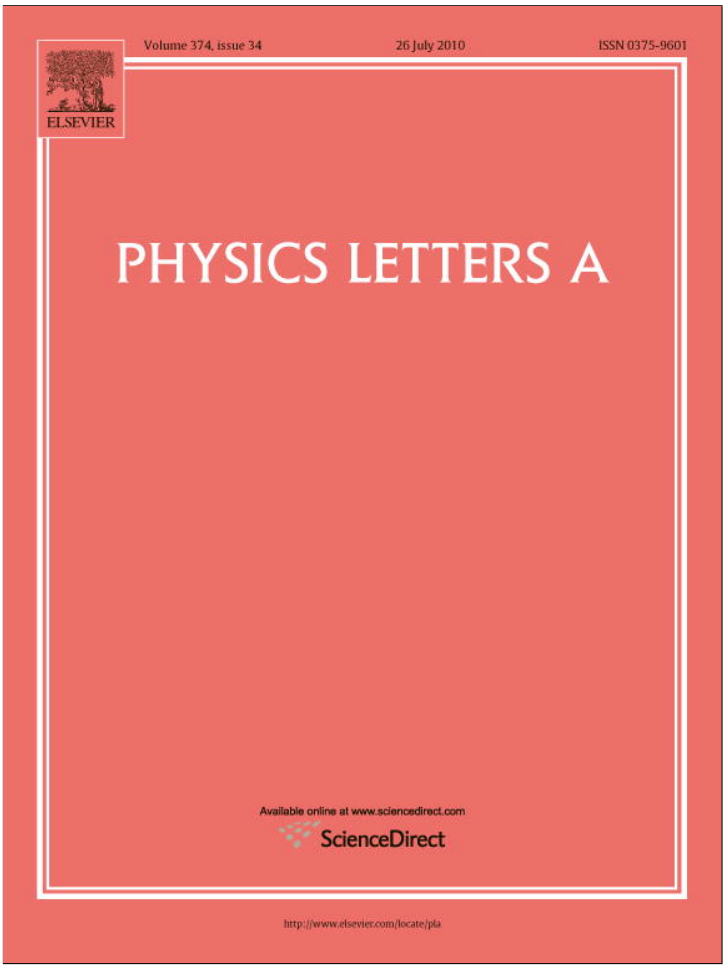

Physics Letters A 374 (2010) 3572–3575

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Kosterlitz–Thouless-like transition in two-dimensional lattices with long-range correlated hopping terms

W.S. Dias [a], F.A.B.F. de Moura [a,*], M.D. Coutinho-Filho [b], M.L. Lyra [a]

[a] Instituto de Física, Universidade Federal de Alagoas, Maceió, AL 57072-970, Brazil
[b] Laboratório de Física Teórica e Computacional, Departamento de Física, Universidade Federal de Pernambuco, Recife, PE 50670-901, Brazil

ARTICLE INFO

Article history:
Received 16 June 2010
Received in revised form 28 June 2010
Accepted 29 June 2010
Available online 9 July 2010
Communicated by V.M. Agranovich

Keywords:
Anderson transition
Localization
Electrons
Transport
Correlated
Disorder

ABSTRACT

We study the Anderson localization in two-dimensional lattices with long-range correlated hopping terms. The hopping energies along one lattice direction will be generated by a superposition of uncorrelated and long-range correlated contributions. Our numerical results strongly suggest the presence of a Kosterlitz–Thouless-like transition above a critical correlation degree.

1. Introduction

Materials with restricted geometry, such as semiconductor quantum-well structures [1], quantum dots and wires [2,3], organic thin films [4], quasiperiodic [5] as well as more general aperiodic structures [6] are nowadays objects of growing interest from both fundamental and practical point of views. An attributive peculiarity of almost all of them is the presence of disorder, which can be of an intrinsic nature (imperfections of the structure itself) as well as originated from a random environment.

