**Journal of Atomic, Molecular, Condensate & Nano Physics**
Vol. 6, No. 3, pp. 187–193, 2015
ISSN 2349-2716 (online); 2349-6088 (print)
Published by RGN Publications

http://www.rgnpublications.com

# Exact Diagonalization Study of Double Quantum Dot System in Zero-bandwidth Limit

Research Article

Haroon* and M. A. H. Ahsan

*Department of Physics, Jamia Millia Islamia* (*Central University*), *New Delhi 110025, India*
***Corresponding author:** haroonjamia@gmail.com

**Abstract.** Using exact diagonalization, we study double quantum dot system with one of the dots attached to the ideal leads acting as source and drain in T-shaped geometry. The leads are incorporated in zero-bandwidth limit by replacing their band structures with one level coinciding with Fermi levels in the respective leads. For the half-filled case, the spin-spin correlation for the dots are calculated numerically at zero as well as finite temperatures. At zero temperature, an antiferromagnetic correlation between the dots is observed for finite values of interdot tunneling matrix-element. The antiferromagnetic correlation between the dots changes remarkably for large values of ondot Coulomb interaction both at zero as well as finite temperatures. The spin-spin correlation between the dots is significantly reduced even for small values of the inderdot Coulomb interaction compared to the ondot Coulomb interaction. At a small value of temperature, the spin-spin correlation between the dots exhibits a (negative) maximum due to contributions coming from thermal excitations to low-lying states.

**Keywords.** Double quantum dot; Spin-spin correlation; Zero-bandwidth limit

**PACS.** 73.21.La; 75.10.-b

**Received:** March 10, 2015 **Accepted:** September 23, 2015



## 1. Introduction

Quantum dots are often referred to as artificial atoms to highlight their two important features namely a small number of electrons present in the dots and the many-body effects. Analogously,

a system of two or more quantum dots coupled together are referred to as artificial molecules [1]. An array of quantum dots may form a two-dimensional artificial crystal which paves the way to create artificially engineered materials [2]. The two unique features of the quantum dot mentioned above lead to properties of a dot change dramatically by adding just one more electron to it. Similar to atomic systems, the electronic states of quantum dots are spatially localized with the corresponding energies quantized. This makes these systems more stable against thermal perturbation. Quantum dots have become the testing ground for many physical phenomena and holds immense potential for device applications [3,4]. During the last few decades, the quantum dot systems have been investigated extensively for their unique properties both theoretically as well as experimentally [5,6].

We consider a *double quantum dot* (DQD) system in T-shaped geometry with one of the dots attached to ideal leads incorporated in *zero-bandwidth* (ZBW) limit. The ZBW limit has the unique advantage that all calculations can be carried out exactly with no approximation to the dot parameters. Earlier studies using ZBW limit for transport through single quantum dot has been found to be consistent with experiments [7,8]. The ZBW limit has also been utilized in the study of two-impurity Anderson model to explain the magnetic correlation between impurities in a metal [9]. The magnetic correlation between the quantum dots in a given geometry can effectively be utilized in device application [10]. In the present work, using exact diagonalization, we calculate spin-spin correlation between the quantum dots at zero as well as finite temperatures to study the magnetic properties of the T-shaped DQD system as a function of tunable parameters of the system like interdot tunneling, hybridization with the leads, etc.

## 2. The Model

The DQD system in T-shaped geometry is taken as shown in Figure 1 where only dot-1 is coupled to the ideal (non-interacting) source and drain leads via the hybridization parameters $V^{s,d}$ and the two dots are tunnel-coupled through the tunneling matrix-element $t$. Besides ondot Coulomb interactions $U_1$, $U_2$ on the two dots, there is an interdot Coulomb interaction $g$. The system can be described by the two-impurity Anderson type Hamiltonian as [11]

$$\mathbf{H} = \mathbf{H_{dqd}} + \mathbf{H_{leads}} + \mathbf{H_{hyb}} \tag{2.1}$$

where the quantum dots are described by $\mathbf{H_{dqd}}$, the non-interacting leads by $\mathbf{H_{leads}}$ and hybridization between the quantum dot-1 and the leads by $\mathbf{H_{hyb}}$.

$$\mathbf{H_{dqd}} = \sum_{j=1,2} \varepsilon_j \sum_{\sigma} c^{\dagger}_{j\sigma} c_{j\sigma} + \sum_{j=1,2} U_j n_{j\uparrow} n_{j\downarrow} + g \sum_{\sigma\sigma'} n_{1\sigma} n_{2\sigma'} + t \sum_{\sigma} \left( c^{\dagger}_{1\sigma} c_{2\sigma} + h.c. \right)$$

$$\mathbf{H_{leads}} = \sum_{l=s,d} \sum_{\mathbf{k},\sigma} \varepsilon^{l}_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}^l\sigma} c_{\mathbf{k}^l\sigma}; \quad \mathbf{H_{hyb}} = \sum_{l=s,d} \sum_{\mathbf{k},\sigma} \left( V^{l}_{\mathbf{k}} c^{\dagger}_{\mathbf{k}^l\sigma} c_{1\sigma} + h.c. \right)$$

The first two terms in $\mathbf{H_{dqd}}$ represent energies of electrons on spin degenerate levels $\varepsilon_j$ on the dots and $U_j$ the ondot Coulomb interaction. The third and the fourth terms in $\mathbf{H_{dqd}}$ represent the interdot Coulomb interaction $g$ and the interdot tunneling matrix-element $t$, respectively. The $\mathbf{H_{leads}}$ describes the non-interacting source and drain leads where $\varepsilon^{l}_{\mathbf{k}\sigma}$ $(l = s,d)$ represents the dispersion relation of their arbitrary continuous energy band structure labeled by

wavevector $\mathbf{k}$. Finally, $\mathbf{H_{hyb}}$ describes the hybridization of dot-1 to the leads with $\mathbf{k}$-dependent hybridization parameters $V^l_{\mathbf{k}}$ $(l = s,d)$.

The ZBW limit of the leads are taken by replacing the arbitrary band structure of the leads $\varepsilon^l_{\mathbf{k}\sigma}$ $(l = s,d)$ by the respective Fermi levels with finite degeneracy [7,9]. In the present work, we consider only one level, the Fermi level, on both the source and the drain leads [8]. The model Hamiltonian (2.1), in the ZBW limit, thus simplifies to

$$\mathbf{H_{ZBW}} = \mathbf{H_{dqd}} + \sum_{l=s,d} \varepsilon^l_F \sum_\sigma c^\dagger_{l\sigma} c_{l\sigma} + \sum_{l=s,d} \left(V^l c^\dagger_{l\sigma} c_{1\sigma} + h.c.\right) \tag{2.2}$$

where the hybridization parameters $V^l_\uparrow = V^l_\downarrow = V^l$ $(l = s,d)$ have been assumed to be independent of the wavevector $\mathbf{k}$ and the spin $\sigma$. The Hamiltonian in (2.2) now describes a four site problem which can be further simplified by taking chemical potential in the two leads equal as $\varepsilon^s_F = \varepsilon^d_F = \varepsilon_F$, the Fermi energy, corresponding to the equilibrium situation [7, 12]. This enables us to transform to the symmetric and antisymmetric combinations [9] of the lead fermionic operators namely $\alpha^\dagger_{s\sigma}|0\rangle = \frac{1}{\sqrt{2}}\left(C^\dagger_{s\sigma} + C^\dagger_{d\sigma}\right)|0\rangle$ and $\alpha^\dagger_{a\sigma}|0\rangle = \frac{1}{\sqrt{2}}\left(C^\dagger_{s\sigma} - C^\dagger_{d\sigma}\right)|0\rangle$ respectively. The Hamiltonian in (2.2) then reduces to a three-plus-one site problem [13]: $\mathbf{H_{ZBW}} = \mathbf{H_{3-site}} + \mathbf{H_{1-site}}$. The problem now remains to solve the Hamiltonian $\mathbf{H_{3-site}} = \mathbf{H_{dqd}} + \varepsilon_F \sum_\sigma \alpha^\dagger_{s\sigma}\alpha_{s\sigma} + \sqrt{2}V \sum_\sigma \left[\alpha^\dagger_{s\sigma} C_{1\sigma} + h.c.\right]$. For different electron fillings in the non-interacting case and the infinitely large $U \to \infty$ limit with $g = 0$, $\mathbf{H_{3-site}}$ can be solved analytically. The $\mathbf{H_{1-site}} = \varepsilon_F \sum_\sigma \alpha^\dagger_{a\sigma}\alpha_{a\sigma}$ with antisymmetric combination of the leads, is the decoupled diagonal term.

