Entanglement in a simple quantum phase transition

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What entanglement is present in naturally occurring physical systems at thermal equilibrium? Most such systems are intractable and it is desirable to study simple but realistic systems that can be solved. An example of such a system is the one-dimensional infinite-lattice anisotropic *XY* model. This model is exactly solvable using the Jordan-Wigner transform, and it is possible to calculate the two-site reduced density matrix for all pairs of sites. Using the two-site density matrix, the entanglement of formation between any two sites is calculated for all parameter values and temperatures. We also study the entanglement in the transverse Ising model, a special case of the *XY* model, which exhibits a quantum phase transition. It is found that the next-nearest-neighbor entanglement (though not the nearest-neighbor entanglement) is a maximum at the critical point. Furthermore, we show that the critical point in the transverse Ising model corresponds to a transition in the behavior of the entanglement between a single site and the remainder of the lattice.

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I. INTRODUCTION

It seems to be a truism in quantum physics that strongly entangled systems exhibit complicated behavior which is difficult to quantify. Two practical examples of this ''principle'' are the conventional superconductor [1,2] and the fractional quantum Hall effect (FQHE) [3]. In both cases, for certain parameter regimes, the system enters a very interesting *entangled* state (the BCS ground state for the superconductor [4,5], and the Laughlin ground state for the FQHE [6]). For many years these systems resisted attempts to understand them using reasoning based on classical methods [7]. It required a major breakthrough, the construction of an insightful ground-state ansatz, to elucidate the physics of both the FQHE and the superconductor. The key feature of both systems, which makes it hard to explain them classically, appears to be that their ground states are *strongly entangled*.

Entanglement is a uniquely quantum property of any *nonlocal* superposition state of two or more quantum systems [12–14]. Such states are typified by the Bell state $|\Psi^-\rangle = (1/\sqrt{2})(|01\rangle - |10\rangle)$. The many curious features of entangled states have motivated considerable research. A remarkable consequence of this work is the emerging understanding of entanglement as a *resource* [12,15], like energy, which can be used to accomplish interesting physical tasks.

The similarities between entanglement and energy appear to be more than just superficial. It turns out to be possible to *quantify* the entanglement present in a given quantum state. This allows the development of quantitative high-level principles governing the behavior of entangled states, independent of their particular physical representation. These principles can be seen as analogous to the laws of thermodynamics governing the behavior of energy, independent of the specific form in which it is given to us. We hope that the quantitative theory of entanglement may provide a powerful unifying framework for the understanding of *complex* quantum systems. This is because, when viewed in terms of their entanglement content, a large number of apparently different states turn out to be equivalent.

This paper is one step in testing the hypothesis [16–19] that the study of complex quantum systems may be simplified by first analyzing the static and dynamic entanglement present in those systems. We will attempt to perform such an analysis in a representative system chosen from condensed-matter physics, specifically, the *XY* model [20]. The signature of complexity in this system is the occurrence of a quantum phase transition.

Quantum phase transitions (QPTs) are a qualitative change in the ground state of a quantum many-body system as some parameter is varied [21,22]. Unlike ordinary phase transitions, which occur at a nonzero temperature, the fluctuations in a QPT are fully quantum. Typically, at the *critical point* in parameter space where a QPT takes place, long-range correlations in the ground state also develop. The existence of a QPT in a quantum many-body system strongly influences the behavior of the system near the critical point, with the development of long-range correlations and a nonzero expectation value for an order parameter [21].

In Ref. [16] it was argued that QPTs are genuinely *quantum mechanical* in the sense that the property responsible for the long-range correlations is entanglement. It was also argued that the system state is strongly entangled at the critical point. It would be desirable, to begin with, to show that systems near quantum critical points can be simply characterized in terms of their entanglement content. Unfortunately, such a proof seems very difficult. We need first to understand the entanglement in such systems before proposing a classification scheme based on entanglement content. At the moment, the most promising technique to study entanglement in critical quantum systems appears to be the renormalization group, which is the standard way to obtain information about systems at and near criticality.

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The renormalization group (RG) is based on the notion that physics at small length scales (and hence higher energy scales) should not affect physics at much larger length scales. The RG is, in fact, a family of methods which can be applied to learn nonperturbative information about strongly interacting systems. The development of the renormalization group (see, for example, Refs. [23,24] for a review) has shown that phase transitions are *universal* in the sense that many properties of the system do not depend on the detailed dynamics of the system under consideration. Instead, using RG techniques, it has been shown that phase transitions depend only on certain global properties, such as symmetry and dimension. We would like to apply the ideas of the RG to calculate entanglement quantities in systems exhibiting a quantum phase transition. To see if this is possible, it is desirable to first carry out exact calculations in order to determine if similar universality properties govern the entanglement present in such systems. The purpose of this paper is therefore to do such calculations for the XY model.

Unfortunately the modern theory of entanglement (see, for example, Refs. [25–28]) is only partially developed, and at the present time can only be applied in a limited number of scenarios. In these limited scenarios, well-developed analytic tools exist to quantify the structure of entanglement present in a system. Two important scenarios are (a) the case of a pure state of a bipartite system, that is, a system consisting of only two components; and (b) a mixed state of two spin-$\frac{1}{2}$ particles.

For this reason, we focus our investigation on two types of calculation for the XY model. The first calculation is of the entanglement between a single site in the lattice and the rest of the system, for the ground state of the model. The second calculation is of the entanglement between two sites of the lattice at arbitrary temperatures and separations, allowing us to determine whether there are truly quantum features present in the two-body correlations in the system. Thus, although we do not obtain an understanding of the three-party and multiparty entanglement present in the system, we do calculate significant partial information characterizing the entanglement.

The entanglement present in condensed-matter systems has been investigated previously by a number of authors [17,19,29–37]. It was considered by Nielsen [17] who studied the Heisenberg model on two sites analytically. An expression for the ground-state entanglement in the infinite one-dimensional (1D) Heisenberg chain was obtained soon after by Wootters [30]. Numerical calculations of entanglement in the Heisenberg model on a small number of sites were carried out by Arnesen *et al.* [31]. Arnesen *et al.* identified parameter regions where there is appreciable *thermal entanglement*, which is entanglement present at nonzero temperatures. Recent studies include the numerical calculation of entanglement in the transverse Ising model on small numbers of sites [33], and analytic computations of entanglement in the XY model on two sites [29] and three sites [34]. Additional studies have been carried out on itinerant fermion systems [14] and other small condensed-matter systems related to the XY model [29,35–37].

The structure of this paper is as follows. In Sec. II the exact solution and calculation of the correlation functions for the XY model is outlined using the Jordan-Wigner transform. The thermal ground-state properties of this system are considered in Sec. III, focusing on the special case of the transverse Ising model, and the role entanglement plays in the quantum phase transition in this model. Thermal entanglement in the transverse Ising model is then calculated in Sec. IV. We conclude in Sec. V, and sketch some possible future research directions.

II. EXACT SOLUTION OF THE XY MODEL

In this section we consider the exact solution of the XY model on N sites, which is facilitated by use of the Jordan-Wigner transform [38]. The observables that are important for the calculation of the entanglement are evaluated in the *large-N* or *thermodynamic* limit. The two fundamental objects constructed in this study are the one- and two-site density matrices. From knowledge of these matrices it is possible to calculate the one- and two-party entanglement occurring in the XY model. The solution of the XY model is well known, and the procedure outlined in this section to solve it follows the standard method [15,16,39,40]. The main result in this section is the explicit construction of the one- and two-party density matrices for the XY model at thermal equilibrium.