Whenever disorder is involved, Anderson's ideas about localization of quasiparticle states come into play [7]. In three dimensions, the states at the center of the quasiparticle energy band remain extended for a relatively weak disorder (of magnitude smaller than the bandwidth), while the other states (in the neighborhood of the band edges) turn out to be exponentially localized. This implies the existence of two mobility edges which separates the phases of extended and localized states [8]. On the contrary, uncorrelated disorder of any magnitude causes localization of all one-particle eigenstates in one dimension (1D) [9] and two dimensions (2D) [10]. However, it was suggested that low-dimensional Anderson models with purely off-diagonal disorder might violate this general statement since a singularity of the density of states (DOS) was found at the band center [11–14]. A throughly analysis of the singularity of the DOS in the 1D Anderson model with off-diagonal disorder and nearest-neighbor interactions showed that the states belonging to this singularity are localized with no tendency of delocalization with increasing chain size [13]. On the other hand, the states belonging to the DOS singularity of the 2D counterpart model display a power-law divergence with the system size, a typical behavior of critical states [14].

Since late eighties, however, it has been realized that extended states may survive on 1D systems if the disorder distribution is correlated [15–23]. Short-range correlated disorder was found to support extended states at special resonance energies. In the thermodynamic limit, such extended states form a set of null measure in the density of states [15–19], implying the absence of mobility edges in these systems. In contrast, systems with long-range correlations in the disorder distribution support a finite fraction of delocalized states [21,22], giving rise to mobility edges. Theoretical predictions of localization suppression on 1D geometries, due to correlations of the disorder distribution, were confirmed experimentally in semiconductor superlattices with intentional correlated disorder [20], as well as in single-mode wave guides with correlated scatterers [23].

A first study of the effects of long-range correlations in the localization properties of $2d$ electronic systems with orthogonal symmetry was performed in Ref. [24]. The authors considered a striped media in the x–y plane with on-site disorder. The on-site energies were generated by a superposition of an uncorre-

* Corresponding author. Tel.: +55 82 3214 1429; fax: +55 82 3214 1645.
E-mail address: fidelis@if.ufal.br (F.A.B.F. de Moura).

0375-9601/$ – see front matter
doi:10.1016/j.physleta.2010.06.063

lated term and a long-range correlated contribution along the y-direction. It was predicted that this system displays a disorder-driven Kosterlitz–Thouless-like MIT in the regime of strong correlations. More recently, the effects of long-range correlations in *both* x- and y-directions, were studied [25–28]. A transfer matrix numerical calculation on a striped geometry, combined with finite-size scaling arguments, confirmed the presence of a correlation induced Kosterlitz–Thouless transition [25]. In addition, by considering the site energies of the $2d$ Anderson Hamiltonian distributed in such a way to have a power-law spectral density $S(k) \propto 1/k^{\alpha_{2d}}$, an exact diagonalization formalism of finite lattices with a square geometry showed that this model displays a phase of low-energy extended states for $\alpha_{2d} > 2$. In this regime, the dynamics associated with the spread of an initially localized wave packet becomes ballistic [26]. Moreover, the exponents governing the collapse of the participation function for low energies ($\xi \propto L^{D_2}$) and the long time decay of the autocorrelation function [$C(t) \propto t^{-\beta}$] were shown to satisfy the scaling relation $D_2 = \beta d$. Furthermore, the scale invariance of the participation function relative fluctuation at the critical point was investigated in Ref. [27]. By using a finite size scaling hypothesis it was shown that the correlation length critical exponent depends on α_{2d}, thus indicating that correlations in the disorder distribution are indeed relevant in this regime, in agreement with the extended Harris criterion.

While the delocalization phenomenon induced by long-range correlations in the on-site potential has been extensively investigated in the literature, the counterpart model with long-range correlated off-diagonal disorder is still quite unexplored. In this work, we report further progress along this direction. We will develop transfer matrix calculations on the $2d$ Anderson model with long range correlated hopping terms. Here, we will consider a striped geometry in the x–y plane with zero on-site potentials. The hopping energies along the y-direction will be generated by a superposition of an uncorrelated term and a long-range correlated one. Combining the transfer matrix calculations with finite-size scaling arguments, we compute the localization length in the thermodynamic limit. We will show that the scaling behavior is compatible with the presence of a Kosterlitz–Thouless metal–insulator transition [25].

