Thermodynamics of a Gas of Deconfined Bosonic Spinons in Two Dimensions

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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 C and the magnetic susceptibility χ at low temperature T in terms of a correlation length $\xi(T)$. Comparing with quantum Monte Carlo results for the J-Q model, which is a candidate for a deconfined Néel–VBS transition, we obtain an almost perfect consistency between C, χ, and ξ. The corresponding expressions for magnon (triplet) excitations are not internally consistent, however, lending strong support for spinons excitations in the J-Q model.

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The excitations of a quantum antiferromagnet are spin waves (magnons) carrying spin $S = 1$. At a conventional quantum phase transition in which the antiferromagnetic (Néel) order parameter vanishes continuously [1, 2], the magnons remain well-defined elementary excitations even at the critical point. The gapped "triplon" excitations in the nonmagnetic phase also have $S = 1$. A different *deconfined quantum critical* (DQC) point has also been suggested [3], in which the magnons of a two-dimensional system fractionalize into independent (deconfined) $S = 1/2$ spinons. In the non-magnetic phase, which in this case is a valence-bond solid (VBS) with spontaneously broken lattice symmetries [4], the spinons are confined into excitations which carry spin $S = 1$ and $S = 0$. The DQC proposal is supported by quantum Monte Carlo (QMC) simulations of a "J-Q" model [5–9] (an $S = 1/2$ Heisenberg model including four-spin or higher-order terms), although deconfined spinons have so far not been explicitly observed. The DQC scenario violates the long-held "Landau rule" according to which an order–order transition breaking unrelated symmetries should be of first order. While there are studies claiming a generic first-order Néel–VBS transition [10, 11], no convincing signs of discontinuities of phase coexistence have have so far been detected in the J-Q model [8].

In this *Letter* we provide evidence for deconfinement in the J-Q model based on its thermodynamic properties. Using a phenomenological ansatz of deconfined bosonic spinons with linear dispersion $\epsilon(k) = ck$ (as in the DQC theory [3]), we derive expressions for the specific heat and the magnetic susceptibility. In addition to the spinon velocity c, these quantities depend on the length scale Λ within which spinons can be regarded as deconfined at temperature $T > 0$. In the $T = 0$ DQC theory [3], this length in the VBS phase diverges as a power of the correlation length, $\Lambda \propto \xi^{1+a}$, where $a > 0$ and the standard correlation length (defined, e.g., in terms of the spin-spin correlation function) diverges as $\xi \propto |q - g_c|^{-\nu}$ as the critical coupling g_c is approached. While the confinement scale Λ is well defined at $T = 0$, where it is also associated with an emergent $U(1)$ symmetry [3, 7], it is at present not clear how this scale enters when there is a finite density of thermally excited spinons. We will here present numerical evidence of an anomalous correction, possibly logarithmic, to the standard divergence $\xi \sim T^{-1/z}$ at g_c (with $z = 1$ expected at a DQC point). We argue that the confinement scale cannot be separated from the spin correlation length at $T > 0$ and use QMC results for $\xi(T)$ in lieu of $\Lambda(T)$ in the spinon-gas expressions. The so predicted $C(T)$ and $\chi(T)$ are almost perfectly satisfied in the critical J-Q model, lending strong support to deconfined spinon excitations.

Quantum-critical models—We will discuss the cases of spinon and magnon excitations in parallel and consider two models in which the two scenarios should be realized. The J-Q model provides a test-case for deconfined spinons and is defined by the hamiltonian [5]

$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q \sum_{\langle ijkl \rangle} C_{ij} C_{kl}, \tag{1}$$

where C_{ij} is a singlet projector; $C_{ij} = 1/4 - \mathbf{S}_i \cdot \mathbf{S}_j$. 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 2×2 plaquette. The ground state has Néel and VBS order for $Q < Q_c$ and $Q > Q_c$, respectively, with $J/Q_c = 0.04498(3)$ according to a recent study [8, 12].

Conventional O(3) $T > 0$ quantum-critical scaling has been studied in the past in various dimerized Heisenberg models (where the hamiltonian itself breaks lattice symmetries) [13–17]. To compare with the J-Q model, we here consider a system with couplings J and $J' > J$, with the stronger ones arranged in columns. A recent high-precision study of this system [12] gave the critical ratio $J'_c/J = 1.90948(4)$. Here we consider $L \times L$ lattices with L up to 512, at $J'/J = 1.9095$ and $J/Q = 0.045$ for the respective models (within the error bars of the best known critical values). The QMC results are free from visible finite-size effects at the temperatures considered.

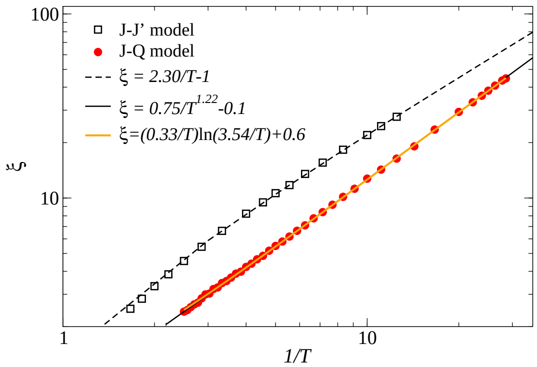

FIG. 1: (Color online) Correlation length versus inverse temperature for the critical J-Q and J-J' models. A fit to $\xi \propto 1/T$ with a constant correction is shown for the $J-J'$ model, while the faster divergence in the J-Q model has been fitted to two different forms—a power-law $1/T^{1+a}$ with $a = 0.22$, as well as $1/T$ with a multiplicative log-correction.

Below we will quote energies in units of $Q = 1$ for the J-Q model and $J = 1$ for the J-J' model.

The spin correlation lengths of the two models (using the standard momentum-space second-moment definition [12]) are shown in Fig. 1. The expected quantum-critical $1/T$ behavior is observed in the J-J' model for $T \lesssim 0.3$, and some of the deviations from this behavior at higher temperatures can be accounted for by a constant correction. In the J-Q model, the divergence is clearly faster. The behavior can be fitted either to a different power-law, $1/T^{1+a}$ with $a \approx 0.22$, or with a multiplicative log-correction to the $1/T$ form. In the standard quantum-criticality scenario [2], a power-law with $a > 0$ would imply a dynamic exponent $z = (1+a)^{-1} < 1$. The susceptibility $\chi \sim T^{2/z-1}$ should then be governed by an exponent $2/z - 1 > 1$. The latter behavior is, however, ruled out by the finding in [8] that χ vanishes as $T \to 1$ slower than T, due to a correction consistent with a factor $\ln(1/T)$. Thus, a log-correction to the $1/T$ form of ξ seems the more likely scenario. Alternatively, the deviation from $1/T$ could be due to a very slowly decaying conventional power-law correction, as was recently found in a different model [18]. We next discuss how the spinon gas scenario relates the correlation length to the susceptibility and the specific heat.

Spinon gas—Our assumption is that the critical system can be described as a gas of bosonic spinons with dispersion $\epsilon(k) = [c^2k^2 + \Delta^2(T)]^{1/2}$ 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 dimerized Heisenberg models), in which case the thermal "gap" Δ is related to the correlation length ξ according to $\Delta \propto 1/\xi \propto T^{1/z}$, with $z = 1$ [1, 2]. The gap corresponds to an infrared cut-off. If the spinons are confined within a length-scale Λ, this should be the scale to use in the gap; $\Delta \propto 1/\Lambda$. We are not, however, able to directly compute Λ at $T > 0$, and it may not even be possible to separate such a length scale from ξ when the density of excited spinons is finite, since these spinons should also contribute to the correlation functions. Here we will therefore assume that the proper length scale to use for $\Delta(T)$ is the correlation length ξ discussed above.

In a magnetic field B, a doubly-degenerate spinon level is split according to

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

where $\mu = 1/2$. This form with $\mu = 1$ holds also for the two shifted $S = 1$ magnon levels (with ϵ_0 not shifted).

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

$$\begin{aligned} M &= \mu F \int \left(\frac{1}{e^{\epsilon_-/T} - 1} - \frac{1}{e^{\epsilon_+/T} - 1} \right) \frac{d^2k}{(2\pi)^2} \\ &= \mu^2 F \frac{TB}{4\pi c^2} \int_0^\infty \frac{x dx}{\sinh^2[\frac{1}{2}\sqrt{x^2 + (\Delta/T)^2}]}. \end{aligned} \qquad (3)$$

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 above with a factor $F = 2$, while for magnons $F = 1$. The integral can be computed exactly, giving

$$\chi = \mu^2 F \frac{T}{\pi c^2} \left(\frac{\Delta/T}{1 - \mathrm{e}^{-\Delta/T}} - \ln(\mathrm{e}^{\Delta/T} - 1) \right). \qquad (4)$$

For magnons at the usual O(3) transition, $\Delta/T \approx 0.96$ has been computed in the large-N (number of components) limit, which gives [2]

$$\chi_1 \approx (1.0760/\pi c^2)T. \qquad (5)$$

For spinons, we assume $\Delta = 1/\xi$ and use the J-Q results for ξ shown in Fig. 1. In the accessible temperature window, it does not matter which of the two fitted forms we use, since they coincide. In (4) we now have $\Delta/T \to 0$ as $T \to 0$, resulting in an infrared divergence of χ/T. To obtain a simple expression we discuss the modified power law written as $\Delta/T = (T/bc)^a$, which gives the low-temperature form

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

where the exponent $a = 0.22$ and the product $bc = 3.70$ from the data in Fig. 1. The log-correction is very interesting, as it was already identified in a recent QMC study of the J-Q model [8]. Using the multiplicative log-correction instead of the modified power-law in ξ gives a double-log divergence of χ/T, which with the appropriate parameters cannot be distinguished from the simple log in the temperature window considered.

The specific heat per unit cell is

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

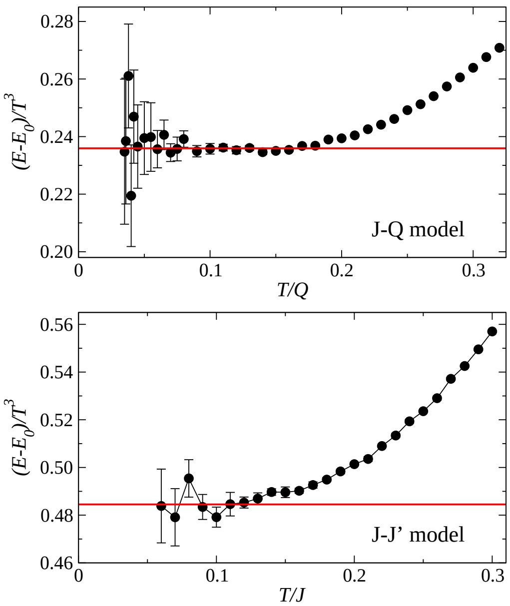

FIG. 2: (Color online) Temperature dependence of the energy E relative to the ground state energy E_0 with the expected leading T^3 dependence divided out. The horizontal lines show the prefactor of the cubic term in the $E(T)$ fits.

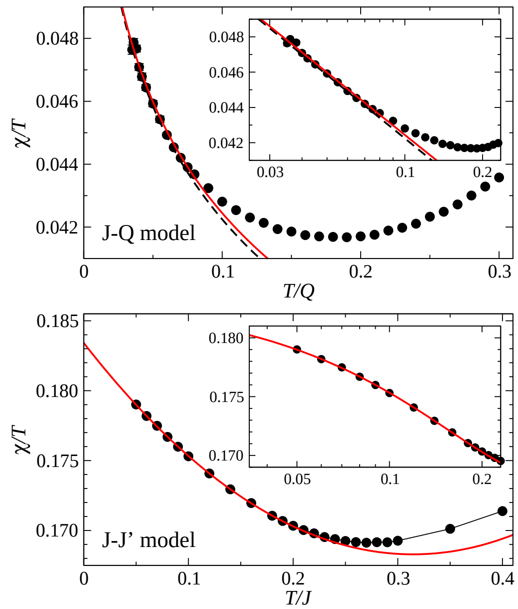

FIG. 3: (Color online) Susceptibility divided by T. In the J-Q graph the dashed curve is Eq. (6) with $a = 0.22$, $c = 2.6$, and $bc = 3.7$. The solid curve is the full form (4) with the same parameters. The curve in the J-J' graph is a second-order polynomial. The insets show the data on log scales.

which for spinons leads to the low-T behavior

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

when the power-law for of ξ is used [and $\zeta(3) \approx 1.20206$]. Note that the log-correction here is not as dramatic as in the susceptibility (6). For the O(3) transition

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

was obtained using the large-N value of Δ/T [2, 19].

Energy and susceptibility fits—Apart from the logarithms arising from the correction to $\xi \sim 1/T$, the differences in the thermodynamics between spinons and magnons arise mainly from the degeneracy factors and μ. Note that once Δ/T has been fixed, by assuming $\Delta = 1/\xi$ and using numerical results for ξ (or using the large-N result for magnons [2, 19]) the velocity c is the only free parameter. We can then test the internal consistency of the picture by fitting QMC data for χ and C. Note that in the case of the J-J' model all quantities should be normalized per two-site unit cell.

We first fit low-T results for the internal energy based on the leading specific heat forms (8) and (9). In addition to the $T > 0$ QMC data, we also use the ground state energy extrapolated to $L = \infty$ based on $T \propto 1/L$ calculations. 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 $c = 2.55$ for the J-Q model and the magnon velocity $c = 1.38$ for the J-J' model (which should be interpreted as $c = \sqrt{c_x c_y}$ 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). It is anyway doubtful whether the spinon gas model can correctly capture subleading corrections.

The susceptibilities of both models are shown in Fig. 3 with T divided out. In the case of the J-J' model, there are significant corrections to the asymptotic $T \to 0$ constant behavior expected with (5). A second-order polynomial fit to the low-T data is shown. The extrapolated $T = 0$ susceptibility corresponds to a spin-wave velocity $c = 1.36$ in (5), in excellent agreement with the value obtained from the energy.

For the J-Q model, we first use (8) with only the leading log-correction and fix $a = 0.22$ and $bc = 3.7$ from the power-law fit to ξ in Fig. 1. The best fit to the low-T susceptibility is achieved with $c = 2.60$, within 2% of the value obtained above from the energy fit. Using the same parameters in full form (4) shows only minor corrections to the asymptotic low-T form, as also shown in Fig. 3.

Using magnon parameters ($F = 1$, $\mu = 1$ instead of $F = 2, \mu = 1/2$) in the J-Q fits leads to a factor 2 in (6) and 3/4 in (8), and, thus, completely inconsistent velocities extracted from C and χ (differing by more than a factor 1.6). The excellent agreement for spinon parameters lends strong support to the spinon-gas picture. It should be noted that we have assumed $\Delta = 1/\xi$ in the fits for the J-Q model, while we may only expect $\Delta = d/\xi$ with d of order 1. Physical observables depend weakly on

d and the consistent c-values extracted from two different quantities justify the use of $d = 1$ *a posteriori*.

Wilson ratio—The Wilson ratio of the J-Q model exhibits a weak $T \to 0$ divergence. From Eqs. (6) and (8) we obtain $W_{1/2} = \chi T/C = w_{1/2}[1 + a\ln(bc/T)]$, with $w_{1/2} = 0.0346(2)$. The log-correction again relies on the particular power-law correction used in the fit to ξ in Fig. 1, and should most likely in actuality be replaced by a double-log corresponding to a log-correction to $\xi \sim 1/T$. For the J-J' model we get $W_1 = 0.1262(6)$, 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 [2] 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 bosonic spinons against QMC data for the critical J-Q model, which is a promising candidate for a DQC point. The correlation length ξ diverges faster than $1/T$ as $T \to 0$ (most likely due to a log-correction) and this can be related to the divergence (log or double-log) of the susceptibility χ/T that was previously observed in the J-Q model [8]. The velocity entering in χ agrees almost perfectly with the velocity needed to fit the specific heat C. Thus, highly non-trivial relationships between ξ, C, and χ predicted from the spinon gas have been confirmed. 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.

Although our study lends support to the DQC scenario for the Néel–VBS transition, the phenomenological approach does not address the mechanism of deconfinement. The anomalous correction to the $1/T$ divergence of ξ is puzzling and may be intimately related to the deconfinement. Log corrections at $T > 0$ should also have counterparts at $T = 0$. Future work 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 point [3], i.e., whether the theory is complete in its present form or whether some ingredient is still missing. No logs were found in large-N treatments of the CP^{N-1} theory [21, 22], but such corrections may appear for small N. A log-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 logs and the Wilson ratio equals 0.0320, which agrees with Ref. 21 (with $\mu = 1/2$).

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 correlation length (with its anomalous correction), these interactions seem to only have very small effects on the thermodynamics.

It would be useful to have an independent estimate of the spinon velocity. A value $c = 2.4(3)$ was extracted for the critical J-Q model in [6], using a cubic space-time geometry in QMC simulations. Although the value agrees well with ours, it is unclear whether the method applies here (but it works for magnons in the Néel state [20]). In future studies we plan to extract c from the imaginary-time dependent spin-spin correlations.

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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