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Thermal Entanglement for Interacting Spin-1/2 Systems and its Quantum Criticality

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In this work, we investigate the thermal entanglement for interacting spin systems $H = 3(\vec{\sigma}_1 \cdot \vec{n})(\vec{\sigma}_2 \cdot \vec{n}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2 + B(\sigma_1^z + \sigma_2^z)$, by varying the parameters of temperature T, direction $\vec{n}$ and magnetic field B.

KEY WORDS: thermal entanglement; spin system; quantum criticality.

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1. INTRODUCTION

Recently entanglement as a valuable resource for quantum information processing (Bennett and DiVincenzo, 2000; Nielsen and Chuang, 2000; Plenio and Vedral, 1998) has attracted a lot of attention from both experimental and theoretical studies (Raimond *et al.*, 2001, 2002). This has provided strong motivation for the investigation probing for the presence of naturally available entanglement among interacting spin systems (Arnesen *et al.*, 2001; Connor and Wootters, 2001; Gunlycke *et al.*, 2001; Saguia and Sarandy, 2003; Wang, 2001), typically in the quantum spin chain systems. Perfect state transfer has been successfully illustrated in spin chains (Christandl *et al.*, 2004), i.e., for an unknown state, which is placed on one site of the chain, can be transmitted to a distant site with fidelity being equal to unity through the dynamical evolution of the spin system. The spin chains are also good candidates for quantum information storing and quantum memories (Bose, 2003; Burgarth and Bose, 2005; Christandl *et al.*, 2005; Yuang and Bose, 2005), quantum computation (Giampaolo *et al.*, in press; Li *et al.*, 2005), quantum clone (Chiara *et al.*, 2004), teleportation (Yeo, 2003; Barjaktarevic *et al.*, in press),

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and so on. Moreover, the realization that entanglement can also affect macroscopic properties (such as the magnetic susceptibility) of bulk solid-state systems (Ghosh *et al.*, 2003; Brukner *et al.*, 2006) has increased the interest in the characterizations of entanglement in terms of macroscopic thermodynamical observables.

Since the entanglement is fragile, the problem of how to create stable entanglement remains a main focus of recent studies in the field of quantum information processing. The thermal entanglement, which differs from other kinds of entanglement by its own advantages of stability, requires neither measurement nor controlled switching of interactions in the preparation process. Therefore the thermal entanglement appeared in various systems is a very attractive topic. In fact, it has been extensively studied for various systems including isotropic Heisenberg chain (Arnesen *et al.*, 2001; Connor and Wootters, 2001; Wang, 2002a,b), anisotropic Heisenberg chain (Wang, 2001; Kamta and Starace, 2002; Zhou *et al.*, 2003; Zhang and Li, 2005), Ising model in an arbitrarily directed magnetic field (Gunlycke *et al.*, 2001; Wang, 2001; Saguia and Sarandy, 2003), and cavity-QED (Mancini and Bose, 2004) since the seminal works of Arnesen *et al.* (2001) Nielsen (1998). However, almost of these models considered previously are approximately governed by the diagonal exchange interactions (i.e., involving only $\sigma_i^\alpha \sigma_j^\alpha$ terms, where $\alpha \in \{x, y, z\}$ and σ_i^α is the Pauli matrix for spin i) (Loss and DiVincenzo, 1998; Kane, 1998; Vrijen *et al.*, 2000). As we all know, spin-orbit coupling introduces the off-diagonal terms into the exchange Hamiltonian (Kavokin, 2001, 2004), whose thermal entanglement hasn't yet been studied. The purpose of this work is to investigate the extended case and compare it with the previous works.