The Hamiltonian for the anisotropic XY model on a 1D lattice with N sites in a transverse field is given by [41]

$$H=-\sum_{j=0}^{N-1}\left(\frac{\lambda}{2}[(1+\gamma)\sigma_j^x\sigma_{j+1}^x+(1-\gamma)\sigma_j^y\sigma_{j+1}^y]+\sigma_j^z\right), \tag{1}$$

where σ_j^a is the ath Pauli matrix ($a=x$, y, or z) at site j, γ is the degree of anisotropy, and λ is the inverse strength of the external field. We assume cyclic boundary conditions, so that the Nth site is identified with the 0th site. The standard procedure used to solve Eq. (1) is to transform the spin operators σ_j^a into fermionic operators via the Jordan-Wigner transform

$$c_i\equiv\prod_{j=0}^{i-1}[-\sigma_j^z]\sigma_i^-, \tag{2}$$

$$c_i^\dagger=\prod_{j=0}^{i-1}[-\sigma_j^z]\sigma_i^+, \tag{3}$$

where

$$\sigma_i^+\equiv\frac{1}{2}(\sigma_i^x+i\sigma_i^y),\quad \sigma_i^-\equiv\frac{1}{2}(\sigma_i^x-i\sigma_i^y). \tag{4}$$

It is easy to verify that c_i satisfy the fermionic anticommutation relations

$$\{c_i,c_j^\dagger\}=\delta_{ij},\quad \{c_i,c_j\}=0. \tag{5}$$

In terms of the fermionic operators, Eqs. (2) and (3), the Hamiltonian Eq. (1) assumes the quadratic form

$$H=\left(\sum_{i,j=0}^{N-1} c_i^\dagger A_{i,j} c_j + \frac{1}{2}\sum_{i,j=0}^{N-1}(c_i^\dagger B_{i,j} c_j^\dagger + \text{H.c.})\right)+N, \quad (6)$$

where $A_{i,i}=-1$, $A_{i,i+1}=-\frac{1}{2}\gamma\lambda=A_{i+1,i}$, $B_{i,i+1}=-\frac{1}{2}\gamma\lambda$, $B_{i+1,i}=\frac{1}{2}\gamma\lambda$, and all the other $A_{i,j}$ and $B_{i,j}$ are zero. The quadratic Hamiltonian Eq. (6) may be diagonalized by making a linear transformation of the fermionic operators,

$$\eta_q=\sum_{i=0}^{N-1}(g_{qi}c_i+h_{qi}c_i^\dagger), \quad (7)$$

$$\eta_q^\dagger=\sum_{i=0}^{N-1}(g_{qi}c_i^\dagger+h_{qi}c_i), \quad (8)$$

where $q=-N/2,-N/2+1,\ldots,N/2-1$ and the g_{qi} and h_{qi} can be chosen to be real. By requiring that the operators η_q obey fermionic anticommutation relations, and that the Hamiltonian Eq. (1) be manifestly diagonal when expressed in terms of the fermionic modes η_q, the following two coupled matrix equations must hold:

$$(A-B)\Phi_q=\omega_q\Psi_q, \quad (9)$$

$$(A+B)\Psi_q=\omega_q\Phi_q, \quad (10)$$

where the components of the two column vectors Φ_q and Ψ_q are given by

$$[\Phi_q]_i=g_{qi}+h_{qi}, \quad (11)$$

$$[\Psi_q]_i=g_{qi}-h_{qi}. \quad (12)$$

The quadratic Hamiltonian Eq. (6), when expressed in terms of the operators η_q, takes the diagonal form

$$H=2\sum_q \omega_q\eta_q^\dagger\eta_q-\sum_q \omega_q, \quad (13)$$

where

$$\omega_q=\sqrt{(\gamma\lambda\sin\phi_q)^2+(1+\lambda\cos\phi_q)^2}, \quad (14)$$

and $\phi_q=2\pi q/N$.

Now that the XY Hamiltonian has been diagonalized we can calculate the one- and two-site density matrices. Much of the remainder of this paper is concerned with the case where the system is at thermal equilibrium at temperature T. The density matrix for the XY model at thermal equilibrium is given by the canonical ensemble $\rho=e^{-\beta H}/\mathcal{Z}$, where $\beta\equiv 1/k_BT$, and $\mathcal{Z}=\mathrm{tr}(e^{-\beta H})$ is the partition function. The thermal density matrix is diagonal when expressed in terms of the Jordan-Wigner fermionic operators η_q. Our interest lies in calculating the quantum correlations present in the system as a function of the parameters β, γ, λ. In general, this problem requires knowledge of all the possible spin-correlation functions. These correlators are typically very difficult to calculate from ρ as it is diagonal in terms of the η_q's, which are complicated nonlocal functions of the original spin operators. Fortunately, the only correlation functions which we require are the one- and two-point correlation functions. The evaluation of these functions has been carried out previously [40,42].

The one- and two-site density matrices may be constructed from the one- and two-point correlation functions, using the *operator expansion* for the density matrix of a system of N spin-$\frac{1}{2}$ particles in terms of tensor products of Pauli matrices. For the single-site density matrix ρ_1 for the first spin—equal, by translational symmetry, to the state ρ_i of a single spin at an arbitrary site—the operator expansion reads

$$\rho_1=\mathrm{tr}_{\hat{i}}(\rho)=\frac{\sum_{\alpha=0}^{3} q_\alpha\sigma_i^\alpha}{2}, \quad (15)$$

where $\mathrm{tr}_{\hat{i}}$ is the partial trace over all degrees of freedom except the spin at site i, σ_i^α are the Pauli matrices acting on the site i with the convention $\sigma_i^0=I_i$, and the coefficients q_α are real. The coefficients q_α are determined by the relation

$$q_\alpha=\mathrm{tr}(\sigma_\alpha^i\rho)=\langle\sigma_\alpha^i\rangle. \quad (16)$$

To completely specify the single-site density matrix requires knowledge of three expectation values ($q_0=1$ because ρ_1 must have trace unity). However, because the Hamiltonian for the XY model Eq. (1) possesses symmetries it is possible to reduce this number to one. First of all, the Hamiltonian is real, so that $\rho_1^*=\rho_1$. As the matrix σ^y is imaginary this means that q_2 must be zero. The second symmetry that the XY Hamiltonian possesses is the global phase-flip symmetry

$$U_{\mathrm{PF}}=\prod_{j=0}^{N-1}\sigma_j^z. \quad (17)$$

This symmetry implies that $[\sigma^z,\rho_1]=0$, so forcing q_3 to be zero. The single-site density matrix ρ_1 is therefore determined solely by q_1.

For the two-site density matrix, which is the joint state of two spins at sites i and j, the operator expansion takes the form

$$\rho_{ij}=\mathrm{tr}_{\hat{ij}}(\rho)=\frac{\sum_{\alpha,\beta=0}^{3} p_{\alpha\beta}\sigma_i^\alpha\otimes\sigma_j^\beta}{4}. \quad (18)$$

The coefficients are determined by the relation

$$p_{\alpha\beta}=\mathrm{tr}(\sigma_i^\alpha\sigma_j^\beta\rho_{ij})=\langle\sigma_i^\alpha\sigma_j^\beta\rangle, \quad (19)$$

so that if the relevant correlation functions are known it is possible to construct the two-site density matrix completely.

The operator expansion Eq. (18) implies that we need sixteen correlation functions to construct the two-site density matrix. However, as in the case of the single-site density matrix, this number can be reduced by appealing to the symmetries of the Hamiltonian. Translational invariance of the

lattice means that the density matrix depends only on the distance $r=|j-i|$ between the spins, that is, $\rho_{ij}=\rho_{0r}$. Reflection symmetry about any site also means that $\rho_{ij}=\rho_{ji}$. Also, since the Hamiltonian is real, $\rho_{ij}^{*}=\rho_{ij}$. Finally, the global phase-flip symmetry implies that $[\sigma_i^z\sigma_j^z,\rho_{ij}]=0$. The symmetries of the XY model require that the only nonzero coefficients in the operator expansion Eq. (18) are p_{00}, p_{03}, p_{30}, p_{11}, p_{22}, and p_{33}. Furthermore, $p_{00}=1$ because the density matrix must have trace unity, and $p_{03}=p_{30}$.

In the thermodynamic limit, $N\to\infty$, sums that appear in the expectation values are replaced by integrals, and the correlation functions for the XY model can be reduced to quadratures [20,40,42,43]. The calculations are rather involved, and we merely summarize the results here. In thermal equilibrium, for arbitrary γ and λ, the transverse magnetization $\langle\sigma^z\rangle$ is given by [40]

$$\langle\sigma^z\rangle=-\frac{1}{\pi}\int_0^{\pi}d\phi(1+\lambda\cos\phi)\frac{\tanh\left(\frac{1}{2}\beta\omega_\phi\right)}{\omega_\phi}, \quad (20)$$

where we abuse notation and write $\omega_\phi\equiv\omega_q$ to indicate the replacement of ϕ_q with the continuous variable ϕ which results from the thermodynamic limit $\phi_q\to\phi$.

