treatment for the Andreev-like interaction on the molecular quantum dot.

Acknowledgements This work is partly supported by the Polish Ministry of Science and Education under the grants NN202187833 and NN202373333.

References

[1] I.L. Aleiner, P.W. Brouwer, and L.I. Glazman, Phys. Rep. **358**, 309 (2002).
H. Haug, A.P. Yauho, Quantum Kinetics in Transport and Optics of Semiconductors (Springer-Verlag, Berlin, 1996).
[2] D. Goldhaber-Gordon, H. Shtrikman, D. Mahalu, D. Abusch-Magder, U. Mairav, and M.A. Kastner, Nature **391**, 156 (1998).
W.G. van der Wiel, S. De Franceschi, T. Fujisawa, J.M. Elzerman, S. Tarucha, and L.P. Kouwenhoven, Science **289**, 2105 (2000).
[3] A.C. Hewson, The Kondo Problem to Heavy Fermions (Cambridge University Press, Cambridge, 1993).
[4] J.R. Schrieffer and P.A. Wolf, Phys. Rev. **149**, 491 (1966).
[5] J. Mravlje, A. Ramsak, and T. Rejec, Phys. Rev. B **72**, 121403 (2005).
L. Arachea and M.J. Rozenberg, Phys. Rev. B **72**, 041301 (2005).
P.S. Cornaglia, H. Ness, and D.R. Grempel, Phys. Rev. Lett. **93**, 147201 (2003).
A.S. Alexandrov and A.M. Bratkovsky, Phys. Rev. B **67**, 235312 (2003).
A.S. Alexandrov, A.M. Bratkovsky, and R.S. Williams, Phys. Rev. B **67**, 075301 (2003).
[6] J. Koch, E. Sela, Y. Oreg, and F. von Oppen, Phys. Rev. B **75**, 195402 (2007).
J. Koch, M.E. Raikh, and F. von Oppen, Phys. Rev. Lett. **96**, 056803 (2006).
[7] A. Taraphder and P. Coleman, Phys. Rev. Lett. **66**, 2814 (1991).
[8] M.J. Hwang, M.S. Choi, and R. Lopez, Phys. Rev. B **76**, 165312 (2007).
[9] M. Gierczak and K.I. Wysokiński, J. Phys. Conf. Ser. **104**, 012005 (2008).
[10] Y. Meir, N.S. Wingreen, P.A. Lee, Phys. Rev. Lett. **70**, 2601 (1993).
[11] J. Ranninger and S. Robaszkiewicz, Physica B **135**, 468 (1985). S. Robaszkiewicz, R. Micnas, and J. Ranninger, Phys. Rev. B **36**, 180 (1987).
R. Friedberg and T.D. Lee, Phys. Rev. B **40**, 423 (1989).
[12] P.W. Anderson, Phys. Rev. Lett. **34**, 953 (1975).
[13] T. Domański, Eur. Phys. J. B **33**, 41 (2003).
T. Domański, J. Ranninger, and J.M. Robin, Solid State Commun. **105**, 473 (1998).
[14] T. Brandes, Phys. Rep. **408**, 315 (2004).
[15] P. Trocha and J. Barnaś, Phys. Rev. B **78**, 075424 (2008); J. Phys.: Condens. Matter **20**, 125220 (2008).