The most general Hamiltonian describing N nearest-neighbor coupled spin-1/2 particles in one dimension is of the form $H = \sum_i \sum_{\alpha,\beta\in\{x,y,z\}} g_{i,i+1}^{\alpha\beta} \sigma_i^\alpha \sigma_{i+1}^\beta$, where $g_{i,i+1}^{\alpha\beta} = (g_{i,i+1}^{\beta\alpha})^*$. There are thus nine independent parameters for each pair of spins $i, i+1$. It is convenient to reexpress H in terms of a scalar part, symmetric part as well as antisymmetric part (Wu *et al.*, 2005). In addition we allow for the presence of a global external magnetic field $\vec{B}$, then the Hamiltonian reads

$$H = \vec{B} \cdot \sum_{i=1}^{N} \vec{\sigma}_i + \sum_{i=1}^{N} \sum_{\alpha=x,y,z} J_\alpha \sigma_i^\alpha \sigma_{i+1}^\alpha + \sum_{i=1}^{N} \vec{A} \cdot (\vec{\sigma}_i \times \vec{\sigma}_{i+1}) + \sum_{i=1}^{N} (\vec{C} \cdot \vec{\sigma}_i)(\vec{C} \cdot \vec{\sigma}_{i+1}) \quad (1)$$

where $\vec{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$, J_α are exchange coupling constants, $\vec{A}$ (the Dzyaloshinskii-Moriya vector in solid-state physics) typically arises from spin-orbit coupling, $\vec{C}$ can arise due to dipole-dipole coupling and other sources.

The paper is organized as follows. Sec II. is the formalism and results. Firstly we calculate the thermal entanglement as a function of temperature with the external magnetic field being zero, in this case the off-diagonal terms won't affect the thermal entanglement because of the isotropic symmetry of the Hamiltonian. Secondly we shall investigate the thermal entanglement with non-vanishing magnetic field. The last section is the conclusion and discussion.

2. FORMALISM AND RESULTS

Let us focus on the Hamiltonian describing two coupled spin-1/2 particles in an external magnetic field $\vec{B} = (0, 0, B)$ with the following form

$$H = 3(\vec{\sigma}_1 \cdot \vec{n})(\vec{\sigma}_2 \cdot \vec{n}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2 + B\left(\sigma_1^z + \sigma_2^z\right), \tag{2}$$

where $\vec{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$ are the Pauli operators for subsystem $i(i = 1, 2)$, $\vec{n} = \vec{r}/r = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, and $\vec{r} = \vec{r}_1 - \vec{r}_2$ is usually the relative coordinate between these two particles. In the absence of B, this kind of Hamiltonian has been appeared in the hyperfine structure of the hydrogen atom, describing interaction between the proton dipole moment and the spin dipole moment of the electron. In the present paper, we would like to play the Hamiltonian (2) as a toy model to investigate the thermal entanglement. For a system in equilibrium at temperature T, the density operator is

$$\rho = \frac{e^{-H/k_B T}}{Z}, \tag{3}$$

where $Z = \mathrm{Tr}[\exp(-H/k_B T)]$ is the partition function and k_B is Boltzmann's constant. For simplicity we set $k_B = 1$. Entanglement of two qubits can be measured by the concurrence

$$C = \max\left(0, 2\lambda_i^{\max} - \sum_{i=1}^{4} \lambda_i\right), \tag{4}$$

where λ_i are the square roots of the eigenvalues of the matrix $R = \rho\sigma_1^y \otimes \sigma_2^y \rho^* \sigma_1^y \otimes \sigma_2^y$, $*$ stands for complex conjugate. The values of concurrence range from zero, for a separable state, to one, for a maximally entangled state. The definition of concurrence (4) is available no matter that ρ is pure or mixed. In the case of a pure state $\rho = |\psi\rangle\langle\psi|$ with $|\psi\rangle = a|0,0\rangle + b|0,1\rangle + c|1,0\rangle + d|1,1\rangle$ the concurrence can be simplified to

$$C(|\psi\rangle) = 2|ad - bc|. \tag{5}$$

The concurrence, as a measurement of entanglement, is invariant under local unitary transformations, i.e.