2. Model and formalism

We consider the $2d$ Anderson Hamiltonian with disordered hopping terms and null on-site energies ($\epsilon_{im} = 0$) on a striped square lattice geometry $L \times M$ [24,25]:

$$H = \sum_{\langle x_1 y_1, x_2 y_2 \rangle} T_{x_1 y_1, x_2 y_2} \big(|x_1, y_1\rangle \langle x_2, y_2| \big), \tag{1}$$

where $|x, y\rangle$ is a Wannier state localized at site (x, y) and $\sum_{\langle x_1 y_1, x_2 y_2 \rangle}$ represents a sum over nearest-neighbor pairs. The matrix $T_{x_1 y_1, x_2 y_2}$ contains the hopping terms along both x- and y-directions. In our calculations, we fix the hopping term along the x-direction as $t_x = 1$. The hopping terms along the y-direction will be generated by a superposition of an uncorrelated contribution and a long-range correlated term,

$$t_y = \tanh(\nu_y + \rho_y) + \langle t_y \rangle. \tag{2}$$

The first term ν_y represents a long-range correlated sequence defined by

$$\nu_y = \zeta(\alpha) \sum_{k=1}^{L/2} \frac{1}{k^{\alpha/2}} \cos\left(\frac{2\pi k y}{L} + \phi_k \right) \tag{3}$$

where ϕ_k are $L/2$ (L even) independent random phases uniformly distributed in the interval $[0, 2\pi]$ and $\zeta(\alpha)$ is a normalization constant which is chosen to have the sequence variance $\sigma = \sqrt{\langle \nu_y^2 \rangle - \langle \nu_y \rangle^2} = 1$. We also shift the sequence in order to have $\langle \nu_y \rangle = 0$. Typically, this sequence is the trace of a $1d$ fractional Brownian motion with a well defined power-law spectrum $S(k) \propto 1/k^{\alpha}$. The second term ρ_y describes L independent random numbers uniformly distributed in the interval $[-W/2, W/2]$. Here we use $\langle t_y \rangle = 2$ to avoid negative hopping terms.

In order to calculate the typical localization length of electrons, we use the finite size scaling method combined with the transfer-matrix technique [24]. We calculate the damping of wave functions in the y-direction for a long strip of size $L \times M$ with L being extremely large ($L \approx 2 \times 10^6$). The periodic boundary condition is adopted in the x-direction. For a given energy E, a $2M \times 2M$ transfer matrix Q_n can be easily set up, mapping the wave-function amplitudes at column $n+1$ to those at column n in the strip. The propagation along the strip is therefore described by the product of transfer matrices

$$P_L = Q_{L-1} Q_{L-2} \cdots Q_2 Q_1. \tag{4}$$

The transfer matrix P_L has M pairs of eigenvalues whose logarithms correspond to the Lyapunov exponents [24,25]. The largest localization length $\lambda(E)$ for a given energy E in a system with a finite width M is given by the inverse of the smallest Lyapunov exponent. In our numerical calculation, we choose L about 2×10^6 so that the self-averaging effect automatically takes care of statistical fluctuations. We estimate and control these fluctuations following the deviations of the calculated eigenvalues of two adjacent iterations. The finally obtained data have statistical errors less than the symbol size in the corresponding figures. We use the standard one-parameter finite-size scaling ansatz [24,25] to obtain the thermodynamic localization length λ_∞. According to the one-parameter scaling theory, the rescaled localization length $\Lambda = \lambda(E)/M$ can be expressed near the critical point in terms of a universal function given by:

$$\Lambda = f(\lambda_\infty / M). \tag{5}$$

We also study some dynamical aspects by examining the time evolution of an initially localized wave packet on a $L \times L$ square lattice. The Wannier amplitudes evolve in time according to the time-dependent Schrödinger equation as ($\hbar = 1$) [26]

$$i \frac{dc_{x,y}(t)}{dt} = t_{y-1} c_{x,y-1}(t) + t_y c_{x,y+1}(t) + c_{x-1,y}(t) + c_{x+1,y}(t), \quad x, y = 1, 2, \ldots, L. \tag{6}$$

We consider a wave packet initially localized at site $x_0 = L/2$, $y_0 = L/2$, i.e. $c_{x,y}(t=0) = \delta_{x,x_0} \delta_{y,y_0}$. The above set of equations were solved numerically by using a high-order method based on the Taylor expansion of the evolution operator $V(\Delta t)$:

$$V(\Delta t) = \exp(-iH\Delta t) = 1 + \sum_{l=1}^{n_o} \frac{(-iH\Delta t)^l}{l!} \tag{7}$$

where H is the Hamiltonian. The wave-function at time Δt is given by $|\Phi(\Delta t)\rangle = V(\Delta t)|\Phi(t=0)\rangle$. The method can be used recursively to obtain the wave-function at time t. The following results were taken by using $\Delta t = 0.05$ and the sum was truncated at $n_o = 20$. This cutoff was sufficient to keep the wave-function norm conservation along the entire time interval considered. We are particularly interested in calculating the wave packet mean-square displacement $\xi(t)$ along the y-direction (the correlated direction) [26]

$$\xi(t) = \sqrt{\sum_{x=1}^{L} \sum_{y=1}^{L} \big[(y - y_0)^2 \big] \big| c_{x,y}(t) \big|^2}. \tag{8}$$

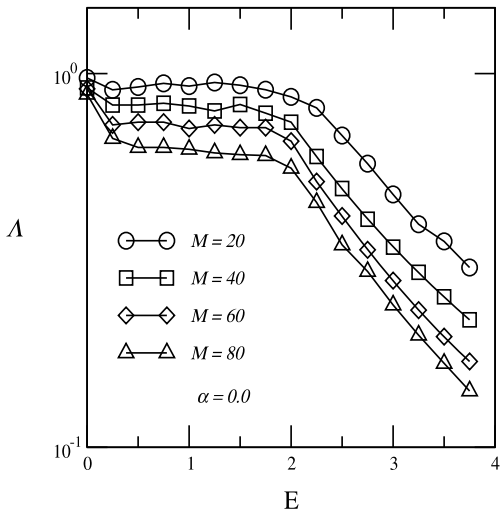

Fig. 1. Rescaled localization length $\lambda(E)/M$ as a function of energy E for $\alpha = 0$ and $M = 20$ up to 80. The curves for smaller M are always above those of larger M throughout the entire range of energies. This feature indicates that there is no mobility edge.

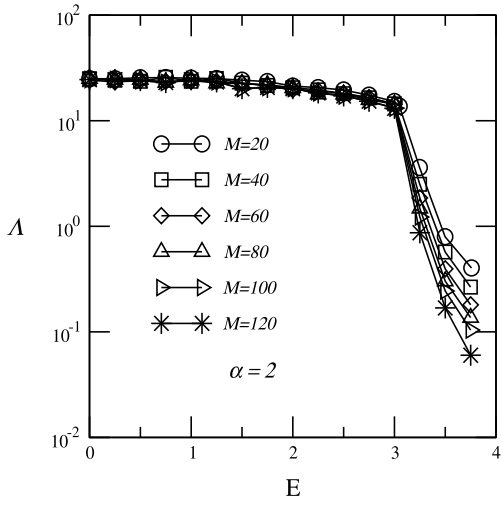

Fig. 2. Rescaled localization length $\Lambda = \lambda(E)/M$ as a function of energy E for $\alpha = 2$ and $M = 20$ up to 120. We can see that all curves merge together for $E < E_c \approx 3$. This behavior signals a metal–insulator transition at $E = E_c$.

3. Results and discussion

All transfer matrix calculations were done for $L \approx 2 \times 10^6$ and $W = 1$. Fig. 1 presents the rescaled localization length $\Lambda = \lambda(E)/M$ as a function of energy E for $\alpha = 0$. the curves of the smaller M are always above those of larger M throughout the entire range of energies, thus indicating that there is no mobility edge and, correspondingly, no metal–insulator transition. In Fig. 2 we show similar data taken from the case of strongly correlated off-diagonal disorder ($\alpha = 2$). This picture has a qualitatively different feature: all curves merge together for $E < E_c \approx 3$. This signals a delocalization phase transition at $E = E_c$. In Fig. 3, we plot the rescaled localization length $\Lambda = \lambda(E)/M$ for a specific energy below E_c ($E = 1$) as a function of M. We can see that the phase transition occurs at $\alpha > 1$, with the rescaled localization length becoming size independent in the regime of large M. In Fig. 4(a) we collect results for the localization length extrapolated to the thermodynamical limit. These estimated values were obtained from the scaling ansatz close to the critical energy $E_c \approx 3$. We successfully

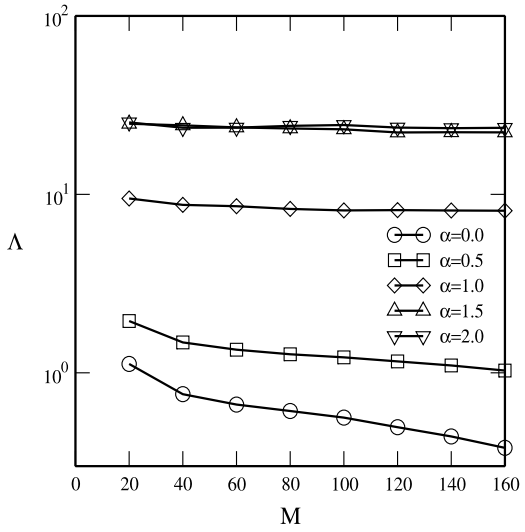

Fig. 3. Rescaled localization length $\Lambda = \lambda(E)/M$ for a specific energy below E_c ($E = 1$) as a function of M. We can see that the phase transition occurs for $\alpha > 1$, characterized by the size independence of the asymptotic scaled localization length.

fit the data with $\lambda_\infty \propto \exp(C/\sqrt{E - E_c})$ with $E_c = 3.00(5)$ indicating a fast decay of the localization length on the insulating side by increasing the deviation from the transition point. This behavior is the typical one for a disorder driven Kosterlitz–Thouless-like transition (KT transition). Using the estimated extrapolated localization lengths, we report in Fig. 4(b) the data for the scaled localization length $\lambda(E)/M$ close to critical energy $E_c = 3.00(5)$ as a function of the proper scaling variable $\lambda_\infty(E)/M$. We have used energy values from $E = 3.20$ up to 3.55 with $\Delta E = 0.05$ and stripe sizes ranging from $M = 20$ up to 120. The fact that all data from distinct energies and system sizes fall into a single curve, without the need of any additional adjusting parameter, reflects the accuracy of the estimated extrapolated localization length and the absence of significant corrections to scaling in the asymptotic regime investigated.

Finally, we show in Fig. 5 results for the time evolution of an initially localized wave-packet in a square lattice with 3000×3000 sites and $\alpha = 0, 1.5$ and 3. Numerical convergence was ensured by conservation of the norm of the wave-packet at every time step, i.e., $1 - \sum_n |c_n(t \to \infty)|^2 \approx 10^{-15}$. The extended states that appear in this model emerge in the regime at which the potential has a strong correlation degree. These are typically non scattered modes thus leading to a ballistic wave-packet spread, $\xi(t) \propto t$. In Fig. 5 we obtain roughly a ballistic spread for $\alpha > 1$. In the long-time, $\xi(t)$ displays a saturation that represents the package arrival at the lattice boundaries.

4. Summary and concluding remarks

In this Letter, we studied the localization properties in 2D striped media with off-diagonal long-range-correlated disorder. The hopping energies along the y-direction were assumed to be composed of a superposition of an uncorrelated disorder term and a long-range correlated random contribution. The long-range correlated terms were distributed in such a way to have a power-law spectral density $S(k) \propto k^{-\alpha}$. By using the well-developed transfer-matrix method we find that the system undergoes a unconventional correlation-driven Kosterlitz–Thouless metal–insulator transition when the hopping disorder distribution exhibits a power-law spectral density $S(k) \propto k^{-\alpha}$ with $\alpha > 1$. This result is in remarkable contrast to the one exhibited by 2D disordered media with uncorrected disorder, which do not display a metal–insulator transition