The two-point correlation functions are given by [42]

$$\langle\sigma_0^x\sigma_r^x\rangle=\begin{vmatrix} G_{-1} & G_{-2} & \cdots & G_{-r} \\ G_0 & G_{-1} & \cdots & G_{-r+1} \\ \vdots & \vdots & \ddots & \vdots \\ G_{r-2} & G_{r-3} & \cdots & G_{-1} \end{vmatrix}, \quad (21)$$

$$\langle\sigma_0^y\sigma_r^y\rangle=\begin{vmatrix} G_1 & G_0 & \cdots & G_{-r+2} \\ G_2 & G_1 & \cdots & G_{-r+3} \\ \vdots & \vdots & \ddots & \vdots \\ G_r & G_{r-1} & \cdots & G_1 \end{vmatrix}, \quad (22)$$

$$\langle\sigma_0^z\sigma_r^z\rangle=4\langle\sigma^z\rangle^2-G_rG_{-r}, \quad (23)$$

where

$$G_r=\frac{1}{\pi}\int_0^{\pi}d\phi\cos(\phi r)(1+\lambda\cos\phi)\frac{\tanh\left(\frac{1}{2}\beta\omega_\phi\right)}{\omega_\phi} - \frac{\gamma\lambda}{\pi}\int_0^{\pi}d\phi\sin(\phi r)\sin(\phi)\frac{\tanh\left(\frac{1}{2}\beta\omega_\phi\right)}{\omega_\phi}. \quad (24)$$

Summarizing, in the thermodynamic limit we may write the single-site density matrix ρ_1 entirely in terms of the transverse magnetization, Eq. (20),

$$\rho_1=\frac{I+\langle\sigma^z\rangle\sigma^z}{2}. \quad (25)$$

Similarly, the two-site density matrix ρ_{0r} can be written entirely in terms of the correlation functions Eq. (21), Eq. (22), Eq. (23), and the transverse magnetization,

$$\rho_{0r}=\frac{I_{0r}+\langle\sigma^z\rangle(\sigma_0^z+\sigma_r^z)+\sum_{k=1}^{3}\langle\sigma_0^k\sigma_r^k\rangle\sigma_0^k\sigma_r^k}{4}. \quad (26)$$

III. GROUND-STATE ENTANGLEMENT FOR THE TRANSVERSE ISING AND *XY* MODELS

In this section we discuss the quantum correlations occurring in the ground state of lattice systems undergoing a quantum phase transition. We argue that the critical point corresponds to the situation where the lattice is *critically entangled*, where, somewhat loosely, we define critically entangled to mean that entanglement is present on all length scales. In Sec. III A we outline the properties of the ground state of the transverse Ising model, which is a simple subclass of the anisotropic XY model. In Sec. III B the contribution to the ground-state correlations from one- and two-party entanglement in the XY model is calculated explicitly in order to illustrate the sharp peak in the entanglement at the critical point. Finally, in Sec. III C we discuss how the properties of shared entanglement may be related to critical quantum lattice systems.

In Ref. [16] it was argued that the physical origin of the correlations which occur in systems exhibiting a quantum phase transition is quantum entanglement. We reproduce the argument of Ref. [16] here in order that this study be self-contained. For concreteness, we restrict our attention to a lattice of spin-$\frac{1}{2}$ particles.

Suppose the ground state of a quantum lattice system was not entangled, that is, it is a product state. Then a simple calculation shows that the spin-spin correlation function $\langle\sigma_i^\alpha\sigma_j^\beta\rangle-\langle\sigma_i^\alpha\rangle\langle\sigma_j^\beta\rangle$ is identically zero. Thus, if the correlation function is nonzero then the ground state must be entangled. Furthermore, we conjecture that large values of the correlation function imply a highly entangled ground state; it is an interesting open problem to prove a precise form of this conjecture.

For general quantum lattice systems the correlation function decays exponentially as a function of the separation $|i-j|$ when the system is far from criticality [21]. When the system is at a critical point, the correlations decay only as a polynomial function of the separation. At this point a fundamental change in the ground state has occurred.

We believe that when a system approaches a critical point, the structure of the entanglement in the ground state undergoes a transition. Further, we conjecture that the nature of this transition is governed by a change in the spatial extent of the entanglement. The entanglement between a single spin and the rest of the lattice away from the critical point must be bounded in finite regions because the correlations are damped exponentially. At the critical point correlations develop on all length scales, and the physical property responsible for these correlations, entanglement, should become present at all length scales as well. We believe that a funda-

mental transition in the nature of the entanglement in the system occurs at this point; in some sense, at the critical point the state is delocalized, compared to the local nature of the entanglement away from the critical point. If this physical picture is correct, there should be evidence of entanglement developing on all length scales in the one- and two-party entanglement results.

As described in detail below, the ground state of the XY model exhibits the features we have described in the previous paragraphs. That is, maximality of the entanglement at criticality, and evidence that a transition in the entanglement structure takes place at the critical point. Although much work remains to be done to flesh out this physical picture, we believe that further research will show that these are generic properties of critical quantum systems.

A. Properties of the transverse Ising model ground state

The ground state of the XY model is very complicated with many different regimes of behavior [40,42]. For the sake of clarity, we focus most of our discussions on the transverse Ising model, which arises as the zero-anisotropy limit $\gamma \rightarrow 1$ in Eq. (1). The reason for this particular choice is because the transverse Ising model is the simplest quantum lattice system to exhibit a quantum phase transition [21]. The central goal in this section is to illustrate the intimate relationship between the entanglement structure of the ground state and the quantum phase transition. In particular, the calculations for the transverse Ising model provide the clearest evidence for the conjecture that the critical point corresponds to the situation where the lattice is most entangled.

The Hamiltonian for the transverse Ising model may be obtained from the XY model Hamiltonian, Eq. (1), by setting $\gamma = 1$,

$$H = -\sum_{j=0}^{N-1} (\lambda \sigma_j^x \sigma_{j+1}^x + \sigma_j^z). \tag{27}$$

The structure of the transverse Ising model ground state changes dramatically as the parameter λ is varied. The dependence of the ground state on λ is quite complicated. However, it is possible to investigate the $\lambda = 0$ and $\lambda \rightarrow \infty$ limits exactly.

When λ approaches zero, the transverse Ising model ground state becomes a product of spins pointing in the positive z direction,

$$|0\rangle_{\lambda \rightarrow 0} \approx \cdots |\uparrow\rangle_j |\uparrow\rangle_{j+1} \cdots. \tag{28}$$

In the $\lambda \rightarrow \infty$ limit the ground state again approaches a product of spins pointing in the positive x direction,

$$|0^+\rangle_{\lambda \rightarrow \infty} \approx \cdots |\rightarrow\rangle_j |\rightarrow\rangle_{j+1} \cdots. \tag{29}$$

The $\lambda \rightarrow \infty$ limit is fundamentally different from the $\lambda = 0$ case because the corresponding ground state is doubly degenerate under the global phase flip, Eq. (17), where

$$|0^-\rangle_{\lambda \rightarrow \infty} \equiv U_{\mathrm{PF}} |0^+\rangle_{\lambda \rightarrow \infty} \approx \cdots |\leftarrow\rangle_j |\leftarrow\rangle_{j+1} \cdots \tag{30}$$

is a second ground state. The $\lambda = 0$ ground state is invariant under the global phase flip. We note that in both limits the ground state approaches a product state.

Using the solutions obtained for the limiting cases of λ we can qualitatively describe the ground state as λ is varied. When λ is small, the exchange term $\sigma_j^x \sigma_{j+1}^x$ may be regarded as a perturbation, and perturbation theory may be used. In this case the ground state becomes a superposition of the unperturbed ground state and low-lying excitations in such a way that the small-λ ground state remains invariant under the global phase flip.

When λ is much greater than one, $1/\lambda$ is a small parameter and perturbation theory may again be used to show that the now-degenerate ground states are a superposition of the unperturbed ground states $|0^{+,-}\rangle$ and low-lying excitations. The degeneracy of the ground state under the global phase flip remains for λ large. (This degeneracy, along with the invariance of the ground state $|0\rangle$ under U_{PF} may be established nonperturbatively [21].)

When $\lambda = 1$ a fundamental transition in the form of the ground state occurs. The symmetry under the global phase flip breaks at this point and the system develops a nonzero magnetization $\langle \sigma^x \rangle \neq 0$ which grows as λ is increased. The magnetization is the *order parameter* which identifies the existence of a new phase.

Now that we have outlined the structure of the ground state for the transverse Ising model as a function of λ, we have a basic physical picture with which to interpret the exact results.

The calculation of the entanglement between a single site and the rest of the lattice requires construction of the single-site density matrix for the ground state. While the single-site density matrix for the thermal state was constructed in Sec. II, there is a distinction between the zero-temperature limit of the thermal density matrix and the ground state, because of the possible ground-state degeneracy. In the following, when referring to the *ground state* of the system, we suppose the system to be in one of the possible degenerate eigenstates $|0^+\rangle$ or $|0^-\rangle$ rather than any other linear combination. It does not matter which of the two is chosen to be ''the'' ground state because all the entanglement quantities calculated in this paper do not depend on the choice, due to the local symmetry connecting the two states. Therefore, without loss of generality, when the system is in the ground state we choose the system to be in the eigenstate $|0^+\rangle$ for $\lambda > 1$ and $|0\rangle$ for $\lambda \leqslant 1$. For simplicity, we will identify $|0^+\rangle$ with $|0\rangle$ when λ is greater than or equal to one.

The *zero-temperature state*, ρ_0, of the XY model may be found by taking the limit $\beta \rightarrow \infty$ of the canonical ensemble,

$$\rho_0 = \lim_{\beta \rightarrow \infty} \frac{e^{-\beta H}}{\mathcal{Z}}. \tag{31}$$

When the ground state is nondegenerate the zero-temperature state is the same as the ground state of the system, $\rho_0 = |0\rangle\langle 0|$. However, if the ground state is degenerate the zero-temperature ensemble becomes an equal mixture of all

the possible ground states. For the transverse Ising model the zero-temperature state may be written

$$\rho_0 = \frac{1}{2}|0^+\rangle\langle 0^+| + \frac{1}{2}|0^-\rangle\langle 0^-|. \tag{32}$$

In order to differentiate between the actual ground state $|0\rangle$ of the XY model and the zero-temperature ensemble we refer to ρ_0 as the *thermal ground state*.

In general, the canonical ensemble ρ possesses the same symmetries as the Hamiltonian Eq. (1). This is a simple consequence of the identity $[U,H]=0$, where U is some unitary or antiunitary operator representing the symmetry operation. The invariance follows from $[U,\rho]=0$, so that $U\rho U^\dagger=\rho$. In particular, while each individual degenerate ground eigenstate may not possess the same symmetries as the Hamiltonian, the thermal ground state ρ_0 has all the same symmetries.

The quantum phase transition in the transverse Ising model separates two different phases, the *paramagnetic* phase where the magnetization $\langle\sigma^x\rangle$ is zero, and the *ferromagnetic* phase where the magnetization becomes nonzero. Associated with the development of a nonzero value for the order parameter $\langle\sigma^x\rangle$ is the breaking of the phase-flip symmetry. The symmetry breaking present in the ground state $|0\rangle$ is a key feature of the quantum phase transition, and is responsible for the development of nonzero order parameter $\langle\sigma^x\rangle$ associated with the ferromagnetic phase. (In practice, small external perturbations force spontaneous symmetry breaking of the phase flip symmetry, and the system will choose one or the other ground state, so this order parameter is, in principle, observable.) This symmetry breaking cannot occur in the thermal ground state. For this reason, we will be most interested in properties of $|0\rangle$ rather that ρ_0. For each of the degenerate ground eigenstates $|0^+\rangle$ and $|0^-\rangle$ the global phase-flip symmetry is broken, so the terms that were set to zero in the operator expansion Eq. (18), as a consequence of the symmetry Eq. (17), may become nonzero.

The single-site density matrix ρ_1 for the ground state of the Ising model is obtained by taking a partial trace over all but one site of $|0\rangle\langle 0|$. In general, because the global phase-flip symmetry may be broken, the operator expansion for ρ_1 is only constrained by the reality condition $\rho_1^*=\rho_1$. Therefore, typically, two parameters are required to specify ρ_1 completely, the magnetization $\langle\sigma^x\rangle$ and the transverse magnetization $\langle\sigma^z\rangle$,

$$\rho_1 = \frac{I+\langle\sigma^x\rangle\sigma^x+\langle\sigma^z\rangle\sigma^z}{2}. \tag{33}$$

It is difficult to calculate the magnetization $\langle\sigma^x\rangle$ of the ground state explicitly because its expression in terms of Jordan-Wigner fermions is nonlocal, but it is possible to obtain $\langle\sigma^x\rangle$ from the large-r limit of the correlation function $\langle\sigma_j^x\sigma_{j+r}^x\rangle$ [43], yielding

$$\langle\sigma^x\rangle = \begin{cases} 0, & \lambda\leqslant 1 \\ (1-\lambda^{-2})^{1/8}, & \lambda>1. \end{cases} \tag{34}$$

The transverse magnetization $\langle\sigma^z\rangle$ is given by the integral Eq. (20) which reduces to an elliptic integral for $\gamma=1$ and $\beta\to\infty$,

$$\langle\sigma^z\rangle = \frac{1}{\pi}\int_0^\pi d\phi \frac{1+\lambda\cos\phi}{\sqrt{1+\lambda^2+2\lambda\cos\phi}}. \tag{35}$$

Armed with knowledge of the appropriate correlation functions we can now proceed to the calculation of the entanglement in the ground state of the XY and transverse Ising models.

B. Ground-state entanglement in the transverse Ising model

Given the modern understanding of entanglement as a physical resource, it makes sense to ask *how much* entanglement there is in a given multipartite state. In order to answer this question the notion of an *entanglement measure* has been developed. A review of work on entanglement measures may be found in Refs. [25–28].

The study of entanglement measures is far from completely developed. There is currently no consensus as to the best method to define an entanglement measure for all possible multipartite states. There are, however, situations where there is an unambiguous way to construct suitable measures. It is these situations that we study in this paper.

When a bipartite quantum system AB is in a pure state there is an essentially unique measure of the entanglement between the subsystems A and B given by the *von Neumann entropy* S [12,44–46]. The von Neumann entropy is calculated from the reduced density matrix ρ_A or ρ_B according to the formula

$$S \equiv -\operatorname{tr}(\rho_A\log_2\rho_A) = -\operatorname{tr}(\rho_B\log_2\rho_B). \tag{36}$$

When either subsystem A or B is a spin-$\frac{1}{2}$ system, S varies from 0 (product state) to $S=1$ (maximally entangled state). For the ground state of the transverse Ising model we regard a single site as subsystem A and the rest of the lattice as subsystem B.

When a bipartite system AB is in a mixed state there are a number of proposals for measures of the entanglement in the state, including, the *entanglement of formation* [12,27], the *distillable entanglement* [12,47], and the *relative entropy of entanglement* [48,49]. Each of these measures has the property that, for pure states of AB, they reduce to the von Neumann entropy. The entanglement of formation $\mathcal{F}(A:B)$ is the best understood of the mixed-state entanglement measures. For this reason, in this paper, we use the entanglement of formation to measure the mixed-state entanglement in the XY model.

The entanglement of formation $\mathcal{F}(\rho)$ for a bipartite mixed-state ρ measures the minimum expected amount of entanglement (as measured by the von Neumann entropy S) required to prepare ρ [50]. Mathematically, this is expressed by the formula

$$\mathcal{F}(\rho) = \inf_{\{q_j,|\psi_j\rangle\}} \langle E\rangle_{\{q_j,|\psi_j\rangle\}}, \tag{37}$$

where $\{q_j, |\psi_j\rangle\}$ is a pure-state decomposition for ρ (i.e., $\rho = \Sigma_j q_j |\psi_j\rangle\langle\psi_j|$) and

$$\langle E\rangle_{\{q_j,|\psi_j\rangle\}} = \sum_j q_j S(\mathrm{tr}_B(|\psi_j\rangle\langle\psi_j|)) \tag{38}$$

is the expected entanglement required to form ρ from the pure-state decomposition $\{q_j, |\psi_j\rangle\}$. The infimum in Eq. (37) runs over all pure-state decompositions of ρ.