$$C(\rho) = C(U_1 \otimes U_2 \rho U_1^\dagger \otimes U_2^\dagger). \tag{6}$$

Firstly, we consider the case with $B = 0$, a direct diagonalization of the Hamiltonian gives all eigenvectors and eigenvalues

$$
\begin{aligned}
&E_1 = 0, && |\psi_1\rangle = \tfrac{1}{\sqrt{2}}(0,\ 1,\ -1,\ 0)^T, && C(|\psi_1\rangle) = 1\\
&E_2 = 2, && |\psi_2\rangle = \tfrac{1}{\sqrt{2}}(e^{-i\phi},\ 0,\ 0,\ e^{i\phi})^T, && C(|\psi_2\rangle) = 1\\
&E_3 = 2, && |\psi_3\rangle = \tfrac{1}{\sqrt{2}}(\cos\theta e^{-i\phi},\ \sin\theta,\ \sin\theta,\ -\cos\theta e^{i\phi})^T, && C(|\psi_3\rangle) = 1\\
&E_4 = -4, && |\psi_4\rangle = \tfrac{1}{\sqrt{2}}(-\sin\theta e^{-i\phi},\ \cos\theta,\ \cos\theta,\ \sin\theta e^{i\phi})^T, && C(|\psi_4\rangle) = 1
\end{aligned} \tag{7}
$$

It is interesting that all eigenvectors are maximally entangled states. According to Eq. (3) the thermal equilibrium state is explicitly given by $\rho = Z^{-1} \sum_{i=1}^{4} \exp(-E_i/T)|\psi_i\rangle\langle\psi_i|$ and $Z = \sum_{i=1}^{4} \exp(-E_i/T)$. Thus the matrix R is obtained and the concurrence C can be calculated. Compared to the direct calculation, the symmetry analysis is helpful to obtain the final result of the concurrence. Because of the rotational symmetry of the Hamiltonian (Connor and Wootters, 2001; Wang and Zanardi, 2002), i.e., $[H, (\vec{\sigma}_1 + \vec{\sigma}_2)\cdot\vec{n}] = 0$, we can argue that the concurrence is independent of $\vec{n}$, called "isotropic." In fact, we can always apply a local unitary transformation $U_{\text{local}} = e^{-i\frac{\theta}{2}\hat{m}\cdot\vec{\sigma}_1} \otimes e^{-i\frac{\theta}{2}\hat{m}\cdot\vec{\sigma}_2}$ to ρ for arbitrary normed vector $\hat{m}$ and this transformation leaves the concurrence invariant according to (6). By choosing $\hat{m} = \vec{n}\times\hat{z}/|\vec{n}\times\hat{z}|$ without loss of generality, from (2) and $U_{\text{local}} H U_{\text{local}}^{\dagger}$ one then immediately arrives at the XXZ Heisenberg chain

$$H = 2\sigma_1^z \otimes \sigma_2^z - \sigma_1^x \otimes \sigma_2^x - \sigma_1^y \otimes \sigma_2^y \tag{8}$$

with the concurrence $C = \max\{0, (e^{4/T} - 1 - 2e^{-2/T})/Z\}$. Obviously, for $B = 0$, Eqs. (2) and (8) share the same concurrence for a fixed temperature T.

Let us briefly review the main results of the thermal entanglement in XXZ Heisenberg chain (Wang and Zanardi, 2002). As Fig. 1 shows, the maximum concurrence arrives at $T = 0$, which implies the maximally entangled state. In fact, since $E_4 = -4$ is the lowest eigenvalue, the thermal state ρ exclusively favors the non-degenerate ground state $|\psi_4\rangle$ at $T = 0$ and thus $C(|\psi_4\rangle) = 1$. With the increasing temperature, the concurrence decreases and eventually reaches zero for a critical temperature T_c^0. Analytic calculation shows that $T_c^0 = -\frac{1}{2}\ln(\sqrt[3]{53 + 6\sqrt{78}} + 1/\sqrt[3]{53 + 6\sqrt{78}} - 1) + \frac{\ln 6}{2} \approx 4.766$. This agrees well with the intuitive argument that temperature serves as a kind of noise which tends to cause a deterioration of quantum correlation.

