Thermodynamics of a gas of deconfined bosonic spinons in two dimensions

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We consider the quantum phase transition between a Néel antiferromagnet and a valence-bond solid (VBS) in a two-dimensional system of \( S = 1/2 \) spins. Assuming that the excitations of the critical ground state are linearly dispersing deconfined spinons obeying Bose statistics, we derive expressions for the specific heat and the magnetic susceptibility at low temperature \( T \). Comparing with quantum Monte Carlo results for the J-Q model, which is a candidate for a deconfined Néel–VBS transition, we find excellent agreement, including a previously noted logarithmic correction in the susceptibility. In our treatment, this is a direct consequence of a confinement length scale \( \Lambda \propto \xi^{1+a} \), where \( \xi \) is the correlation length and \( a > 0 \) (with \( a \approx 0.2 \) in the model).

**Spinon gas**—Our assumption is that a system with couplings tuned to the \( T = 0 \) quantum-critical point can be described as a gas of bosonic spinons with dispersion \( \epsilon(k) = \sqrt{c^2k^2 + \Delta^2(T)} \) at \( T > 0 \). This dispersion is valid for magnons at a conventional O(3) quantum phase transition between the Néel state and a disordered state (e.g., in dimmerized Heisenberg models [13–19]), in which case the thermal “gap” \( \Delta \) is related to the correlation length \( \xi \) according to \( \Delta \propto 1/\xi \propto T^z \), with \( z = 1 \) [1, 2]. At the DQC point \( \xi \propto 1/T \) is also expected, but the spinon gap should be given by the larger confinement length, \( \Delta \propto 1/\Lambda \propto T^{1+a} \). Effectively, the gap is used as an infrared cut-off in momentum space.

The \( T = 0 \) confinement exponent \( a \) was previously estimated using QMC results for the finite-size scaling of the U(1)-Z_4 cross-over of the VBS order-parameter symmetry (a hallmark of the DQC theory [5]) of a variant of the J-Q model. The result was \( a = 0.20 \pm 0.05 \). It is unclear whether the \( T > 0 \) confinement exponent should be the same, however. Here we leave \( a \) as a free parameter along with the velocity \( c \) and write the gap as

\[
\Delta = m_{1/2}T (T/c)^a,
\]

where the constant \( m_{1/2} \) should be close to 1. In the case of magnons, it is known that \( \Delta = m_1T \), with the mean-field value \( m_1 \approx 0.96 \) [2] in good agreement with QMC calculations of observables (e.g., the magnetic susceptibility) which depend on this constant [2, 16].

In a magnetic field \( B \), the spinon level is split into

\[
\epsilon_{\pm}(k) = \sqrt{c^2k^2 + \Delta^2} \pm \mu B \equiv \epsilon(k) \pm \mu B,
\]

where \( \mu = 1/2 \). This form with \( \mu = 1 \) holds also for
the two shifted magnon levels (with \( \epsilon_0 \) not shifted). In the CP\(^1\) DQC theory [3], there are both spinons and anti-spinons, which contribute equally to thermodynamic properties. We take this into account with a factor \( F = 2 \), while for magnons \( F = 1 \).

With the boson occupation number \( n(\epsilon) = 1/(e^{\epsilon/T} - 1) \) the magnetization per lattice site for small \( B \) is:

\[
M = \mu F \int \left( \frac{1}{e^{\epsilon/T} - 1} - \frac{1}{e^{\epsilon - \Delta/T} - 1} \right) \frac{d^2k}{(2\pi)^2} = \mu^2 F \frac{T B}{4\pi c^2} \int_0^\infty \frac{xdx}{\sinh^2 \left( \frac{1}{2} \sqrt{x^2 + (\Delta/T)^2} \right)}. \tag{3}
\]

The integral can be computed exactly,

\[
\int_0^\infty \frac{xdx}{\sinh^2 \left( \frac{1}{2} \sqrt{x^2 + p^2} \right)} = \frac{4p}{1 - e^{-p}} - 4 \ln(e^p - 1), \tag{4}
\]

where \( p = \Delta/T \). For magnons at the usual O(3) transition, \( p = m_1 \approx 0.96 \) and the susceptibility is [2]

\[
\chi_1 \approx (1.0760/\pi c^2)T. \tag{5}
\]

For spinons, if there is indeed an anomalous exponent \( a > 0 \) in Eq. (4), then \( \Delta/T \to 0 \) as \( T \to 0 \) and we can use the expansion of (4) around \( p = 0 \), giving

\[
\chi_{1/2} = \frac{T}{2\pi c^2} \left[ 1 + a \ln \left( \frac{c}{T} \right) + \frac{1}{24} \left( \frac{T}{c} \right)^2 \right]. \tag{6}
\]

Here we have used \( m_{1/2} = 1 \) in (4), and the next correction to \( \chi_{1/2} \) is of order \( (T/c)^4 \). The logarithmic correction is very interesting, as it was already identified in a recent QMC study of the J-Q model [8].

The specific heat per site is

\[
C_S = (2S + 1)F \int \epsilon(k) \frac{\partial n(\epsilon)}{\partial T} \frac{d^2k}{(2\pi)^2}, \tag{7}
\]

which for \( S = 1/2 \) leads to the low-\( T \) behavior

\[
C_{1/2} = \frac{2T^2}{\pi c^2} \times \left[ 6\zeta(3) - \left( \frac{T}{c} \right)^2 a \left[ \frac{3}{2} + a + a(1 + a) \ln \left( \frac{c}{T} \right) \right] \right], \tag{8}
\]

where we have again used \( m_{1/2} = 1 \) and \( \zeta(3) \approx 1.20206 \). Note that the log-correction is multiplied by a power and is not as dramatic as in the susceptibility (4). For the O(3) transition, \( S = F = 1 \) in (4) gives, at low \( T \) \[2,20\],

\[
C_1 = \frac{36\zeta(3)}{5\pi c^2}T^2. \tag{9}
\]

Apart from the logarithms, the differences in the thermodynamics between spinons and magnons arise mainly from the degeneracy factors and \( \mu \). The log correction to \( \chi_{1/2} \) in (6) is significant, however, and should be a decisive fingerprint of the deconfined spinon gas.

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**Quantum-critical models**—A promising model exhibiting a Néel–VBS transition is the J-Q model, which in its simplest form is defined by the Hamiltonian [8]

\[
H = -J \sum_{ij} C_{ij} - Q \sum_{ijkl} C_{ijkl}, \tag{10}
\]

where \( C_{ij} \) is a singlet projector; \( C_{ij} = 1/4 - S_i \cdot S_j \).

In the J (Heisenberg) term \( ij \) are nearest neighbors on the square lattice, while in the Q term \( ij \) and \( kl \) form opposite edges of a 2 \( \times \) 2 plaquette. There is mounting evidence [2,24] of a continuous \( T = 0 \) transition in this system between a Néel state for \( (J/Q) < (J/Q)_c \) and a VBS for \( (J/Q) > (J/Q)_c \), with \( (J/Q)_c \approx 0.045 [8] \).

To ensure pure critical behavior when testing the above spinon gas predictions, it is necessary to know the critical coupling ratio \( (J/Q)_c \), to high precision. Here we use the correlation lengths \( \xi_s \) and \( \xi_d \) extracted from, respectively, the spin-spin and dimer-dimer (four-spin) correlation functions. QMC calculations were carried out on \( L \times L \) lattices with \( L = 2 \) at inverse temperature \( \beta = Q/T = L \) (in [8]). At a DQC point, \( \xi_s/L \) and \( \xi_d/L \) should be size independent for large \( L \). Curves plotted versus \( J/Q \) for two different system sizes, e.g., \( L = 2L \) should then cross each other at some value \( (J/Q)_L \), which can be different for \( \xi_s/L \) and \( \xi_d/L \) but in both cases should approach \( (J/Q)_c \) when \( L \to \infty \).

Such crossing points are shown in Fig. 1. Due to the slow convergence, it is difficult to extrapolate precisely. There is, however, a remarkable feature of these data: The \( \xi_s/L \) and \( \xi_d/L \) crossing points approach an apparent common asymptotic value at the same rate but from different sides. Their average exhibits almost no size dependence, and one can therefore obtain a much better critical-point estimate than what might initially have been expected. The result based on the four largest-\( L \) points (which agree completely within statistical errors) is \( (J/Q)_c \approx 0.04498(3) \). Here we will use \( J/Q = 0.045 \).
Conventional O(3) $T > 0$ scaling has been studied in the past in various dimerized Heisenberg models (where the Hamiltonian itself breaks lattice symmetries and no other symmetries are broken in the disordered phase) [14,17]. To compare with the J-Q model, we consider a system with couplings $J$ and $J’ > J$, with the stronger ones arranged in columns. This model was the subject of a recent high-precision study [19], which gave the critical ratio $(J'/J)_c = 1.9096(2)$. A further improved estimate is now available, $(J'/J)_c = 1.90948(4)$ [21]. We use $J'/J = 1.9095$ and carry out more detailed comparisons with the O(3) theory than in past studies. In this case all quantities should be normalized per two-site unit cell.

Energy fits—We first fit low-$T$ results for the internal energy based on the leading specific heat forms (5) and (9). QMC calculations were carried out using sufficiently large lattices ($L \leq 512$) to eliminate finite-size effects in the range of temperatures considered. We also use the ground state energy extrapolated to $L = \infty$ based on $\beta = L$ results. For the J-Q model at $J/Q = 0.045$, the result is $E_0/Q = -0.8740318(4)$, while the J-J’ model with $J'/J = 1.9095$ has $E_0/J = -1.740507(2)$ per unit cell. Fig. 2 shows $E(T)$ after $E_0$ has been subtracted and $T^3$ has been divided out. The low-$T$ behavior gives the spinon velocity $c = 2.55Q$ for the J-Q model and the magnon velocity $c = 1.38J$ for the J-J’ model (which should be interpreted as $c = \sqrt{\chi_\perp \chi_{||}}$ since the J-J’ model is anisotropic). While there are corrections to the $T^3$ behavior in Fig. 2, the low-$T$ results for the J-Q model are not sufficiently accurate to test the correction in (8).

Neglecting the power-law correction in (8) and fixing the magnetic correction (which was found to describe the data well in [5]), gives $c = 2.48Q$ and $a = 0.20$. In both cases, including also the very small power-law correction in (8) changes $\chi_{1/2}/T$ by less than 1% and barely affects the extracted parameters.

We have set $m_{1/2} = 1$ in (8) throughout the above analysis, while we may only expect $m_{1/2} \approx 1$ [as with the constant $m_1$ in the conventional O(3) theory]. Physical observables depend only weakly on $m_{1/2}$, however, and the consistent $c$-values extracted from two different quantities justify the use of $m_{1/2} = 1$ a posteriori.

Wilson ratio—The Wilson ratio of the J-Q model exhibits a log divergence. From Eqs. (9) and (8) and the

It is anyway doubtful whether the spinon gas model can correctly capture subleading corrections.

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Wilson ratio—The Wilson ratio of the J-Q model exhibits a log divergence. From Eqs. (9) and (8) and the
parameters of the fits (taking $c$ from the energy fit and $a$ from the susceptibility fit with $c$ fixed) we get $W_{1/2} = \chi T/C = w_{1/2} [1 + a \ln(c/T)]$, with $w_{1/2} = 0.0346 \pm 0.0002$, $c = 2.55 \pm 0.02$, and $a = 0.222 \pm 0.005$. For the J’ model we get $W_1 = 0.1262 \pm 0.0006$, in good agreement with $W_1 = 0.1243$ from Eqs. (5) and (9). Including the next term in the $1/N$ expansion of the large-$N$ O(3) theory makes this agreement worse by several percent, however. Note that if the log-correction is disregarded, $W_{1/2}$ is only about 1/4 of $W_1$.

**Conclusions and discussion**—We have tested a model of non-interacting (deconfined) bosonic spinons against QMC data for the J-Q model, which is a promising candidate for a DQC point. The most notable result is that a confinement length $\Lambda$ diverging as $1/T^{1+\alpha}$ with $\alpha > 0$ leads to a logarithmic correction to the susceptibility $\chi$, as was previously observed in the J-Q model [8]. The velocity entering in $\chi$ agrees with the velocity needed to fit the specific heat. The anomalous exponent $a \approx 0.22$ is in good agreement with an estimate based on a completely different analysis at $T = 0$ [3], which suggests that the $T = 0$ and $T > 0$ exponents indeed are the same (which is unclear in the DQC theory, in which no anomalous $T > 0$ exponent has been discussed [3, 22]). The critical behavior does not fit the standard O(3) picture with $S = 1$ excitations [2], which we have investigated here in the context of a dimerized model.

The agreement between the critical J-Q model and the non-interacting spinon gas is remarkable, considering that the spinons in the DQC theory are only marginally deconfined (with interactions mediated by the gauge field) [3]. Apparently, beyond their underlying role in determining the anomalous exponent $a$ in Eq. (1), these interactions only have very small effects on the thermodynamics. A treatment similar to the spinon gas considered here has been applied to the $S = 1/2$ Heisenberg chain (with the important difference that the spinons there obey Fermi statistics) [23]. Known results, including logarithmic corrections, were reproduced.

It would be useful to have an independent estimate of the spinon velocity. A velocity $c = 2.4 \pm 0.3$ was extracted for the critical J-Q model in [8], using a criterion for cubic-space-time geometry in QMC simulations. Although the value is in good agreement with ours, it is unclear whether their method applies to spinons (while it should evidently not for magnons). In future studies we will extract $c$ from imaginary-time dependent spin-spin correlations.

Our study lends support to the DQC scenario [3] for the Néel–VBS transition, although the phenomenological approach does not address the mechanism of deconfinement (only tests the consequences). Log corrections at $T > 0$ should also have counterparts at $T = 0$. Further work along these lines will hopefully explain, e.g., anomalous corrections to the spin stiffness of the J-Q model [8] and its impurity response [9]. An important missing link is how these corrections could arise from the CP$^1$ field theory of the DQC proposal [3], i.e., whether this theory is complete in its current form or whether some ingredient is still missing. No log corrections were found in large-$N$ treatments of the CP$^{N-1}$ theory [22, 24], but it is possible that these corrections appear only for small $N$. A logarithmic enhancement of the susceptibility was found in a U(1) gauge theory with fermions [23]. In that case, there is also a correction to the specific heat, which makes the Wilson ratio non-divergent. The spinon gas approach with Fermi statistics gives no log corrections and the Wilson ratio equals 0.0320, which is identical (with $\mu = 1/2$) to the value in Ref. 22.

We finally note that there are no indications of a first-order transition in the J-Q model (with previous claims [10, 11] not supported by later results [8, 9]). As a matter of principle, however, extremely weak discontinuities cannot be ruled out based on numerical data alone (though the first-order scenario appears increasingly unlikely). What we have shown here is that, regardless of the ultimate nature of the transition, spinons are deconfined on length scales sufficiently large to have significant consequences for the thermodynamics.

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