### Spin-spin Correlation

The magnetic properties of the system can be studied by calculating spin-spin correlation using grand canonical ensemble where the chemical potential is adjusted in such a way that the system contains a fixed average number of electrons [13]. Alternatively, one can use canonical ensemble as the two approaches are equivalent [9, 13]. At zero temperature, the spin-spin correlation between the dots is calculated as $\langle \lambda^g_{N,S,S_z}|\mathbf{S_1}\cdot\mathbf{S_2}|\lambda^g_{N,S,S_z}\rangle$ where $|\lambda^g_{N,S,S_z}\rangle$ is the $N-$electron ground state and $\mathbf{S_1}\cdot\mathbf{S_2} = \frac{1}{2}\left(S^+_i S^-_j + S^-_i S^+_j\right) + S^z_i S^z_j$ with $S^{+/-}_i = C^\dagger_{i\uparrow/\downarrow} C_{i\downarrow/\uparrow}$ and $S^z_i = \frac{1}{2}\left(n_{i\uparrow} - n_{i\downarrow}\right)$. The finite temperature spin-spin correlation between the dots is calculated in canonical ensemble as $\langle \mathbf{S_1}\cdot\mathbf{S_2}\rangle = Tr\left(\langle S_1\cdot S_2\rangle e^{-\beta \mathbf{H_{ZBW}}}\right)/Z_c$ where $Z_c = Tr(e^{-\beta \mathbf{H_{ZBW}}})$ is the canonical partition function and $\beta = 1/k_B T$.

## 3. Numerical Results

For the system described by the four-site Hamiltonian $\mathbf{H_{ZBW}}$ in (2.2) in ZBW limit, we calculate spin-spin correlation between the quantum dots for the half-filled case using canonical ensemble [14]. The four electron basis states in spin subspaces $S = 0,1,2$ are used for numerical calculation. The dimensionality of the full Hilbert space is 70 and the Hamiltonian matrix is block diagonalized into one $20 \times 20$ matrix corresponding to $S = 0$ and $S_z = 0$, three $15 \times 15$ matrices corresponding to $S = 1$ and $S_z = +1, 0, -1$ respectively, and five $1 \times 1$ matrices corresponding to $S = 2$ and $S_z = +2, +1, 0, -1, -2$ respectively. Since there is no magnetic field,

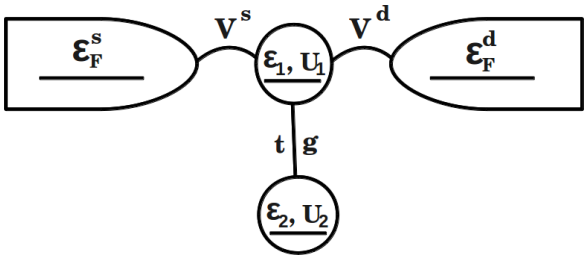
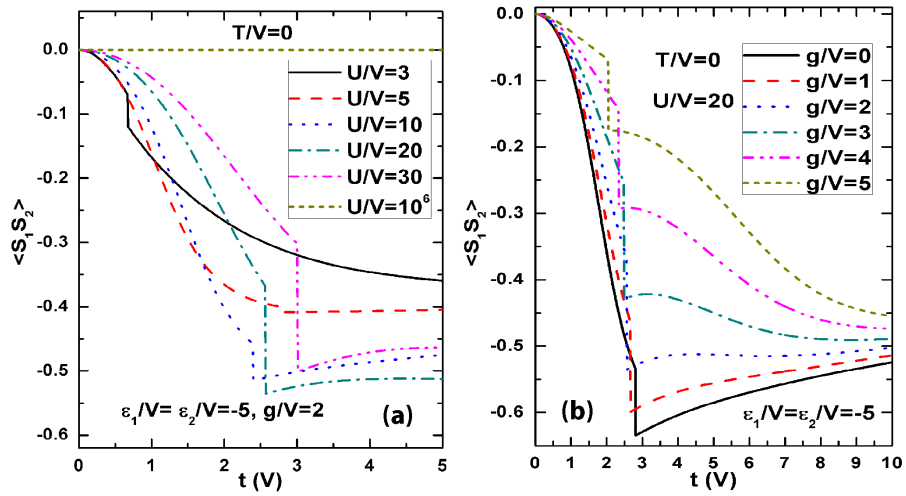



**Figure 1.** Schematic diagram of DQD system in T-shaped geometry. Only dot-1 is coupled to the source and drain leads through hybridization parameters $V^{s,d}$. In the ZBW limit, there is only one level−the Fermi level− on each of the leads. Dots 1 and 2 are tunnel-coupled through the matrix-element $t$. The dot energies are given by $\varepsilon_1$ and $\varepsilon_2$ whereas $U_1$ and $U_2$ are the respective ondot Coulomb interactions. The parameter $g$ denotes the interdot Coulomb interaction.

the Hamiltonian is spin conserving. This allows the eigenvectors of the three matrices to be spin-rotated within the subspace $S = 1$ corresponding to $S_z = -1, 0, +1$ using spin raising/lowering operators, resulting in three-fold $(2S+1)$ degenerate eigenvalues [13]. Similarly, the eigenstates in $S = 2$ subspace are five-fold degenerate. In our calculations, we have fixed Fermi energies of the source and the drain leads equal to zero, $\varepsilon_F^s = \varepsilon_F^d = 0$. The dot levels are kept at $\varepsilon_1 = \varepsilon_2 = -5$ and equal ondot Coulomb interactions $U_1 = U_2 = U$ are assumed on the two dots, the hybridization parameter $V$ is taken as the unit of energy. By varying the remaining parameters i.e. the interdot tunneling-matrix element $t$, the ondot Coulomb interaction $U$ and the interdot Coulomb interaction $g$, the system is studied here both at zero as well as the finite temperatures.



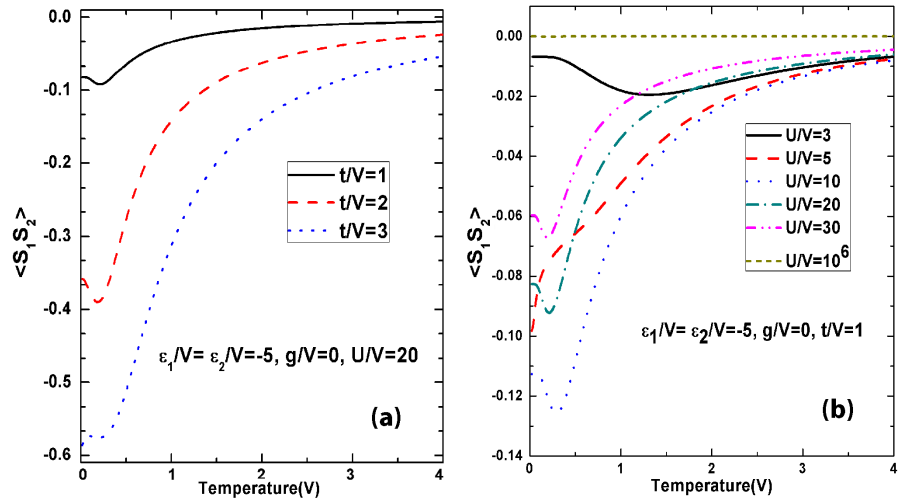

(a) (b)

**Figure 2.** Zero temperature spin-spin correlation $\langle \mathbf{S_1} \cdot \mathbf{S_2} \rangle$ between the dots *versus* interdot tunneling matrix-element $t$. (a) The plots with $g = 2$ correspond to six different values of ondot interaction: $U = 3$−solid line; $U = 5$−dashed line; $U = 10$−dotted line; $U = 20$−dash-dotted line; $U = 30$−dash double dotted line; $U = 10^6$−short-dashed line. (b) The plots with $U = 20$ correspond to six different values of interdot Coulomb interaction: $g = 0$−Solid line; $g = 1$−dashed line; $g = 2$−dotted line; $g = 3$−dash-dotted line; $g = 4$−dash double dotted line and $g = 5$−short-dashed line.