Secondly, we apply a nonzero magnetic field along the z-direction. In this case we have only the rotational symmetry along the z-direction, in other words, the isotropy will only hold on in the xy-plane, and the concurrence is now only

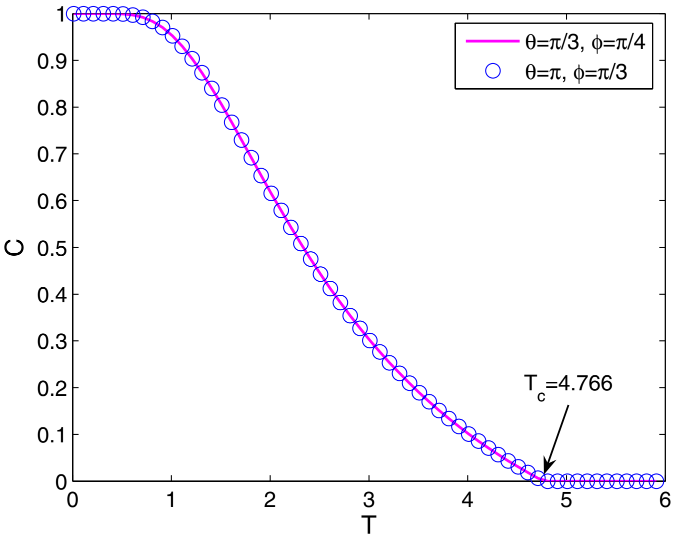

Fig. 1. The concurrence C vs the temperature T where $B = 0$. C decreases from one, for $T = 0$, to zero, for the critical temperature $T_c^0 \approx 4.766$. The concurrence C is isotropic, i.e. independent of the direction $\vec{n}$.

dependent on θ but independent on ϕ. Without loss of generality, one may choose $\phi = 0$, i.e., $\vec{n} = (\sin\theta, 0, \cos\theta)$, and from Eq. (2) one immediately obtains

$$H = (3\sin^2\theta - 1)\sigma_1^x\sigma_2^x - \sigma_1^y\sigma_2^y + (3\cos^2\theta - 1)\sigma_1^z\sigma_2^z + 3\sin\theta\cos\theta\left(\sigma_1^x\sigma_2^z + \sigma_1^z\sigma_2^x\right) + B\left(\sigma_1^z + \sigma_2^z\right). \tag{9}$$

The fourth term is an off-diagonal interaction. Except it the above Hamiltonian is nothing but the XYZ Heisenberg chain under a homogeneous magnetic field. The exact eigenvalues of Hamiltonian in Eq. (9) are

$$\begin{aligned} E_1 &= 0, \\ E_2 &= \frac{1}{3}Q + \frac{P}{Q}, \\ E_3 &= -\frac{1}{6}Q - \frac{P}{2Q} - i\frac{\sqrt{3}}{2}\left(\frac{1}{3}Q - \frac{P}{Q}\right), \\ E_4 &= -\frac{1}{6}Q - \frac{P}{2Q} + i\frac{\sqrt{3}}{2}\left(\frac{1}{3}Q - \frac{P}{Q}\right), \end{aligned} \tag{10}$$

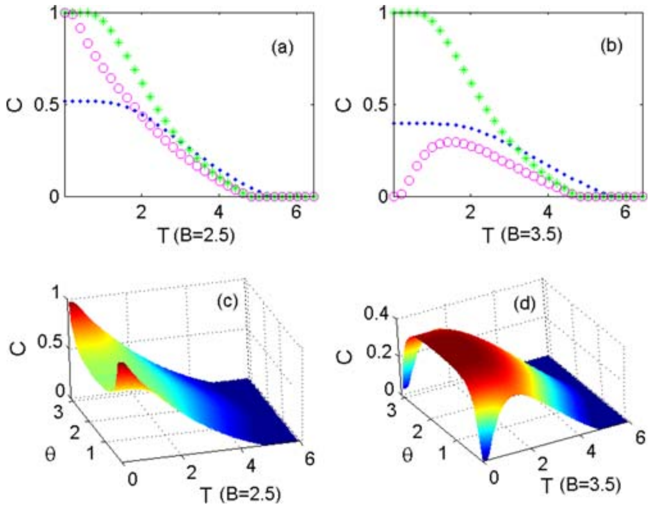

Fig. 2. (a) & (b): The concurrence C vs the temperature T when the external magnetic field $B = 2.5,\ 3.5$, respectively. The lines represent: green-dot, along x-axis; pink-circle, along z-axis; blue-star, $B = 0$ for comparison. (c) & (d): The concurrence C vs the temperature T and θ when the external magnetic field $B = 2.5,\ 3.5$, respectively. For $\theta = 0$ there is a critical magnetic field $B_c = 3$ turning C from 1 to 0.

where $P = 12 + 4B^2$ and complex number $Q = (-216 - 108B^2 + 324B^2\cos^2\theta + 12\sqrt{-27B^4 - 12B^6 - 972B^2\cos^2\theta - 486B^4\cos^2\theta + 729B^4\cos^4\theta})^{1/3}$. Obviously the external magnetic field also modifies the concomitant ground state and thus affects the concurrence.

In Fig. 2 we plot the dependence of the concurrence C on the temperature T as well as θ. Just as before, T still plays the role of noise and deteriorate the entanglement. Now the anisotropy exhibits a few interesting behaviors. Given a lower magnetic field $B = 2.5$ (Fig. 2a), the concurrence along the z-axis declines from its maximum 1 at $T = 0$ to zero at the critical temperature $T_c^z = T_c^0$, and is less than the concurrence when $B = 0$ on the whole. But along the x-axis (also along the y-axis) the concurrence varies from its maximum, far less than 1, to zero at a certain critical temperature $T_c^{xy} > T_c^0$. This means that the parallel field and the transverse field (or say the off-diagonal term) demonstrate obviously different effects on the entanglement. At some higher temperature, the concurrence along the x-axis surprisingly exceeds the concurrence when $B = 0$.

In the case of a higher magnetic field $B = 3.5$ (Fig. 2b), a markable difference is that the concurrence along the z-axis is reduced to zero at $T = 0$. As is shown below, this is due to the suppression of B, having its origin in the change of eigenvalues and eigenvectors. However, the concurrence gains its nonzero values as the temperature increases and finally resumes zero at $T_c^z = T_c^0$.

In Fig. 2c and d, we also plot the concurrence along other directions when $B = 2.5$ and $B = 3.5$, respectively. They show intergradation between $\theta = 0$ and $\theta = \pi/2$. Particularly, there are two characteristics to be emphasized on. One is that only along the z-axis would the concurrence be reduced to zero at $T = 0$ when the magnetic field exceeds a critical value, called B_c. The Hamiltonian along the z-axis can be simplified into XXZ chain and thus $B_c = 3$ exactly. We here just want to point out its uniqueness with respect to θ. In fact, the entanglement at $T = 0$ is firstly determined by the competition of eigenvalues. Except along the z-axis the eigenvalue E_4 under the magnetic field would keep the lowest while its corresponding eigenvectors $|\psi_4\rangle$ carries some entanglement, as the numerical result shows.

The other characteristic arises when we turn to the criticality of the temperature. We have shown that $T_c^z = T_c^0$ and $T_c^{xy} > T_c^0$. The intergradation of T_c, as we expect, is gradual, just as Fig. 3 shows. When $\theta = \frac{\pi}{2}$, T_c arrives its maximum, i.e., the two-spin system along the xy-plane is most robust to the temperature. This illuminates the fact that a transverse external field can partially weaken the destructive effect of thermal fluctuation and enhance the entanglement. Additionally, there is an evidence that the critical temperature is a monotonous function of B. The larger the magnetic field is, the larger the critical temperature becomes.

We now want to show the dependence of the concurrence C on B. At a lower temperature $T = 1$ (Fig. 4a), C along the z-axis is more than the one along the x-axis (also along the y-axis) when B is lower but decreases quickly when B rises

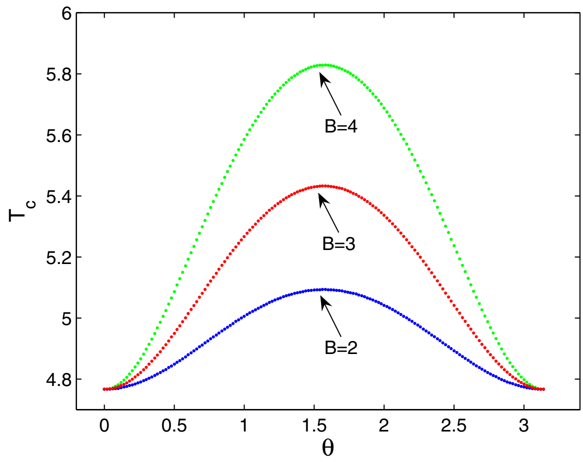

Fig. 3. The critical temperature T_c vs θ.

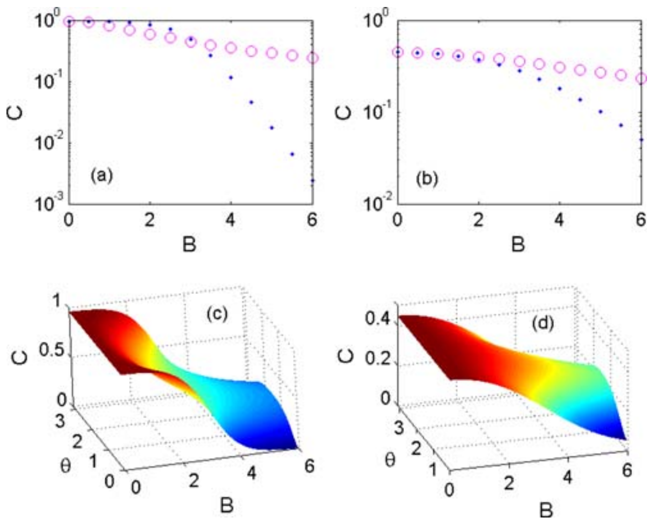

Fig. 4. (a) & (b): The concurrence C vs the magnetic field B when the temperature $T = 1,\ 2.5$, respectively. The lines represent: blue-dot, along z-axis; pink-circle, along x-axis. (c) & (d): The concurrence C vs the magnetic field B and θ when the temperature $T = 1,\ 2.5$, respectively.

up. However, not like the behavior of temperature, there is no such a critical value B_c. Along any directions C just gradually declines and remains a non-vanishing value for large B, though this value is practically useless. At a higher temperature $T = 2.5$ (Fig. 4b), the only difference is that C along the z-axis is wholly less than C along the x-axis. We may also regard the magnetic field as some kind of noise which tend to cause a deterioration of quantum correlation. However, just as Fig. 2d shows, B together with T won't play the superposition of their individual contributions to C. T sometimes even counterwork the suppression of B while B may tamper the destructive effect of T. In Fig. 4c and d, we also plot the concurrences along other directions when $T = 1$ and $T = 2.5$, respectively. They exhibit intergradation between $\theta = 0$ and $\theta = \pi/2$.

3. CONCLUSION AND DISCUSSION

In conclusion, we investigated quantitatively the thermal entanglement properties of a pair of interacting spin-1/2 systems via the Hamiltion $H = 3(\vec{\sigma}_1 \cdot \vec{n})(\vec{\sigma}_2 \cdot \vec{n}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2 + B(\sigma_1^z + \sigma_2^z)$, which includes an off-diagonal terms. The familiar Heisenberg XXZ and XYZ chains are shown as special form of our model in the absence (presence) of the magnetic field with the help of symmetry analysis. We have determined the dependence of entanglement, in terms of “concurrence,” on various parameters like the external magnetic field, the direction between the two spins as well as temperature. We find that the temperature and the magnetic field can affect the feature of the thermal entanglement significantly. High temperature may ruin the entanglement while the increasing magnetic field just reduces it. Together the temperature and the magnetic field doesn’t cooperate with each other to destruct the entanglement. At a certain temperature, the transverse magnetic field (or say the off-diagonal term) is most helpful for entanglement. In other words, the entanglement may be enhanced under an off-diagonal interaction. Meanwhile, the entanglement may be reproduced by thermal fluctuation from the spoiling by high magnetic field.

