Entanglement Induced Phase Transitions

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(Received November 8, 2018)

Starting from the canonical ensemble over the space of pure quantum states, we obtain an integral representation for the partition function. This is used to calculate the magnetisation of a system of $N$ spin-$\frac{1}{2}$ particles. The results suggest the existence of a new type of first order phase transition that occurs at zero temperature in the absence of spin-spin interactions. The transition arises as a consequence of quantum entanglement. The effects of internal interactions are analysed and the behaviour of the magnetic susceptibility for a small number of interacting spins is determined.

PACS Numbers: 03.65.Bz, 05.30.Ch, 02.40.Ft

In classical statistical mechanics, a phase transition is a phenomenon characteristic of systems having internal interactions [1]. Indeed, if the form of the internal energy is reasonably idealised, there is a wide range of models describing phase transitions at finite temperatures that can be solved exactly [2]. The situation is similar for quantum systems, though exact solutions are typically difficult to obtain in this case [3].

One distinguishing feature of quantum systems in this context is the existence of entanglement. This gives rise to a colossal increase in the state space volume for combined systems. Furthermore quantum entanglement can be viewed in itself as a form of internal interaction between the constituent particles of the system. It is natural therefore to inquire whether entanglement has any role to play in critical phenomena.

In this letter we consider an entangled system of distinguishable spin-$\frac{1}{2}$ particles, weakly interacting with a heat bath. A general integral formula for the partition function is obtained and used to analyse the magnetisation and the magnetic susceptibility of the system. In particular we show that the magnetisation of

$$M \sim \frac{1}{2} N \mu - (2^N - 1) \frac{k_B T}{B},$$

where $\mu$ is the magnetic moment of an individual particle, $B$ is the applied magnetic field, $T$ is the temperature of the heat bath, and $k_B$ is Boltzmann’s constant. The $N$-dependence of the magnetisation points, in the thermodynamic limit $N \to \infty$, to the possible existence of a first order phase transition at zero temperature in the absence of spin-spin interactions. This is a phenomenon with no classical counterpart, indicating that entanglement may have an effect similar to that of a mean-field which enhances critical phenomena.

Let $\psi^\alpha$ be a state vector in a complex Hilbert space $\mathcal{H}$. A physical observable, such as the Hamiltonian $H^\beta_\gamma$, is represented by a linear operator acting on $\mathcal{H}$. If a system is in the state $\psi^\alpha$, then the quantum expectation of an operator $F^\alpha_\beta$ in that state is $\langle \hat{F} \rangle = \overline{\psi}_\alpha F^\alpha_\beta \psi^\alpha / \psi^\alpha \psi^\alpha$, where $\overline{\psi}_\alpha$ is the complex conjugate of $\psi^\alpha$. The expectation $\langle \hat{F} \rangle$ is unaltered under transformations of the form $\psi^\alpha \to \Lambda \psi^\alpha$, where $\Lambda$ is any nonvanishing complex number. In other words, the Hilbert space formulation of quantum mechanics carries an extra complex degree of freedom given by the overall scale and phase. It is convenient, therefore, to introduce the space of equivalence classes of vectors in $\mathcal{H}$ modulo complex scale transformations. This is the projective Hilbert space $\mathcal{PH}$: a point in $\mathcal{PH}$ corresponds to all the points on a ray through the origin of $\mathcal{H}$, except the origin itself. We refer to $\mathcal{PH}$ as the space of pure quantum states.

For definiteness, let us take $\mathcal{H}$ to be an $(n+1)$-dimensional complex Hilbert space. Then the corresponding state space is the $n$-dimensional complex projective space $\mathbb{C}P^n$. The state space $\mathbb{C}P^n$, when regarded as a real manifold $\Gamma$ of dimension $2n$, is equipped with a natural symplectic structure, as well as a Riemannian structure known as the Fubini-Study metric [4]. Each point $x$ in $\Gamma$ represents a ray in $\mathcal{H}$. Conversely, suppose we assign to each point $x$ in $\Gamma$ a nonvanishing element $\psi^\alpha(x)$ in the ray corresponding to $x$. Then given any observable $F$ acting on $\mathcal{H}$, we can construct a real-valued biquadratic function $F(x)$ on $\Gamma$ given by the expectation of $F^\alpha_\beta$ in the state $\psi^\alpha(x)$. It is straightforward to verify that $F(x)$ is independent of the particular choice of cross-section $\psi^\alpha(x)$.