At the current time, there is no simple way to calculate the entanglement of formation Eq. (37) for mixed states of bipartite systems AB where the dimension of A or B is three and above. However, for the case where both subsystems A and B are spin-$\frac{1}{2}$ particles there exists a simple formula from which the entanglement of formation can be calculated [51]. In this case the entanglement of formation is given in terms of another entanglement measure, the *concurrence* C [27,51,52]. The entanglement of formation varies monotonically with the concurrence.

The entanglement S between a single site and the rest of the lattice represents the collective contibutions of the entanglement between the given site and all other sites in the lattice. Unfortunately, the single-site entanglement does not tell us how the entanglement is shared out. For example, $S = 1$ could mean that the site in question is maximally entangled with a neighboring site, *or*, entangled with many sites. In the transverse Ising model it appears that S is related to the onset of correlations in a fairly direct way (see below), and to reflect this we speak of S as ''measuring'' how entangled the lattice is.

We should point out that this situation is by no means typical. It is quite common for the ground state of a condensed-matter system to possess strong nearest-neighbor entanglement and no long-range correlations (see, for example, the models constructed by Affleck, Kennedy, Lieb, and Tasaki (AKLT) discussed in Ref. [53]). Analysis of the entanglement in various AKLT models carried out by the authors has shown that, in fact, the single-site entanglement is *constant* for all parameter values even though long-range correlations develop and vanish. The entanglement in these models (and many other condensed-matter systems) is, in general, not revealed from knowledge of the single-site density matrix. What is really needed—but which has not yet been developed—to study these models is an entanglement measure which can take account of the way entanglement is shared out.

At the critical point, $\lambda_c = 1$, of the transverse Ising model there is a fundamental transition in the structure of the ground state. The correlation function $\langle\sigma_i^\alpha\sigma_j^\beta\rangle - \langle\sigma_i^\alpha\rangle\langle\sigma_j^\beta\rangle$ decays polynomially as a function of separation at this point (the dominant term has exponent $-\frac{1}{4}$) while for all other values of λ this decay is exponential. Interestingly, one could argue that the correlation function itself actually constitutes an entanglement measure for pure states as it transforms as a tensor under local unitary operations and is zero for product states. As argued earlier, the change in the correlation function signals a fundamental change in the entanglement present in the ground state. This change is reflected in the single-site entanglement S for the ground state which appears in Fig. 1. The single-site entanglement varies from zero at $\lambda = 0$, where the ground state is a product, to a maximum at the critical point $\lambda = 1$. As the limit $\lambda \to \infty$ is approached S also approaches zero because the ground state again approaches product form. The single-site von Neumann entropy for the thermal ground state of the transverse Ising model is also shown in Fig. 1. Unlike the ground-state case, the entropy approaches unity in the limit $\lambda \to \infty$. This is because the thermal ground state approaches an equal mixture of two pure states (the eigenstates $|0^+\rangle$ and $|0^-\rangle$) in this limit. The single-site entropy is not measuring the entanglement content of the thermal ground state in this limit, rather it is measuring the degree of mixedness of the thermal ground state.

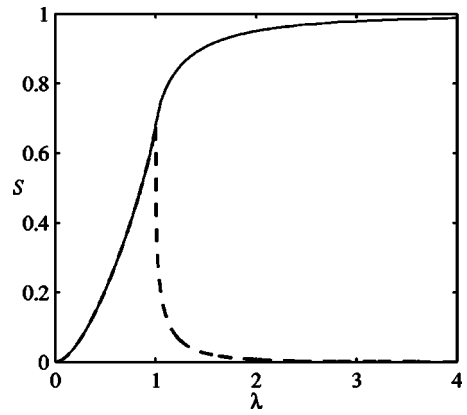

FIG. 1. Single-site entropy S for the thermal ground state ρ_0 (solid line) and the single-site entanglement for the ground state $|0^+\rangle$ (dashed line) of the transverse Ising model.

It is an intriguing fact that systems with quite different microscopic dynamics may behave equivalently at criticality. Further, their behavior depends only on the dimension of the system and the symmetry of the order parameter. The character of this behavior is captured by a small number of *universal* quantities whose behavior at criticality is completely described in terms of a unique *single* number, a *critical exponent*. The equivalence of physically different systems and their simple dependence on certain global properties at criticality is known as *universality*. One of the triumphs of twentieth century physics was the development of the RG, which provided an explanation for the emergence of universality in critical systems.

If we are to suppose that S is a universal quantity which could be studied via the RG then we should be able to find a critical exponent for S. In other words, near the critical point we should be able to write something like

$$S \propto |\lambda - \lambda_c|^\gamma, \tag{39}$$

where γ is the critical exponent for S. Unfortunately, this is not possible. As we describe below, the single-site entanglement is two sided, so that *two* numbers are needed to specify S like Eq. (39) near the critical point, one for each of the two ways of approaching $\lambda_c = 1$. In this way we see that the single-site entanglement is *not* a universal quantity.

The two-sided behavior of the single-site entanglement arises because the single-site density matrix depends on both the magnetization and the transverse magnetization. In the region near $\lambda \leqslant 1$ only the transverse magnetization is nonzero and the single-site entropy rises linearly. At the critical point the magnetization becomes nonzero and increases as $\lambda^{1/8}$. This becomes the dominant term in the expression for the single-site entanglement, and so the decay of the single-site entanglement is faster than linear in the region near $\lambda > 1$.

If there exist universal quantities related to the entanglement in critical quantum systems, then it is likely that they are derived from entanglement measures that satisfy additional properties beyond the set usually regarded as ''essential'' for an entanglement measure (see, for example, Refs. [45,48]). There are two main reasons why we make this assertion. The first arises from the inability of the single-site entanglement to distinguish between neighboring and distributed entanglement. In order to distinguish between these differing scenarios, a good entanglement measure for critical quantum systems should take account of how the entanglement is shared out. The second reason is that, as we argue below, the single-site entanglement is not *rescalable*. If a quantity is to be renormalizable it is necessary that it be rescalable. That is, it must be possible to collect degrees of freedom together, calculate the collective value of the quantity, and then rescale (or ''renormalize'') the collective value. A renormalizable entanglement measure should be rescalable in this way.

We should be a little more precise in our definition of rescalability for entanglement measures. Say we wish to calculate the bulk entanglement of a block of spins $s_1, s_2, \ldots, s_m$ in a lattice with the rest of the lattice, L. If the entanglement measure $\mathcal{G}$ (for example, $\mathcal{G}$ could be the entanglement of formation) used to calculate this entanglement is to be rescalable then, in the very least, it must satisfy the *extensivity relation*

$$\mathcal{G}(s_1, s_2, \ldots, s_m : L) \geqslant \mathcal{G}(s_1 : L) + \cdots + \mathcal{G}(s_m : L). \quad (40)$$

This inequality expresses the idea that the entanglement of a collection of spins with the rest of the lattice should be *at least as great* as the sum of the entanglements of each spin with L. If an entanglement measure does not satisfy the extensivity relation Eq. (40) then it is not clear how to rescale the bulk value of the entanglement.

Summarizing, the failure of the single-site entanglement to be universal may be due to the facts that: (a) it does not distinguish localized from distributed entanglement; and (b) it is not rescalable, in a sense that we can now make explicit. To do this, note first that it has previously been shown that the entanglement of formation does not satisfy Eq. (40) [54]. If we regard the single-site entanglement S as the entanglement of formation $S = \mathcal{F}(s_1, L)$ between a single spin s_1 and the rest of the lattice L, it seems unlikely that it will be a universal quantity. [There do exist other entanglement measures which reduce to the von Neumann entropy for pure states [12,15,48,49]. It is an open question whether they satisfy Eq. (40).]

There are indications [54], however, that the *square* of the concurrence *is* extensive. Perhaps a suitable generalization of the concurrence will turn out to be the best quantity for studying universal properties of entanglement. Evidence that this is the case has recently been obtained by Osterloh *et al.* [55] where they found that a quantity related to the concurrence *is universal* for the transverse Ising and XY models. It would be interesting to investigate this behavior and see if it arises because of the possible extensivity properties of the concurrence. Note, incidentally, that universal behavior in the concurrence does not necessarily imply universal behavior for the entanglement of formation, for the latter is only a function of the former in the special case of a two-qubit system.

The determination of what entanglement is shared by two sites in the lattice requires a measure of the two-party entanglement present in mixed states. We will henceforth use the concurrence C to measure the two-party mixed-state entanglement between two spins. The concurrence of two spin-$\frac{1}{2}$ particles may be calculated from their density matrix ϱ via the formula

$$C(\varrho) = \max[0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4], \quad (41)$$

where the λ_i are the eigenvalues in decreasing order, of the Hermitian matrix $R \equiv \sqrt{\sqrt{\varrho}\,\tilde{\varrho}\,\sqrt{\varrho}}$, and $\tilde{\varrho} = (\sigma^y \otimes \sigma^y)\varrho^*(\sigma^y \otimes \sigma^y)$. The concurrence varies from $C = 0$ for a separable state to $C = 1$ for a maximally entangled state [56].

The two-site density matrices for the ground state of the XY model are difficult to calculate when there is ground-state degeneracy. This is because the magnetization $\langle \sigma^x \rangle$ becomes nonzero as the phase-flip symmetry is broken, and it becomes necessary to include the correlation function $\langle \sigma_0^x \sigma_r^z \rangle$ in the operator expansion Eq. (18). The $\langle \sigma_0^x \sigma_r^z \rangle$ correlation function is nonlocal when expressed in terms of the Jordan-Wigner fermionic operators and there is no simple way to derive it from other correlators. As a result of this difficulty we do not calculate the two-site density matrix for the ground state, instead, all two-site calculations are performed with respect to the thermal ground state. However, because the thermal ground state for the transverse Ising model takes the special form Eq. (32), it is possible to place bounds on the entanglement that can occur between two sites in a degenerate ground state.

The entanglement between pairs of sites for the thermal ground state of the transverse Ising model shares many of the same features of the single-site entanglement. The entanglement, as measured by the concurrence, between neighboring sites and next-nearest neighboring sites is shown in Fig. 2 and Fig. 3, respectively. All other pairs have zero two-party entanglement because the correlation functions drop below the threshold for a positive concurrence. In both cases the entanglement rises from zero in the limits $\lambda = 0$ and $\lambda \to \infty$ to a maximum value near the critical point $\lambda = 1$. When $\lambda \leqslant 1$, the ground state coincides with the thermal ground state so that the two-site entanglement results are the same in this case. Note that the maximum does not occur *exactly* at the critical point $\lambda = 1$. At first site this may appear to contradict our earlier conjecture that we expect entanglement to be the

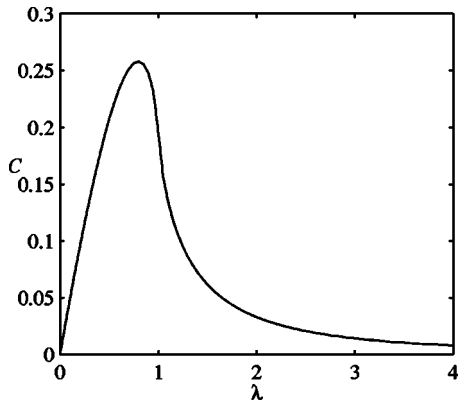

FIG. 2. Nearest-neighbor concurrence C at zero temperature for the transverse Ising model.

greatest at the critical point. In fact, as explained in Sec. III C, the reason for this is that the results here are for two-site entanglement, and are not inconsistent with the conjecture that the *total* entanglement in the lattice is a maximum at the critical point.

The entanglement E_{0j} between any two sites, 0 and j, and the rest of the lattice, can also be calculated for the parameter regimes where the ground state of the XY model is unique (e.g., $\lambda<1, \quad \gamma=1$). We have not included the results of such calculations as we are not able to calculate E_{0j} outside of the region $\lambda<1, \quad \gamma=1$. In addition, qualitatively, for $\lambda<1, \quad \gamma=1$ the results for E_{0j} are very similar to single-site entanglement results in Fig. 1.

It is interesting to see what effect the ground-state degeneracy has on the two-site entanglement in the ground state. As mentioned, it is not possible to study the two-site entanglement for $\lambda>1$. Despite this difficulty, for λ above the critical value, we can place a lower bound on the two-site entanglement in a degenerate ground state. This may be achieved by observing that the concurrence measure C is *convex* [51], which means that

$$C\left(\sum_{i=1}^{n} p_i\rho_i\right)\leqslant\sum_{i=1}^{n} p_i C(\rho_i), \tag{42}$$

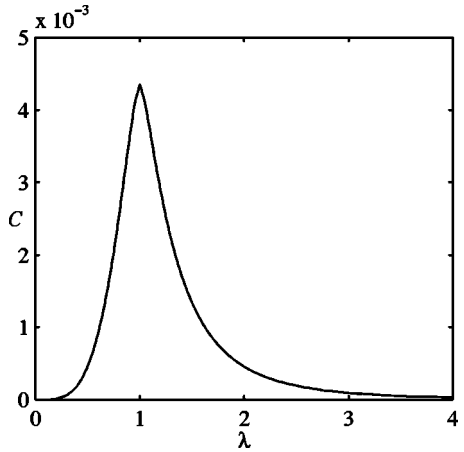

FIG. 3. Next-nearest-neighbor concurrence C at zero temperature for the transverse Ising model.

where p_i is any probability distribution and ρ_i a set of two-site density matrices. If we apply this inequality to the thermal ground state, Eq. (32), we obtain $C(\rho_{0r}) \leqslant \frac{1}{2}C(\mathrm{tr}_{\hat{0}r}(|0^+\rangle\langle 0^+|))+\frac{1}{2}C(\mathrm{tr}_{\hat{0}r}(|0^-\rangle\langle 0^-|))$. The global phase flip is a local unitary operation, so that the concurrence of each term in the right-hand side (RHS) of the inequality is the same, that is

$$C(\rho_{0r})\leqslant C(\mathrm{tr}_{\hat{0}r}(|0^+\rangle\langle 0^+|)). \tag{43}$$

In this way we see that the two-party entanglement in the ground state is at least as large as the two-party entanglement in the thermal ground state.

C. Critical quantum systems and the constraints of shared entanglement

The maximum value of the concurrence between neighboring sites does not occur at the critical point. This seemingly contradicts the idea that the strength of the correlations is proportional to the entanglement, and that therefore the entanglement should be maximal at the critical point. However, as we will discuss in this subsection, there are reasons based on the properties of shared entanglement to expect that this maximum should occur away from the critical point.

It is well known that there are limitations to the amount of entanglement that may be distributed amongst three or more subsystems [30,54,57–61]. This class of problem, that is, the determination of how much two-party entanglement can be distributed amongst a given number of parties, is known as an *entanglement-sharing* problem. The simplest example of this is the situation of three parties A, B, and C. If A is maximally entangled with B then it is not possible for A and C or B and C to share any two-party entanglement. Entanglement sharing is relevant to the quantum phase transition in the transverse Ising model as it provides a fundamental bound on the amount of entanglement that may be distributed amongst the sites. The existence of such a bound means that as the overall entanglement in the lattice is increased, some sites become pairwise more disentangled. An example where this occurs is in a system approaching a critical point.

As the critical point is approached in the transverse Ising model the correlation length begins to increase. What occurs physically is that each site develops entanglement with its neighboring sites. When the system gets closer to the critical point each site begins to develop entanglement with its next-nearest neighbors and so on. When the system is not at the critical point the entanglement between a single site and the rest of the lattice is localized within some region because the correlations are exponentially damped for large enough separation. At the critical point this is no longer the case; there are appreciable correlations between a single site and every other site. However, the entanglement associated with this correlation must be distributed in such a way that it satisfies the constraints of entanglement sharing.

We conjecture that saturating the constraints of shared entanglement is a natural symmetry for critical quantum systems. There are many ways to saturate the constraints of shared entanglement. One way is to saturate the constraint expressed by Eq. (40). Another way is to maximize the av-

erage of the two-party entanglements between all pairs. In the second case the saturating state for n qubits has been constructed [60] (the two-party entanglement is given by $C=2/n$ for all pairs).

We now provide an example of the type of heuristic that one might adopt to motivate the saturation conjecture. In order to do this we need to use ideas based on the renormalization group. The RG works by successively collecting together subsystems of a lattice and eliminating degrees of freedom from these collections. For example, suppose a system A is composed of n qubits $A=A_1,\ldots,A_n$. A typical RG step would involve collecting together two qubits A_j and A_{j+1}, and discarding two degrees of freedom from the A_jA_{j+1} subsystem (i.e., *renormalizing* A_jA_{j+1}). The renormalized system is a single qubit, written A_j'. This type of RG step is often performed simultaneously on all the pairs of A. It is known [23,24] that quantum critical points correspond to *fixed points* of the RG, i.e., where the state of the system is symmetric under a RG step. For this reason, the state of a system at a quantum critical point is said to be *scale invariant* or *self-similar*.

Suppose that a system A is composed of four qubits $A_1,\ldots,A_4$. Consider the extensivity relation Eq. (40) (which we assume to be generally true) for the first qubit A_1,

$$\mathcal{G}(A_1:A_2A_3A_4)\geqslant\mathcal{G}(A_1:A_2)+\mathcal{G}(A_1:A_3)+\mathcal{G}(A_1:A_4). \tag{44}$$

We are going to provide a speculative argument that as A is renormalized this inequality will tend toward saturation.

To do this we suppose the following two facts.

(1) The left-hand side of Eq. (44) does not change if a pair, say A_2A_3, is renormalized, $A_2A_3\mapsto A_2'$, i.e.,

$$\mathcal{G}(A_1:A_2A_3A_4)=\mathcal{G}(A_1:A_2'A_4). \tag{45}$$

(2) The renormalized entanglement $\mathcal{G}(A_1:A_2')$ is given by the expression

$$\mathcal{G}(A_1:A_2')=\mathcal{G}(A_1:A_2A_3)=\mathcal{G}(A_1:A_2)+\mathcal{G}(A_1:A_3)+\mathcal{G}(A_1:A_2:A_3), \tag{46}$$

where $\mathcal{G}(A_1:A_2:A_3)$ is an associated measure of purely three-party entanglement [62].

The additional assumption we make in (2) is that if the purely three-party entanglement, as measured by $\mathcal{G}(A_1:A_2:A_3)$, is added to the RHS of the extensivity relation, Eq. (40), for three qubits then the inequality becomes an equality. For further details on why this should be the case see Ref. [54].

Consider the *deficit* Δ between the left and right sides of the extensivity relation before a renormalization step,

$$\Delta\equiv\mathcal{G}(A_1:A_2A_3A_4)-\mathcal{G}(A_1:A_2)-\mathcal{G}(A_1:A_3)-\mathcal{G}(A_1:A_4). \tag{47}$$

If the pair A_2A_3 is renormalized the deficit Δ' between the left- and right-hand sides of Eq. (44) after the RG step will be less than the original deficit, i.e., $\Delta'\leqslant\Delta$. This follows from

$$\begin{aligned}\Delta'&=\mathcal{G}(A_1:A_2'A_4)-\mathcal{G}(A_1:A_2')-\mathcal{G}(A_1:A_4),\\&=\mathcal{G}(A_1:A_2A_3A_4)-\mathcal{G}(A_1:A_2A_3)-\mathcal{G}(A_1:A_4),\\&=\mathcal{G}(A_1:A_2A_3A_4)-\mathcal{G}(A_1:A_2)-\mathcal{G}(A_1:A_3)\\&\quad-\mathcal{G}(A_1:A_4)-\mathcal{G}(A_1:A_2:A_3),\\&=\Delta-\mathcal{G}(A_1:A_2:A_3).\end{aligned} \tag{48}$$

If there is three-party entanglement then the only fixed point is $\Delta=0$, i.e., saturation of the extensivity relation.

Generalizing this argument to an infinite lattice, we see that as RG steps are continually applied, the deficit between left and right sides will continue to decrease until it reaches zero at a fixed point of the RG (a quantum critical point), that is, saturation of the entanglement sharing inequality.

There is a lot that is questionable with the preceding argument. For example, the two assumptions 1 and 2 we made about the behavior of entanglement under renormalization may not be correct. The biggest problem our saturation conjecture faces is that, as we will show, the entanglement sharing inequality is *not* saturated for the critical transverse Ising model. Nonetheless, we believe that a more rigorous argument similar to the one we have made here will provide the correct picture of the entanglement distribution at a quantum critical point.

We should mention that the RG procedure we have employed to discuss the saturation conjecture is well known in the condensed-matter literature where it is referred to as the *real-space renormalization group* (RSRG) [39]. When the RSRG is applied, in the way we have described it, to study the critical transverse Ising model it is known that it does not generate a very good approximation to the state of the system at criticality [39]. Improvements to the scheme involve collecting larger blocks of subsystems instead of just pairs. To account for this obviously requires a refinement of our argument. This means that the failure of the entanglement sharing inequality to be saturated at the critical point may be an artifact of the renormalization scheme we have chosen.

In the light of this interpretation it is interesting to compare the entanglement calculations for the transverse Ising model at criticality to the lattice calculations of Wootters and O'Connor [30,57]. In the critical case $\lambda_c=1$ the correlation functions for the transverse Ising model are known explicitly as functions of r [43],

$$\langle\sigma_0^x\sigma_r^x\rangle=\left(\frac{2}{\pi}\right)^r 2^{2r(r-1)}\frac{H(r)^4}{H(2r)}, \tag{49}$$

$$\langle\sigma_0^y\sigma_r^y\rangle=-\frac{\langle\sigma_0^x\sigma_r^x\rangle}{4r^2-1}, \tag{50}$$

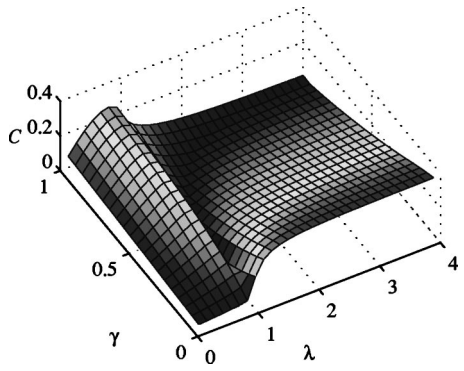

FIG. 4. Nearest-neighbor concurrence C at zero temperature for the XY model.

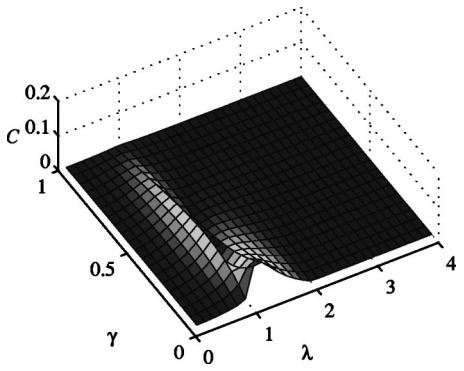

FIG. 5. Next-nearest-neighbor concurrence C at zero temperature for the XY model.

$$\langle \sigma_0^z \sigma_r^z \rangle = \frac{4}{\pi} \frac{1}{4r^2-1}, \tag{51}$$

$$\langle \sigma^z \rangle = \frac{2}{\pi}, \tag{52}$$

where $H(r)=1^{r-1}2^{r-2}\cdots(r-1)$. The concurrence at the critical point is nonzero for both $r=1$ and $r=2$ where it is given by, respectively, 0.1946 and 0.0044. These values should be compared with the values obtained by O'Connor and Wootters in their study [57] of the concurrence in chains and rings of qubits. They maximized the entanglement between nearest neighbors of a translationally invariant ring of spin-$\frac{1}{2}$ degrees of freedom. Wootters and O'Connor were attempting to saturate the bounds of entanglement sharing by maximizing the entanglement of nearest-neighbors subject to the symmetry of translational invariance. They found a maximal nearest-neighbor concurrence value of 0.4345 for an infinite ring, which is greater than the critical value for the transverse Ising model. This result alone does not imply that the critical transverse Ising model is less entangled than the ring considered in Refs. [30,57], indeed, if the conjecture made in the preceding paragraph is true then the ring would be much less entangled than the critical transverse Ising model. The reasoning for this is that the critical transverse Ising model is conjectured to maximize the entanglement between all pairs subject to translational invariance while the chains and rings of Wootters and O'Connor only maximize entanglement between nearest neighbors. One means of determining whether this is the case would be to calculate the correlation function for the ring. On the basis of the arguments made in this study, we expect that the correlations will decay exponentially with separation for the ring.

The entanglement in the thermal ground state of the general XY model may be calculated simply, following the method outlined in Sec. II. Following Barouch [42], which is where the correlation functions Eq. (21), Eq. (22), and Eq. (23) were calculated, only the region $0 \leqslant \gamma \leqslant 1$ is considered here. The concurrence between nearest-neighbor and next-nearest neighbor sites is shown in Fig. 4 and Fig. 5, respectively. The concurrences are a complicated function of the parameters, reflecting the competition between the various different noncommuting terms in the Hamiltonian as the parameters are varied.

The completely isotropic limit, $\gamma=0$, is the most interesting parameter region besides the transverse Ising model. Direct calculation along the lines already presented shows that two-party entanglement exists between all pairs for all separations at this point. Wootters [63] has made a study of the correlations in one- and two-dimensional lattices and he has found interesting connections between the two-party correlations in the isotropic XY model and the bounds of entanglement sharing. Further investigations along these lines could provide evidence that critical quantum lattice systems are maximally entangled in the sense of entanglement sharing.

IV. THERMAL ENTANGLEMENT IN THE TRANSVERSE ISING MODEL

In this section we discuss the entanglement present in the thermal state of the transverse Ising model. We find that the largest amount of entanglement is present in the parameter region close to the critical point. This region is found to correspond with the *quantum critical* region introduced by Sachdev (p. 58 of Ref. [21]). We also find parameter values for which the entanglement *increases* as the temperature is increased. Finally, we discuss the persistence of quantum effects in the thermal state as the temperature is increased.

It is desirable to determine when a condensed-matter system will behave quantum-mechanically. This is particularly important because the validity of various ansatz methods depends on whether they take account of possible quantum effects. When a system is in its ground state, quantum effects will certainly be important, as evidenced by the quantum phase transition in the XY model. The zero-temperature calculations of the last section represent a highly idealized situation, however, it is unclear whether they have any relevance to the system at a nonzero temperature. It turns out that the properties of a quantum system for low temperatures are strongly influenced by nearby (in parameter space) quantum critical points [21,22]. It is tempting to attribute the effect of nearby critical points to persistent mixed-state entanglement in the thermal state. In order to investigate this, we calculate the two-party entanglement present at a nonzero temperature T.

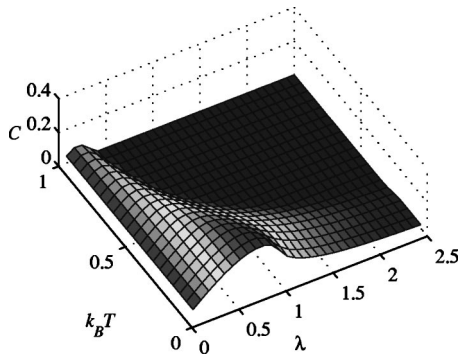

FIG. 6. Nearest-neighbor concurrence C at nonzero temperature for the transverse Ising model.

The two-site density matrices constructed in Sec. II are valid for all temperatures. Using these matrices it is possible to study the purely two-party entanglement present at thermal equilibrium because the concurrence measure of entanglement can be applied to arbitrary mixed states. The regions where there is appreciable two-party entanglement give at least a partial indication of where quantum effects may be important. We again emphasize the transverse Ising model for this section. The influence the critical point has on the entanglement structure at nonzero temperatures is particularly clear for this model.

The entanglement between nearest-neighbor and next-nearest-neighbor sites in the Ising model at nonzero temperature appears in Fig. 6 and Fig. 7, respectively. The entanglement is nonzero only in a certain region in the $k_BT-\lambda$ plane. It is in this region that quantum effects are likely to dominate the behavior of the system. The entanglement is largest in the vicinity of the critical point $\lambda=1$, $k_BT=0$. This region corresponds, approximately, to the *quantum critical* regime identified by Sachdev [21]. Sachdev found, by using a very different argument, that quantum effects would be important in this regime. The correspondence of these two regions provides evidence that the entanglement content plays an important role in the emergence of quantum behavior in naturally occurring quantum systems.

There are two notable features of the two-site thermal entanglement results. The first feature is that, for certain values of λ, the two-site entanglement can increase as the temperature is increased (e.g., $\lambda=1.4$, Fig. 6). This effect has previously been observed in finite-size calculations [17,31] for the Heisenberg model. The occurrence here of the same effect implies that it is not an artifact of the truncation of a lattice. The second feature is the existence of appreciable entanglement in the system for temperatures k_BT above the ground-state energy gap Δ. It has been argued [22] that quantum systems behave *classically* when the temperature exceeds all relevant frequencies. For the transverse Ising model the only relevant frequency is given by the ground-state energy gap $\Delta\equiv\hbar\omega$. The presence of entanglement in the system for temperatures above the energy gap indicates that quantum effects may persist past the point where they are usually expected to disappear.

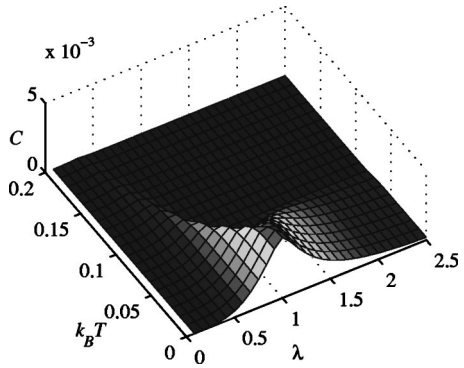

FIG. 7. Next-nearest-neighbor concurrence C at nonzero temperature for the transverse Ising model.

A comparison should be made between the results obtained here and the numerical calculations of concurrence in the Ising model on a finite number of sites [33]. The calculations that were performed in Ref. [33] were implemented on a maximum of seven sites. The concurrence between nearest neighbors obtained by Gunlycke *et al.* (Figs. 2 and 5 of Ref. [33]) is in qualitative agreement with the results obtained here. However, as there is no phase transition for the finite-size Ising model the dominance of the critical point was not as sharp in the calculations of Ref. [33].

V. SUMMARY AND FUTURE DIRECTIONS

The one- and two-party entanglement present in the ground and thermal states of the XY model has been calculated. It should be stressed that the calculations in this study are analytic and, furthermore, they are for the thermodynamic limit of a quantum lattice system.

We have argued that the critical point of a quantum lattice system corresponds to the situation where the lattice is maximally entangled. Evidence for this conjecture was found in the single-site entanglement results for the ground state of the transverse Ising model. We have also argued that the constraints of shared entanglement are important for critical quantum systems, and we have found possible evidence of such constraints playing a role in the two-party entanglement results for the transverse Ising model. The entanglement present at thermal equilibrium was also studied, and an approximate correspondence between the quantum critical regime identified by Sachdev and the regions where the two-party entanglement is nonzero was found. Parameter values where the entanglement increases as the temperature is increased were also found.

We have focused on the transverse Ising model throughout this study, although the calculations presented also cover the XY model. The transverse Ising model is interesting because it is the simplest system to exhibit a quantum phase transition, and it is relatively easy to identify the structure of the entanglement present in this system. The importance of the critical point in this system is also particularly clear. The XY model has many parameter regimes where it behaves differently, so it is very likely that more interesting phenomena may be found in other parameter regions.

Entanglement calculations in this study have been restricted to time-independent scenarios. However, the dy-

namic correlation functions have been calculated for the Ising and XY models for certain values of λ. It is possible and may be interesting to calculate the time evolution of the entanglement in these models and thus identify truly quantum dynamics.

The calculations in this study are intended as a point of reference for the development of an understanding of the entanglement in critical quantum systems. Rather frustratingly, the present incomplete understanding of entanglement measures has prevented us from performing many of the calculations we would like to do in order to check the many conjectures made in this paper. Further progress on the general quantitative theory of entanglement should enable these conjectures to be checked in the future. We believe that entanglement plays a central role in the emergence of long-range correlations at the critical point of such systems, and that a fruitful interplay between the theory of entanglement and critical quantum phenomena may result from further study. In particular, it would be interesting to make *universal* statements about the character of entanglement at the critical point, and to examine whether the constraints of entanglement sharing impose physical limitations on the behavior that can occur in such a system.

Note added. Recently we learned of related work done independently by Osterloh *et al.* [55].

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