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REFERENCES

Arnesen, M. C., Bose, S., and Vedral, V. (2001). *Physical Review Letters* **87**, 017901.
Barjaktarevic, J. P., McKenzie, R. H., Links, J., and Milurn, G. J. (in press). eprint quant-ph/0501180.
Bennett, C. H. and DiVincenzo, D. P. (2000). *Nature* **404**, 247.
Bose, S. (2003). *Physical Review Letters* **91**, 207901.
Brukner, C., Vedral, V., and Zeilinger, A. (2006). *Physical Review A* **73**, 012110.
Burgarth, D. and Bose, S. (2005). *Physical Review A* **71**, 052315.
Chiara, G. D., *et al.* (2004). *Physical Review A* **70**, 062308.
Christandl, M., *et al.* (2005). *Physical Review A* **71**, 032312.
Christandl, M., Datta, N., Ekert, A., and Landahl, A. J. (2004). *Physical Review Letters* **92**, 187902.
Connor, O’ and Wootters, W. K. (2001). *Physical Review A* **63**, 052302.
Daniel, M. M. and Lidar, A. (2005). *Physical Review Letters* **94**, 040507.
Ghosh, S., Rosenbaum, T. F., Aeppli, G., and Coppersmith, S. N. (2003). *Nature (London)* **425**, 48.
Giampaolo, S. M., *et al.* (in press). eprint quant-ph/0503107.
Gunlycke, D. *et al.* (2001). *Physical Review A* **64**, 042302.
Kamta, G. L. and Starace, A. F. (2002). *Physical Review Letters* **88**, 107901.
Kane, B. E. (1998). *Nature (London)* **393**, 133.
Kavokin, K. V. (2001). *Physical Review B* **64**, 075305
Kavokin, K. V. (2004). *Physical Review B* **69**, 075302.
Li, Y., *et al.* (2005). *Physical Review A* **71** 022301
Loss, D. and DiVincenzo, D. P. (1998). *Physical Review A* **57**, 120.
Mancini, S. and Bose, S. (2004). *Physical Review A* **70**, 022307.
Nielsen, M. A. (1998). PhD Dissertation, The University of New Mexico, eprint quant-ph/0011036.
Nielsen, M. A. and Chuang, I. L. (2000). *Quantum Computation and Quantum Information*, Cambridge University Press, Cambridge.
Plenio, M. B. and Vedral, V. (1998). *Contemporary Physics* **39**, 431.
Raimond, J. M., *et al.* (2001). *Reviews of Modern Physics* **73**, 565.
Raimond, J. M., *et al.* (2002). *Vedral, Reviews of Modern Physics* **74**, 197.

Saguia, A. and Sarandy, M. S. (2003) *Physical Review A* **67**, 012315.
Vrijen, R., *et al*. (2000). *Physical Review A* **62**, 012306.
Wang, X. (2001). *Physical Review A* **64**, 012313.
Wang, X. (2002). *Physical Review A* **66**, 044305
Wang, X. (2002b). *Physical Review A* **66**, 034302.
Wang, X. and Zanardi, P. (2002). *Physics Letters A* **301**, 1.
Wu, L.-A., Bandyopadhyay, S., Sarandy, M. S., and Lidar, D. A. (2005). *Physical Review A* **72**, 032309.
Wu, L.-A., Sarandy, M. S., and Lidar, D. A. (2004). *Physical Review Letters* **93**, 250404.
Yeo, Y. (2003). *Physical Review A* **68**, 022316.
Yuang, M.-H. and Bose, S. (2005). *Physical Review A* **71**, 032310.
Zhang, G. F. and Li, S. S. (2005). *Physical Review A* **72**, 034302.
Zhou, L., Song, H. S., Guo, Y. Q., and Li, C. (2003). *Physical Review A* **68**, 024301.
Zhou, X., *et al*. (2002). *Physical Review Letters* **89**, 197903.