When we shift emphasis from $\mathcal{H}$ to $\Gamma$, the role of the complex number is taken over by the symplectic structure, given by a nondegenerate skew-symmetric tensor field, and the Schrödinger equation can be expressed in Hamiltonian form. The formulation of quantum mechanics on the state space $\Gamma$ thus bears a striking resemblance to classical Hamiltonian mechanics, with the additional constraint that the Hamiltonian $H(x)$ in quantum mechanics is of the special form $H(x) = H^\beta_\gamma \Pi^\alpha_\beta(x)$, where

$$\Pi^\alpha_\beta(x) = \frac{\overline{\psi}_\alpha(x) \psi^\beta(x)}{\psi^\gamma(x) \psi^\gamma(x)}.$$
is the projection operator corresponding to the pure state \( x \in \Gamma \).

The fact that the space \( \Gamma \) of pure states is the quantum phase space makes \( \Gamma \) the appropriate space in which to consider the effects of quantum entanglement. In this letter our interest is in the weak coupling limit between a quantum system and an environment with which it is in thermal equilibrium. Specifically, we would like to know how to characterise thermal equilibrium states on \( \Gamma \), that is, to find an ensemble \( \rho(x) \) over \( \Gamma \) that describes the distribution of wave functions. This question has been addressed in [3], where it is shown that, if we assume the resulting distribution over \( \Gamma \) maximises the Shannon entropy associated with \( \rho(x) \), then the equilibrium ensemble is given by the Gibbs measure

\[
\rho(x) = \frac{e^{-\beta H(x)}}{Z(\beta)},
\]

where \( \beta = 1/k_B T \), and

\[
Z(\beta) = \int_{\Gamma} e^{-\beta H(x)} dV
\]

is the partition function. Here \( dV \) is the volume element arising from the Fubini-Study metric on \( \Gamma \). More specifically, we have

\[
dV = \frac{D^n \bar{\psi} D^n \psi}{(\bar{\psi}_\alpha \psi^\alpha)^{n+1}}
\]

for the phase space volume element, where

\[
D^n \psi = \epsilon_{\alpha \beta \gamma \cdots} \bar{\psi}_\alpha d\psi_\beta d\psi_\gamma \cdots d\psi_\delta
\]

and \( \epsilon_{\alpha \beta \gamma \cdots} \) is the totally skew-symmetric tensor.

The interpretation of the distribution (3) is as follows. For each pure state \( x \in \Gamma \) we compute the expectation \( H(x) \) of the Hamiltonian operator, conditioned on that pure state. For thermal equilibrium the probability that the quantum system is in the pure state \( x \) is given by the internal energy

\[
U(\beta) = \int_{\Gamma} H(x) \rho(x) dV,
\]

which is equivalent to the trace formula \( H^\beta_\alpha \rho^\beta_\alpha \), where \( \rho^\beta_\alpha \) is the density matrix associated with the distribution (3), given by

\[
\rho^\beta_\alpha = \int_{\Gamma} \rho(x) \Pi^\beta_\alpha(x) dV.
\]

It follows by a standard identity that \( U = -\partial \ln Z/\partial \beta \). Therefore, we would like to obtain an explicit expression for the partition function \( Z(\beta) \), in order to determine properties of the thermodynamic functions.

For the computation of the partition function, it is convenient to revert to the homogeneous coordinates \( \psi^\alpha (\alpha = 0, 1, \cdots, n) \) on the complex projective space \( \mathbb{C} P^n \). Then, we observe that the integration in (3) can be lifted to \( \mathbb{C} P^{n+1} \) with a spherical constraint \( \bar{\psi}_\alpha \psi^\alpha = 1 \), which gives us

\[
Z(\beta) = \int_{\mathbb{C} P^{n+1}} \delta(\bar{\psi} \psi - 1) e^{-\beta H^\beta_\alpha \bar{\psi}_\alpha \psi^\beta} d^{n+1} \bar{\psi} d^{n+1} \psi.
\]

Moreover, if we choose a basis such that the Hamiltonian operator is diagonal and substitute the standard identity \( \partial / \partial \beta = -\beta / \partial \beta \), then the \( \mathbb{C} P^{n+1} \)-integration becomes a Gaussian and we obtain

\[
Z(\beta) = \int_{-\infty}^{\infty} (2\pi)^n e^{-i \beta \xi} d\xi
\]

where \( E_k \) are the energy eigenvalues. In obtaining (10) we transform from complex coordinates \( \psi^\alpha \) to real coordinates, which makes the integration involved for each energy eigenvalue \( E_k \) in (9) a double Gaussian. If we analytically continue \( \xi \) to the lower half-plane, then the integral decreases exponentially and we can close the contour and apply the residue theorem to evaluate the integral. The result is

\[
Z(\beta) = \sum_{\text{res}} e^\lambda \left( \prod_{k=0}^{n} \frac{1}{\lambda + 3 \pi} \right).
\]

where we have written \( \lambda = -\beta \xi \) and we have discarded the physically unimportant factors of \( 2\pi \).