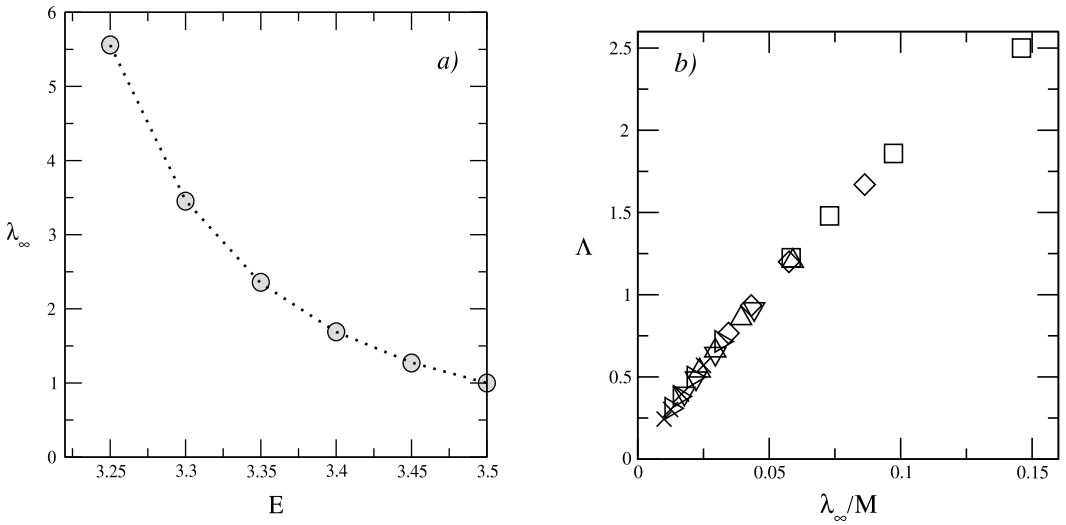

Fig. 4. (a) Fit of the extrapolated localization length $\lambda_\infty \propto \exp(C/\sqrt{E-E_c})$ with $E_c = 3.00(5)$. This scaling behavior in typical of a Kosterlitz–Thouless transition. (b) Data collapse of the scaled localization length in the universal scaling form, thus supporting the accuracy of the estimated extrapolated localization lengths.

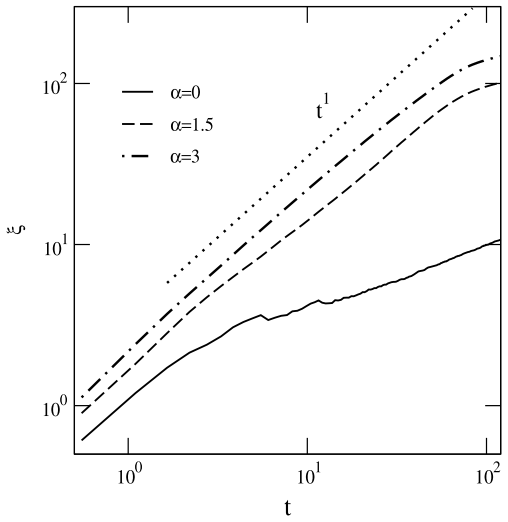

Fig. 5. The mean-square displacement $\xi(t)$ of a one-electron wave-packet computed in a square lattice with 3000×3000 sites and $\alpha = 0, 1.5$ and 3. A nearly ballistic spread ($\xi(t) \propto t$) takes place in the regime of strong correlations in the longitudinal hopping distribution ($\alpha > 1$).

for any amount of disorder. In addition, we followed the time evolution of an initially localized wave-packet. Within our numerical precision, we found that associated with the metal–insulator transition, a ballistic wave-packet propagation takes place. We hope that the present work will stimulate further studies on semiconductors and superlattices with intentional long-range correlated off-diagonal disorder.

Acknowledgements

This work was financially supported by CNPq-Rede Nanobioestruturas, CAPES, FINEP, PRONEX/CNPq/FAPEAL and FACEPE.