We first examine the effects of ondot and interdot Coulomb interactions at zero temperature on spin-spin correlation $\langle \mathbf{S_1} \cdot \mathbf{S_2} \rangle$ between the spins associated with the two dots. The interdot tunneling matrix-element $t$ allows the transfer of electronic charge between the dots. Figure 2(a) shows the variation of zero temperature spin-spin correlation $\langle \mathbf{S_1} \cdot \mathbf{S_2} \rangle$ between the the dots *versus* interdot tunneling matrix-element $t$ at six different values of ondot Coulomb interaction $U$. At $t = 0$, the two dots decouple and the spin-spin correlation between the dots vanishes. It is seen that finite interdot tunneling matrix-element $t$ causes *antiferromagnetic* (AF) correlation between the dots and this can be understood through the following consideration. At zero temperature, the ground state of the system is non-magnetic with total spin $S = 0$. In order to avoid the additional cost of energy $U$ due to ondot Coulomb repulsion, the two dots remain singly occupied in the ground state. Moreover, to facilitate the hopping between the quantum dots via the tunneling matrix-element $t$, the spins on the two dots will be required to be opposite due to Pauli exclusion principle. The remaining two spins on the leads are appropriately aligned to make the total spin zero ($S = 0$) for the four electron system. This forces the ground state to have a structure where with increasing $t$, the statistical weights of those basis states increase in which the dots are singly occupied and the electrons on the two dots have antiparallel spins. It is to be noted from Figure 2(a) that the AF correlation (with negative values) increases steeply for small values of interdot tunneling $t$ ($< U$) and for moderate values ($\leq 5$) the correlation saturates to a value depending the value of $U$. For $U \leq (|\varepsilon_1| = |\varepsilon_2|)$, the dots can possibly have double occupancy with opposite spins and the interdot tunneling causes the transfer of one of the spins to the other dot leading to AF correlation between the dots. For $U > (|\varepsilon_1| = |\varepsilon_2|)$, the AF correlation between the dots exhibits an abrupt increase (becomes more negative) when the $\left(4t^2/U\right) > 1$, as is evident from plots for $U/V = 10, 20, 30$ in Figure 2(a). For very large values of ondot Coulomb interaction $U/V = 10^6 \sim \infty$, the ratio $4t^2/U$ becomes vanishingly small for any value of $t$ and the probability amplitude of hopping between the dots is greatly suppressed.

We now examine how the interdot Coulomb interaction $g$ affects the spin-spin correlation between the dots. We observed in Figure 2(b) that the effect of interdot tunneling matrix-element $t$ becomes significant for large values of ondot Coulomb interaction $U > (|\varepsilon_1| = |\varepsilon_2|)$, we therefore choose one such value, $U = 20V$. Figure 2(b), shows the zero temperature spin-spin correlation $\langle \mathbf{S_1} \cdot \mathbf{S_2} \rangle$ between the dots *versus* interdot tunneling matrix-element $t$, for six different values of interdot Coulomb interaction $g$. It is observed that the interdot Coulomb interaction $g$ significantly reduces the AF correlation between the dots. This can plausibly be understood as: since the interdot Coulomb interaction $g$ suppresses the transfer of charge between the dots resulting in reduction of the statistical weight of those basis states in the ground state where the two dots are singly occupied with their spins opposite. Comparing Figure 2(b) with Figure 2(a), it can clearly be seen that even small values of the interdot Coulomb interaction $g$ compared to the ondot Coulomb interaction $U$ shows significantly large change in spin-spin correlation between the dots.

We now examine the effect of temperature. In Figure 3(a), we have plotted the spin-spin correlation $\langle \mathbf{S_1} \cdot \mathbf{S_2} \rangle$ between the dots *versus* temperature for three different values of interdot tunneling matrix-element $t$. At zero temperature, the magnetic correlation is finite and AF in nature since the interdot tunneling matrix-element $t$ is finite. Further, the magnetic correlation increases with increasing values of interdot tunneling matrix-element $t$. At a small value of




(a) (b)

**Figure 3.** Spin-spin correlation $\langle \mathbf{S_1} \cdot \mathbf{S_2} \rangle$ between the quantum dots *versus* temperature $T$. (a) The plots corresponds to three different values of interdot tunneling matrix-element: $t = 1-$solid line ; $t = 2-$dashed line and $t = 3-$dotted line at $U = 20$ and $g = 0$. (b) At $g = 0$ and $t = 1$, the plots corresponds to six different values of ondot interaction: $U = 3-$Solid line; $U = 5-$dashed line; $U = 10-$dotted line; $U = 20-$dash-dotted line; $U = 30-$dash double dotted line and $U = 10^6-$short-dashed line.

temperature ($T \ll 1$, in units of $V$), the AF correlation exhibits a (negative) maximum; this is due to the fact that the temperature causes excitations to available low-lying states giving additional contribution [9, 13]. As the temperature is increased further ($T > 1$), the spin-spin correlation between the dots is destroyed due to thermal excitations.

Lastly we examine how the ondot Coulomb interaction affects the thermal excitations. In Figure 3(b), we show the spin-spin correlation $\langle \mathbf{S_1} \cdot \mathbf{S_2} \rangle$ between the dots *versus* temperature for six different values of ondot Coulomb interaction $U$, at fixed interdot tunneling matrix-element, $t = 1$. For small values of ondot Coulomb interaction $U = 3, 5 \leq (|\varepsilon_1| = |\varepsilon_2|)$, a (negative) maximum in the AF correlation does not appear as the low-lying states are not accessible at small temperatures $T \ll 1$. For $U = 10, 20, 30 > (|\varepsilon_1| = |\varepsilon_2|)$, a maximum in the form of a (negative) peak appears in the AF correlation. This is due to the fact that the ondot interaction $U > (|\varepsilon_1| = |\varepsilon_2|)$ causes the low-lying excited states to be accessible at small temperatures. The AF correlation falls off exponentially with temperature.

## 4. Conclusion

The ZBW limit is applied to the ideal leads connected to DQD system in T-shaped geometry to study the magnetic correlation between the dots. The effects of interdot tunneling matrix-element, ondot Coulomb interaction, interdot Coulomb interaction on spin-spin correlation between the dots are examined at zero as well as finite temperatures. It is observed that, at zero temperature, the dots are coupled antiferromagnetically for finite values of interdot tunneling matrix-element, regardless of the values of other dot parameters like interdot, ondot Coulomb interactions. Further, for large values of ondot Coulomb interaction $U > (|\varepsilon_1| = |\varepsilon_2|)$, the AF correlation between the dots is significantly affected by the interdot tunneling matrix-

element. It is also seen that for infinitely large values of ondot Coulomb interaction, the AF correlation between the dots vanishes. The spin-spin correlation between the dots reduces significantly even for small values of interdot Coulomb interaction compared to the ondot Coulomb interaction, $g \ll U$. For finite temperatures it is observed that, for small values of temperature, the spin-spin correlation shows a (negative) maximum due to thermal excitation from the ground state to the low-lying excited states whereas for large values of temperature, the spin-spin correlation falls off exponentially. The spin-spin correlation between the dots can thus be tuned by manipulating system parameters also the geometry of the quantum dots and may have applications in realizing qubits for quantum computation.

## Acknowledgements.

Haroon is thankful to Jawaharlal Nehru Memorial Fund(JNMF), Teen Murti House, New Delhi, for providing fellowship for a part of the work.

## Competing Interests

The authors declare that they have no competing interests.

## Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

## References

[1] Wu, Jiang, Wang, Zhiming M., *Quantum Dot Molecules*, Springer-Verlag, New York, 2014.

[2] K. Shiraishi, H. Tamura and H. Takayanagi, Appl. Phys. Lett. 78, 3702 (2001).

[3] D. Loss and D.P. DiVincenzo, Phys. Rev. A, **57**, 120 (1998).

[4] Wang, Zhiming M., *Quantum Dot Devices*, Springer-Verlag New York, 2012.

[5] A.D. Yoffe, Adv. Phys., 2001, **50**, 1 (2001).

[6] W.G. van der Wiel, S. De Franceschi, J.M. Elzerman, T. Fujisawa, S. Tarucha and L.P. Kouwenhoven, Review of Modern Physics, **75**, 1 (2003).

[7] R. Allub and C.R. Proetto, Physical Review B, **62**, 10923 (2000).

[8] R. Allub and C.R. Proetto, Solid State Communications, **117**, 429-434 (2001).

[9] R. Allub, Physical Review B **67**, 144416 (2003).

[10] L.P. Kouwenhoven, D.G. Austing and S. Traucha, Rep. Prog. Phys., **64**, 701 (2001).

[11] S. Alexander and P.W. Anderson, Phys. Rev. A, **133**, 1594 (1964).

[12] B.R. Bulka and T. Kostyrko, Physical Review B, **70**, 205333 (2004).

[13] R. Allub, J. Phys. Condens. Matter, **20**, 445208 (2008).

[14] B.R. Alascio, R. Allub and A. Aligia, J. Phys. C: Solid St. Phys., **13**, 2869-2879 (1980).