Formula (11) for the partition function is valid for any quantum system that can be modelled by a finite dimensional state space. In particular, if there is no degeneracy in the energy eigenvalues, then we find that the partition function reduces to the following simple expression:

\[
Z(\beta) = \sum_{k=0}^{n} e^{-\pi E_k} \left( \prod_{l=0}^{n} \frac{1}{\beta E_l - E_k} \right).
\]

This formula is applicable, for example, to the case of a single spin-\( \frac{1}{2} \) particle in a magnetic field, for which we can write \( E_k = -(\frac{1}{2} - k) \mu_B, \) where \( k = 0, \cdots, n \). Then we have

\[
Z = \frac{1}{n!} \left( \frac{\sinh \frac{1}{2} \mu_B}{\frac{1}{2} \mu_B} \right)^n
\]

for the partition function. Interestingly, this is identical to the expression one obtains for \( n \) classically indistinguishable, independent (disentangled) spin-\( \frac{1}{2} \) particles in a magnetic field. In the spin-\( \frac{1}{2} \) case (i.e. \( n = 1 \)), as was addressed in [4], the magnetisation energy is given by

\[
U = k_B T - \frac{1}{2} \mu_B \coth \frac{1}{2} \beta \mu_B.
\]
Let us now apply the result (11) to a system of distinguishable spin-$\frac{1}{2}$ particles (e.g., electrons on a lattice) in a magnetic field. Classically, if the particles are not interacting, then the resulting partition function factors, and we obtain the same magnetisation per particle as in the single particle case. However, quantum mechanically, this is no longer the case, because of the existence of quantum entanglement. That is, even in the absence of direct interactions, the presence of entanglement implies that the particles are not independent. For example, if the system consists of two spin-$\frac{1}{2}$ particles, any entangled state (such as the singlet state) gives rise to a nonvanishing Boltzmann weight through formula (3).

For $N$ noninteracting spin-$\frac{1}{2}$ particles, the Hamiltonian operator is

$$\hat{H} = -\mu B \sum_{i=1}^{N} \hat{s}_{iz} = -\mu B \hat{S}_z,$$

where $\hat{S} = \sum_{i=1}^{N} \hat{s}_i$. Note that, although the total number of eigenstates is given by $2^N$, the corresponding eigenvalues are highly degenerate. In particular, there are only $N + 1$ distinct energy eigenvalues, given by $\epsilon_k = -\left(\frac{k}{2} - k\right) \mu B$, where the index $k$ runs from 0 to $N$. The degree of degeneracy associated with the eigenvalue $\epsilon_k$ is $NC_k$. Using this energy spectrum, we have determined the magnetisation of the system per particle for $N$ up to five, with the resulting plot given in Fig. 1.

The results in Fig. 1 show that, even in the absence of spin-spin interactions, the existence of quantum entanglement gives rise to nontrivial thermal expectation values—a result that has no classical counterpart. Furthermore, it also indicates that, in the thermodynamic limit $N \to \infty$, the gradient of the magnetisation at zero temperature diverges. If this were the case, then we would obtain a first order phase transition at $T = 0$ such that the value of magnetisation would jump from 0 to 1/2 as $T \downarrow 0$. However, because the formula (11) is not guaranteed to be valid in the thermodynamic limit, we cannot prove the existence of a phase transition. Nevertheless, we may consider the asymptotic behaviour of the magnetisation in the low temperature limit, and study how the resulting expression depends on $N$. In particular, as $T \to 0$ the contribution from the residue arising from the ground state energy dominates the partition function. Thus we find

$$Z \sim e^{-\beta \epsilon_0} \prod_{k=1}^{N} \frac{1}{[\beta(\epsilon_k - \epsilon_0)]^{NC_k}}$$

$$= a_N(\beta \mu B)^{1 - 2^N} \exp \left(\frac{N}{2} \beta \mu B\right),$$

where $a_N$ is independent of $\beta$. Then using $M = \beta^{-1} \partial \ln Z / \partial B$, we obtain the behaviour of the magnetisation as given in (1). This result is valid for an arbitrarily large but finite $N$, in the limit $T \to 0$, and agrees with the numerical results in Fig. 1. In particular, the coefficient of $T$ diverges exponentially in $N$, strongly pointing towards the existence of a transition.

The phase transition implied by the foregoing analysis is, of course, rather artificial, in the sense that the transition takes place at zero temperature, and that the magnetisation can take only two distinct values. This is not surprising however because the model we have considered has no spin-spin interactions. If we include interactions in order to have a finite temperature transition, then we expect the decrease of $M/N$ with increasing $N$ at fixed $T$, as observed in Fig. 1, is suppressed.

We now turn to study a highly interacting system in which derivations of thermodynamic functions are analytically tractable. In particular, we consider the quantum Ising model on a complete graph, rather than the conventional square-lattice models. Therefore, the Hamiltonian operator is now given by

$$\hat{H} = -\mu B \sum_{i=1}^{N} \hat{s}_{iz} - J \sum_{i>j}^{N} \hat{s}_i \cdot \hat{s}_j$$

$$= -\mu B \hat{S}_z - \frac{1}{2}J(\hat{S}^2 - \frac{3}{4}N),$$

without loss of generality, we can assume that the total number $N = 2n$ of the spins is even. Then (11) gives us

$$Z(\beta) = \sum_{\text{residues}} e^{\lambda} \left( \prod_{s=0}^{n} \prod_{m=-s}^{s} \frac{1}{(\lambda + \beta \epsilon_m(s))^{d_{2n}(s)}} \right),$$

where

$$\epsilon_m(s) = -\mu B - \frac{1}{2}J(s(s + 1) - \frac{3}{4}s)$$

and $d_{2n}(s) = 2nC_{n-s} - 2nC_{n-s-1}$. The ground state energy, in particular, is given by $E_0 = \epsilon_n(n)$.
With the expression \( (18) \) at hand, we can consider the behaviour of thermodynamic functions. In particular, for a system of interacting spins, we can determine the second moment, namely, the magnetic susceptibility of the system. Using the definition \( \chi = (1/N) \partial M/\partial B \) for the magnetic susceptibility, we analysed numerically the behaviour of \( \chi \) for a range of values of \( N \). The results are shown in Fig. 2, indicating the vanishing of the second moment at \( T = 0 \) and \( T \to \infty \), as well as a peak at finite temperature, the sharpness of which increases with \( N \).

There are two regimes of \( (18) \) which can be explored analytically. The first is the case of weak coupling in the low temperature limit. More precisely, when \( J/\mu_B \leq 2/N \), the residue coming from the ground state energy is again the leading contribution to the partition function as \( T \to 0 \). If one calculates the magnetisation per particle, then, as conjectured, the decrease of \( M/N \) with increasing \( N \) at fixed \( T \) is suppressed. However, the analytic result obtained is of limited use for large \( N \), because the restriction on \( J \) means one is simultaneously taking \( J \) to zero.

The second regime is the strong coupling limit \( J \to \infty \). In this limit, the system is effectively quenched, so we expect to observe little impact from quantum entanglement. When we calculate the partition function, we find, for \( J/\mu_B \gg 1 \), that the main contribution to \( Z \) is due to the residues arising from the \( 2n+1 \) states that have \( s = n \). Furthermore, the energy difference between states of differing \( s \) can be treated as independent of \( \mu_B \). Specifically we have

\[
Z \sim \sum_{k=-n}^{n} e^{-\beta \epsilon_k(n)} \left( \prod_{s=0}^{n-1} \prod_{m=-s}^{s} \frac{1}{[\beta(\epsilon_m(s) - \epsilon_k(n))]^{2n+1}} \right) \times \prod_{l=-n}^{n} \frac{1}{\beta(\epsilon_l(n) - \epsilon_k(n))} \]

\[
\simeq \frac{e^{\frac{1}{2} \beta JN(n-\frac{1}{2})}}{N!^{2^{N-1}}(\mu_B)^N} \sum_{k=-n}^{n} N C_{n-k} (-1)^{n-k} e^{k \beta \mu_B} \]

\[
= a_N \left( J \right) e^{\frac{1}{2} \beta J N (N-1)} \sinh^N \left( \frac{1}{4} \beta \mu_B \right). \tag{20}
\]

It is now straightforward to determine the magnetic susceptibility:

\[
\frac{\chi}{\mu/B} = \left[ 1 - \left( \frac{\frac{1}{4} \beta \mu_B}{\sinh \frac{1}{4} \beta \mu_B} \right)^2 \right] k_B T / \mu_B. \tag{21}
\]

That this result is independent of \( N \) is not surprising since we are considering interacting spins on a complete graph in the strong coupling limit. The effect of quantum entanglement is thus washed out in this limit.

In summary, we have obtained an expression for the partition function of a finite quantum system in thermal equilibrium, when the equilibrium states are obtained by maximising the Shannon entropy on the space of pure states. We applied this result to study the thermal expectation of the magnetisation and magnetic susceptibility of a system of \( N \) spin-1/2 particles. In the case of noninteracting spins, we were able to determine explicitly the effect arising from quantum entanglement. In reality, individual particles forming magnetic substances are not likely to be fully entangled. Nevertheless, there are partial entanglements within a system, and entanglements appear to have the effect of enhancing phase transitions.

DCB gratefully acknowledges financial support from The Royal Society.

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