Thermodynamics of the Ishimori-Haldane-Faddeev ferromagnetic chain: The field-dependent case

N. Theodorakopoulos, N. C. Bacalis, and Z. Xiong
Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vas. