Quantum Information Review
An International Journal

http://dx.doi.org/10.12785/qir/020102

Role of Quantum Discord and Entanglement in an Infinite Spin Chain

J. Batle[1,*] *and M. Abdel-Aty*[2,3,*]

[1] Departament de Física, Universitat de les Illes Balears, 07122 Palma de Mallorca, Spain
[2] Mathematics Department, College of Science, Bahrain University, Bahrain
[3] Department of Mathematics, Faculty of Science, Sohag University, 82524 Sohag, Egypt

Received: 9 Jun. 2013, Revised: 5 Oct. 2013, Accepted: 7 Oct. 2013
Published online: 1 Jan. 2014

Abstract: We review thermal properties of quantum correlations in the *thermodynamic limit* with reference to the XY-model. Although this model has been the subject of active entanglement-research, the bulk of the pertinent work refers to finite instantiations. As a consequence, the temperature cannot be properly defined in such circumstances, a problem that is overcome here. Our effort includes the interesting role of the quantum discord notion.

Keywords: Quantum Entanglement, Quantum Discord

1 Introduction

The tern nonlocality-entanglement-quantum discord is of obvious interest and possesses technological implications (see, for instance, [1]).

We revisit here the relation between quantum discord and entanglement in an infinite system, namely, the XY model (thermodynamic limit [2]), that, like the celebrated Ising and Heisenberg models, is one of the paradigmatic systems in statistical mechanics. Although this model has been the subject of active entanglement-research, the bulk of the pertinent work refers to finite instantiations (for a very illustrative example see, for instance, [3]). There is thus a gap in our thermal-discord knowledge that we intend to overcome here. Although the notion of quantum discord was proposed by Ollivier and Zurek [4] (see also [5]) some 10 years ago and much interesting work has been published in the ensuing decade, the concept remains somewhat elusive in regards as just what are the correlation it describes. Thus, studying the entanglement-discord correlations at high T may perhaps serve some enlightening purpose.
Since the formalization by Werner [6] of the modern concept of quantum entanglement it has become clear that there exist entangled states that comply with all Bell inequalities (BI). This entails that nonlocality, associated to BI-violation, constitutes a non-classicality manifestation exhibited only by just a subset of the full set of states endowed with quantum correlations. Later, exciting work by Zurek, Ollivier, Arnesen, Vedral, etc. (see for example, [4,5]) established that not even entanglement captures all aspects of quantum correlations. A new information-theoretical measure was introduced, quantum discord, that corresponds to a new facet of the "quantumness" that arises even for non-entangled states. Indeed, it turned out that the vast majority of quantum states exhibit a finite amount of quantum discord.

In some cases, however, entangled states are useful to solve a problem if and only if they violate a Bell inequality [7]. Moreover, there are important instances of non-classical information tasks that are based directly upon non-locality, with no explicit reference to the quantum mechanical formalism or to the associated concept of entanglement [8]. Last, but certainly not least, recent research indicates that quantum discord is also a valuable resource for the implementation of non-classical information processing protocols [9,10,11,12,13]. On the light of these developments, it becomes imperative to conduct a systematic exploration of the connections between the tripod members.

* Corresponding author e-mail: jbv276@uib.es, amisaty@gmail.com

It is thus our intention to study the interplay of entanglement and quantum discord for the XY model in the thermodynamic limit. To such an effect we will consider, after giving some background in Section II, the correlations existing between a pair of qubits located at two given sites (Section III)). Finally, some conclusions are drawn in Section IV.

2 Background

The Hamiltonian of the anisotropic one-dimensional spin-$\frac{1}{2}$ XY model in a transverse magnetic field h (N particles) reads

$$H = \sum_{j=1}^{N} [(1+\gamma)S_x^j S_x^{j+1} + (1-\gamma)S_y^j S_y^{j+1}] - h\sum_{j=1}^{N} S_z^j, \quad (1)$$

where $\sigma_u^j = 2S_u^j$ ($u = x,y,z$) are the Pauli spin-$\frac{1}{2}$ operators on site j, $\gamma \in [0,1]$ and $\sigma_u^{j+N} = \sigma_u^j$. The model (1) for $N = \infty$ is completely solved by applying a Jordan-Wigner transformation [2,15], which maps the Pauli (spin 1/2) algebra into canonical (spinless) fermions. The system (except for the isotropic case $\gamma = 0$) undergoes a paramagnetic-to-ferromagnetic quantum phase transition (QPT) [16,17] driven by the parameter h at $h_c = 1$ and $T = 0$. It is well known that near factorization a characteristic length scale naturally emerges in the system, which is specifically related with the entanglement properties and diverges at the critical point of the fully isotropic model [18].

Quantum discord [9,4] constitutes a quantitative measure of the "non-classicality" of bipartite correlations as given by the discrepancy between the quantum counterparts of two classically equivalent expressions for the mutual information. More precisely, quantum discord is defined as the difference between two ways of expressing (quantum mechanically) such an important entropic quantifier. Let ρ represent a state of a bipartite quantum system consisting of two subsystems A and B. If $S(\rho)$ stands for the von Neumann entropy of matrix ρ and ρ_A amd ρ_B are the reduced ("marginal") density matrices describing the two subsystems, the quantum mutual information (QMI) M_q reads [4]

$$M_q(\rho) = S(\rho_A) + S(\rho_B) - S(\rho). \quad (2)$$

This quantity is to be compared to another quantity $\tilde{M}_q(\rho)$, expressed using conditional entropies, that classically coincides with the mutual information. To define $\tilde{M}_q(\rho)$ we need first to consider the notion of conditional entropy. If a complete projective measurement Π_j^B is performed on B and (i) p_i stands for $Tr_{AB}\Pi_i^B \rho$ and (ii) $\rho_{A||\Pi_i^B}$ for $[\Pi_i^B \rho \Pi_i^B / p_i]$, then the conditional entropy becomes

$$S(A|\{\Pi_j^B\}) = \sum_i p_i S(\rho_{A||\Pi_i^B}), \quad (3)$$

and $\tilde{M}_q(\rho)$ adopts the appearance

$$\tilde{M}_q(\rho)_{\{\Pi_j^B\}} = S(\rho_A) - S(A|\{\Pi_j^B\}). \quad (4)$$

Now, if we minimize over all possible Π_j^B the difference $M_q(\rho) - \tilde{M}_q(\rho)_{\{\Pi_j^B\}}$ we obtain the quantum discord Δ, that quantifies non-classical correlations in a quantum system, *including those not captured by entanglement*. One notes then that only states with zero Δ may exhibit strictly classical correlations. Among many valuable discord-related works we just mention two at this point that are intimately related to the present one, e.g., Batle et al. [19].

3 Two qubits in the infinite XY model

The general two-site density matrix is expressed as

$$\rho_{ij}^{(R)} = \frac{1}{4}\left[I + \sum_{u,v} T_{uv}^{(R)} \sigma_u^i \otimes \sigma_v^j\right]. \quad (5)$$

$R = j - i$ is the distance between spins, $\{u,v\}$ denote any index of $\{\sigma_0, \sigma_x, \sigma_y, \sigma_z\}$, and $T_{uv}^{(R)} \equiv \langle \sigma_u^i \otimes \sigma_v^j \rangle$. Due to symmetry considerations, only $\{T_{xx}^{(R)}, T_{yy}^{(R)}, T_{zz}^{(R)}, T_{xy}^{(R)}\}$ do not vanish. Barouch *et al* [15] have provided exact expressions for two-point quantum correlations, together with details of the dynamics associated with an external field $h(t)$. For the purposes of this paper, we will consider only systems which at time $t = 0$ are in thermal equilibrium at temperature T. We have then the (canonical ensemble) expression $\rho(t = 0) = \exp[-\beta H]$, where $\beta = 1/kT$ and k is the Boltzmann constant. Following [15], one obtains $T_{xx}^{(1)} = G_{-1}, T_{yy}^{(1)} = G_1, T_{zz}^{(1)} = G_0^2 - G_1 G_{-1} - S_1 S_{-1}$, and $T_{xy}^{(1)} = S_1$, where

$$\begin{aligned} G_R = {} & \frac{\gamma}{\pi}\int_0^{\pi} d\phi \sin(R\phi) \frac{\tanh\left[\frac{1}{2}\beta\Lambda(h_0)\right]}{\Lambda(h_0)\Lambda^2(h_f)} \\ & \times[\gamma^2 \sin^2\phi + (h_0 - \cos\phi)(h_f - \cos\phi) \\ & -(h_0 - h_f)(h_f - \cos\phi)\cos(2\Lambda(h_f)t)] \\ & -\frac{1}{\pi}\int_0^{\pi} d\phi \cos(R\phi) \frac{\tanh\left[\frac{1}{2}\beta\Lambda(h_0)\right]}{\Lambda(h_0)\Lambda^2(h_f)} \\ & \times[\{\gamma^2 \sin^2\phi + (h_0 - \cos\phi)(h_f - \cos\phi)\}(\cos\phi - \\ & h_f) - (h_0 - h_f)\gamma^2 \sin^2\phi \cos(2\Lambda(h_f)t)], \end{aligned} \quad (6)$$

$$S_R = \frac{\gamma(h_0 - h_f)}{\pi}\int_0^{\pi} d\phi \sin(R\phi) \sin\phi \frac{\sin[2\Lambda(h_f)t]}{\Lambda(h_0)\Lambda(h_f)}, \quad (7)$$

with $\Lambda(h) = [\gamma^2 \sin^2\phi + (h - \cos\phi)^2]^{1/2}$. G_R is the two-point correlator appearing in the pertinent Wick-calculations and $M_z = \frac{1}{2}G_0$. The two-spin correlation functions are given by [15]

$$\langle\sigma_x^i\sigma_x^{i+R}\rangle = \begin{vmatrix} G_{-1} & G_{-2} & \cdots & G_{-R} \\ G_0 & G_{-1} & \cdots & G_{-R+1} \\ \vdots & \vdots & \ddots & \vdots \\ G_{R-2} & G_{R-3} & \cdots & G_{-1} \end{vmatrix}, \quad (8)$$

$$\langle\sigma_y^i\sigma_y^{i+R}\rangle = \begin{vmatrix} G_1 & G_0 & \cdots & G_{-R+2} \\ G_2 & G_1 & \cdots & G_{-R+3} \\ \vdots & \vdots & \ddots & \vdots \\ G_R & G_{R-1} & \cdots & G_1 \end{vmatrix}, \quad (9)$$

$$\langle\sigma_z^i\sigma_z^{i+R}\rangle = 4\langle\sigma_z\rangle^2 - G_R G_{-R}, \quad (10)$$

where $R = j - i$ (distance between spins). In the case where more than two particles are considered, the previous correlators no longer possess their previous Toeplitz matrix structure [20].

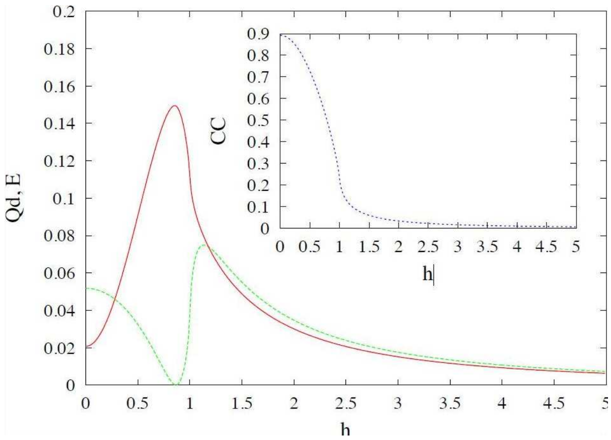

Fig. 1: Plot of quantum discord QD (upper solid curve) and entanglement of formation E (lower dashed curve) vs the external magnetic field h for two qubits in infinite the XY model (nearest neighbors), with anisotropy $\gamma = \frac{1}{2}$ at T=0. The region around the factorizing field h_f concentrates maximum QD. Inset depicts the corresponding classical correlations CC vs h. See text for details.

Let us write the two qubit states $\rho_{ij}^{(R)}$ (5) in the computational basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ as

$$\frac{1}{4}\begin{pmatrix} 1+4M_z+T_{zz} & 0 & 0 & T_{xx}-T_{yy}-i2T_{xy} \\ 0 & 1-T_{zz} & T_{xx}+T_{yy} & 0 \\ 0 & T_{xx}+T_{yy} & 1-T_{zz} & 0 \\ T_{xx}-T_{yy}+i2T_{xy} & 0 & 0 & 1-4M_z+T_{zz} \end{pmatrix}. \quad (11)$$

It turns out that states $\rho_{ij}^{(R)}$ in (11) are of such special aspect that the quantum discord QD turns out to be to be

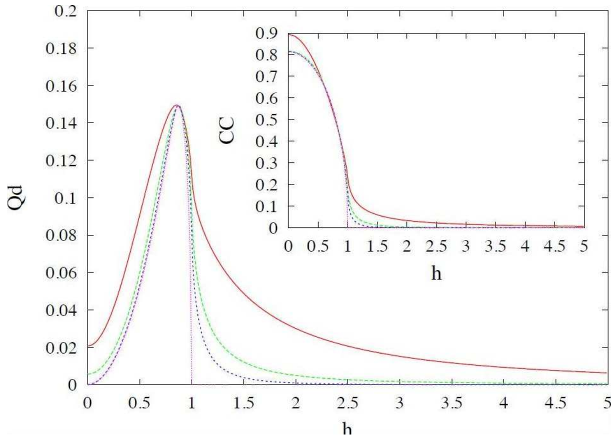

Fig. 2: Plot of QD for the same settings as in Fig. 1 for different relative distances $R = 1$ to 2, 3 and ∞ between spins. The further they are separated, the more they collapse into a single curve, which is zero for $h > 1$. Notice that E rapidly tends to zero for all h in the limit $R \to \infty$, while the corresponding QD remain finite. A similar behavior occurs for CC as depicted in the inset. See text for details.

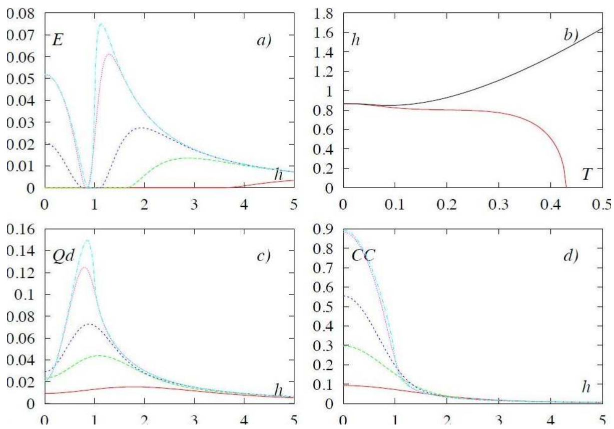

Fig. 3: (a) Value for E vs h for finite temperatures T=0.01,0.1,0.3,0.5,1 (from top to bottom) for $R = 1$ and $\gamma = \frac{1}{2}$. Notice how the region of null entanglement spreads form a point (at the factorising field $h_f = \sqrt{1-\gamma^2}$) to a region. (b) Plot of the aforementioned region of zero entanglement. The upper and lower curves define de limits of h for a given T where null E is found. This figure resembles a phase diagram-like plot where the regions of zero and nonzero entanglement are defined. (c) QD exhibits a particular behavior as T increases which tend to be maximum within the limits of zero entanglement. (d) CC vs h plot for the same temperatures. An overall decreasing tendency is apparent. See text for details.

analytically given (see Ref. [21]). Nevertheless, the concomitant QD can be easily obtained, in different fashion, as follows. The most general parameterization of the local measurement that can be implemented on one qubit (let us call it B) is of the form $\{\Pi_B^{0'} = I_A \otimes |0'\rangle\langle 0'|, \Pi_B^{1'} = I_A \otimes |1'\rangle\langle 1'|\}$. More specifically we have

$$|0'\rangle \leftarrow \cos\alpha|0\rangle + e^{i\beta'}\sin\alpha|1\rangle$$
$$|1'\rangle \leftarrow e^{-i\beta'}\sin\alpha|0\rangle - \cos\alpha|1\rangle, \quad (12)$$

which is obviously a unitary transformation –rotation in the Bloch sphere defined by angles (α,β')– for the B basis $\{|0\rangle,|1\rangle\}$ in the range $\alpha \in [0,\pi]$ and $\beta' \in [0,2\pi)$. After some cumbersome calculations, it turns out that the expression for a minimum discord Δ of the Introduction exhibits a positive and nonsingular Hessian, convex for the relevant range of values of (α,β'). Our expression possesses thus a unique global minimum, that occurs when the concomitant partial derivatives vanish. It can be proved that this happens whenever we have $(\sin\alpha = \frac{\sqrt{2}}{2}, \sin\beta' = 0)$ in the previous expression.

The present results correspond to pairwise entanglement and quantum discord for the infinite XY model at any temperature, including zero-one. This implies that one does not really need to "solve" the model in the sense of sufficiently augmenting the number of spins in the chain for the results to be thermally relevant. T here is an *actual*, thermometer-measurable temperature, since we are tackling a "real" thermodynamic system. This is to be confronted to the vast XY-literature associated to finite spin-numbers, where T is not, strictly speaking, well-defined in the thermodynamics sense.

A comparison between the discord QD and the entanglement of formation E at $T = 0$ is displayed in Fig. 1 (from now on we shall take the Boltzmann constant $k = 1$). QD and E are depicted versus the external magnetic field h (anisotropy $\gamma = \frac{1}{2}$) for the nearest neighbor configuration $R = 1$. Remarkably enough, the QD measure exhibits a maximum in the vicinity of the factorizing field $h_f = \sqrt{1-\gamma^2}$. Both QD and E seem to decay in the same fashion. The classical correlations (CC) for the same configuration are depicted in the inset of Fig. 1. Notice that all quantities here considered, i.e., QD, E, or CC, are ultimately described in terms of several G_Rs for all configurations, so that they all diverge at the QPT (for $h = 1$) in the same way.

As an illustration consider the magnetization given by $M_z(h) = \frac{1}{2}G_0 = \frac{\partial}{\partial h}\frac{1}{2\pi}\int_0^{\pi} d\phi[\gamma^2\sin^2\phi + (h-\cos\phi)^2]^{1/2}$. For $\gamma = 1$ we have $M_z(h) = \frac{\partial}{\partial h}\left(\frac{2(h+1)}{2\pi}E\left[\frac{2\sqrt{h}}{h+1}\right]\right) = \frac{1}{2\pi}\left[\frac{h-1}{h}K\left(\frac{2\sqrt{h}}{h+1}\right) + \frac{h+1}{h}E\left(\frac{2\sqrt{h}}{h+1}\right)\right]$, where $K(E)$ is the complete elliptic integral of the first(second) kind. Since $\frac{d}{dh}M_z$ diverges in logarithmic way at $h = 1$, as also do the divergence of K and the first derivatives of E, QD, and CC. In other words, they all signal the presence of a $h = 1$-QPT at zero temperature (except for the isotropic case $\gamma = 0$). In fact, the possibility of detecting a QPT at finite T by using QD has been recently considered by Werlang *et al.* [22]. They perfom an interesting analysis of the role of the temperature and QD in several quantum systems. We remember that a different concept such as nonlocality –as measured by the maximum violation of the well known Clauser-Horne-Shimony-Holt Bell inequality– was also considered as a QPT in [20] (also in the context of the XY-model). In the present work we do not focus attention on this particular issue of QPTs, but study instead the comparison between entanglement and quantum discord for finite and infinite systems at non-zero temperature.

Fig. 2 depicts the the same quantities as Fig. 1 for several configurations. As we increase the relative distance from $R = 1$ to 2, 3, and ∞, the corresponding QD's diminishes and also decays in faster and faster fashion with h. Notice that while entanglement (not shown here) globally diminishes, QD only tends to vanish for $h > 1$ and $R = \infty$. The inset here depicts the CC for the same configurations. They decreasing in the same fashion. While E tends to zero, both QD and CC remain nonzero, regardless of the distance between spins along the infinite chain.

As soon as we introduce a non-zero temperature things drastically change. In Fig. 3 we display several quantities at different temperatures ($T = 0.01, 0.1, 0.3, 0.5, 1$): $R = 1$ and $\gamma = \frac{1}{2}$. Fig. 3(a) depicts the entanglement of formation E for states $\rho_{ij}^{(R)}$ (5) versus the magnetic field h as we increase the temperature. T lowers and broadens the region of null entanglement from a point at the factorizing field h_f ($T = 0$) to finite intervals centered at h_f. Eventually, E becomes finite at higher values of h. This temperature-generated entanglement is depicted quantitatively in Fig. 3(b), where the region of zero entanglement extends from a point at zero T to a finite-sized region as T grows. The aforementioned region ceases to be finite beyond a critical temperature that depends on the particular R's and γ's involved therein. We discern some resemblance with a phase diagram: within the area encompassed by the two curves of Fig. 3(b) no entanglement is detected. It is surprising that, for the whole region, QD globally diminishes and tends to be concentrated in the null-E region, as can be seen in Fig. 3(c). These facts allow one to readily appreciate how different is the behavior of entanglement vis-a-vis that of QD. The role of classical correlations can be observed in Fig. 3(d). For the same set of temperatures employed above CC decreases i) as we augment T and ii) for increasing values of h, a behavior different from that of entanglement: while CC never vanishes, it is larger wherever $E = 0$. Both E and CC coexist for high values of h. We are dealing with a system for which, as we increase the temperature, entanglement survives –although barely– for high values of h. This fact clearly affects the existence of finite discord- or CC-values. Recall that this was the case already at $T = 0$. The role of the factoring field h_f in defining higher or lower values of QD becomes crucial. To further analyze the nontrivial relation between entanglement E and quantum discord QD at finite T it would enlightening to consider a physical system for which E would increase with the temperature. Such is the Heisenberg model's scenario, also a statistical mechanical model used in the study of critical points and phase transitions of magnetic systems [23,5].

4 CONCLUSIONS

We have compared entanglement E and quantum discord QD for magnetic systems at finite temperatures, comparing their behavior with that of classical correlations as well. It is clear that, some similarities notwithstanding, E and QD behave in quite different fashion in the thermodynamic limit. Although they represent the same magnitude for pure states, their differences are enhanced in realistic models such as the one studied here. The distinction we are trying to establish here is blurred in the case of finite systems. We conclude that for realistic systems E and QD should both be studied in independent fashion, as they reflect on different aspects of the quantum world.

ACKNOWLEDGEMENTS

J. Batle acknowledges fruitful discussions with J. Rosselló and M. del M. Batle, and partial support under project No. FIS2011-23526 (MINECO) and FEDER (EU). Aty: bla-bla..

References

[1] Nielsen M A and Chuang I L, *Quantum Computation and Quantum Information* (New York: Cambridge University Press), (2002).
[2] Lieb E, Schultz T and Mattis D, *Ann. of Phys.*, **16**, 407 (1961).
[3] Amit Kumar Pal and Indrani Bose, *Quantum Discord in the Ground and Thermal States of Spin Clusters* arXiv: 1012.0650.v3.
[4] Ollivier H and Zurek W H, *Phys. Rev. Lett.*, **88**, 017901 (2001).
[5] Arnesen M C, Bose S and Vedral V, *Phys. Rev. Lett.*, **87**, 017901 (2001).
[6] Werner R F, *Phys. Rev. A.*, **40,** 4277 (1989).
[7] Brukner C, Zukowski M and Zeilinger A, *Phys. Rev. Lett.*, **89,** 197901 (2002)
[8] Barrett J, Hardy L and Kent A, *Phys. Rev. Lett.*, **95**, 010503 (2005); Acín A, Gisin N and Masanes Ll, *Phys. Rev. Lett.*, **97**, 120405 (2006); Acín A et al, *Phys. Rev. Lett.*, **98**, 230501 (2007).
[9] Dakic B, Vedral V and Brukner C, *Phys. Rev. Lett.*, **105**, 190502 (2010).
[10] Ferraro A, Aolita L, Cavalcanti D, Cucchietti F M and Acín A *Phys. Rev. A.*, **81**, 052318 (2010).
[11] Datta S, *Phys. Rev. Lett.*, **100**, 050502 (2008).
[12] Lu S and Fu S, *Phys. Rev. A.*, **82**, 034302 (2010).
[13] Datta S arXiv [quant-ph] 1003.5256.
[14] Chandler D, *Introduction to Modern Statistical Mechanics* (New York: Oxford University Press), (1987); Mermin N D and Wagner, H *Phys. Rev. Lett.*, **17**, 1133 (1966); Olsson P, *Phys. Rev. B.*, **52**, 4526 (1995); Teitel S and Jayaprakash C, *Phys. Rev. B.*, **27**, 598 (1983).
[15] Barouch E, McCoy B and Dresden M, *Phys. Rev. A.*, **2**, 1075 (1970); Barouch E and McCoy B, *Phys. Rev. A.*, **3**, 786 (1971).
[16] Recall that a QPT is a qualitative change that occurs in the ground state of a many-body system due to modifications either in the interactions among its constituents or due to the effect of an external probe.
[17] Sachdev S, *Quantum Phase Transitions* (Cambridge: Cambridge University Press), (1999).
[18] Baroni F, Fubini A, Tognetti V and Verrucchi P, *J. Phys. A: Math. Theor.*, **40**, 9845 (2007).
[19] Batle J et al, arXiv:quant-ph/1103.0704, (2011).
[20] Batle J and Casas M, *Phys. Rev. A.*, **82**, 062101 (2010).
[21] Batle J and Casas M, e-print arXiv:quant-ph/1102.4653, and references therein.
[22] Werlang T *et al*, *Phys. Rev. Lett.*, **105**, 095702 (2010).
[23] Baxter R J, *Exactly solved models in statistical mechanics* (London: Academic Press), (1982).

Mahmoud Abdel-Aty completed his doctorate in quantum optics at Max-Plank Institute of Quantum Optics, Munch, Germany in 1999. After his analytical study of quantum phenomena in Flensburg University, Germany, 2001-2003, as a post doctorate visitor, he joined the Quantum Information Group at Sohag University in 2004, where he led the quantum optics group. He received the D. Sc. (Doctor of Science), in 2007. Now he is a visiting Professor at Lund University, Sweden and regular associate at ICTP, Italy. He is especially well known for seminal contributions to theories of quantum measurement, nanomechanical modeling, highly non-classical light, practical information security, and optical implementations of quantum information tasks. His current research interests include quantum resources, optical and atomic implementations of quantum information tasks and protocols. He is the Editor-in-Chief of Applied Mathematics & Information Sciences (an International Journal, USA), an editorial board member for several international journals. He has published over 174 papers in international refereed journals, two books and five book chapters. He has awarded several national and international prizes, from Italy, Jordan, Kwait and Egypt.