References

[1] G. Khitrova, H.M. Gibbs, F. Jahnke, M. Kira, S.W. Koch, Rev. Mod. Phys. 71 (1999) 1591.
[2] See contributions to in: G.W. Briant, G.S. Solomonm (Eds.), Optics of Quantum Dots and Wires, Artech House, Boston, 2005.
[3] T. Brandes, Phys. Rep. 408 (2005) 315.
[4] J.R. Tischler, M.S. Bradly, Q. Zhang, T. Atay, A. Nurmiko, V. Bulović, Org. Electronics 8 (2007) 94.
[5] E.L. Albuquerque, M.G. Cottam, Phys. Rep. 376 (2003) 225;
E.L. Albuquerque, M.G. Cottam, Polaritons in Periodic and Quasiperiodic Structures, Elsevier, Amsterdam, 2004.
[6] E. Maciá, Aperiodic Structures in Condensed Matter, CRC Press, Boca Raton, 2009.
[7] P.W. Anderson, Phys. Rev. 109 (1958) 1492.
[8] N.F. Mott, J. Non-Cryst. Solids 1 (1968) 1.
[9] N. Mott, W.D. Twose, Adv. Phys. 10 (1961) 107.
[10] E. Abrahams, P.W. Anderson, D.C. Licciardello, T.V. Ramakrishnan, Phys. Rev. Lett. 42 (1979) 673.
[11] G. Theodorou, M.H. Cohen, Phys. Rev. B 13 (1976) 4597.
[12] H. Fidder, J. Knoester, D.A. Wiersma, J. Chem. Phys. 95 (1991) 7880.
[13] G.G. Koslov, V.A. Malyshev, F. Domínguez-Adame, A. Rodríguez, Phys. Rev. B 58 (1998) 5367.
[14] A. Eilmes, R.A. Roemer, M. Schreiber, Physica B 296 (2001) 46.
[15] J.C. Flores, J. Phys.: Condens. Matter 1 (1989) 8471.
[16] D.H. Dunlap, H.-L. Wu, P.W. Phillips, Phys. Rev. Lett. 65 (1990) 88.
[17] P.W. Phillips, H.-L. Wu, Science 252 (1991) 1805.
[18] A. Sánchez, F. Domínguez-Adame, J. Phys. A: Math. Gen. 27 (1994) 3725;
A. Sánchez, E. Maciá, F. Domínguez-Adame, Phys. Rev. B 49 (1994) 147.
[19] E. Diez, A. Sánchez, F. Domínguez-Adame, Phys. Rev. B 50 (1994) 14359;
F. Domínguez-Adame, E. Diez, A. Sánchez, Phys. Rev. B 51 (1995) 8115.
[20] V. Bellani, E. Diez, R. Hey, L. Toni, L. Tarricone, G.B. Parravicini, F. Domínguez-Adame, R. Gómez-Alcalá, Phys. Rev. Lett. 82 (1999) 2159.
[21] F.A.B.F. de Moura, M.L. Lyra, Phys. Rev. Lett. 81 (1998) 3735;
F.A.B.F. de Moura, M.L. Lyra, Phys. Rev. Lett. 84 (2000) 199;
F.A.B.F. de Moura, M.L. Lyra, Physica A 266 (1999) 465.
[22] F.M. Izrailev, A.A. Krokhin, Phys. Rev. Lett. 82 (1999) 4062.
[23] U. Kuhl, F.M. Izrailev, A.A. Krokhin, H.-J. Stöckmann, Appl. Phys. Lett. 77 (2000) 633.
[24] W.-S. Liu, T. Chen, S.J. Xiong, J. Phys.: Condens. Matter 11 (1999) 6883.
[25] W.-S. Liu, S.Y. Liu, X.L. Lei, Eur. Phys. J. B 33 (2003) 293.
[26] F.A.B.F. de Moura, M.D. Coutinho-Filho, E.P. Raposo, M.L. Lyra, Europhys. Lett. 66 (2004) 585.
[27] I.F. dos Santos, F.A.B. F de Moura, M.L. Lyra, M.D. Coutinho-Filho, J. Phys.: Condens. Matter 19 (2007) 476213.
[28] F.A.B.F. de Moura, M.L. Lyra, F. Domínguez-Adame, V.A. Malyshev, J. Phys.: Condens. Matter 19 (2007) 056204.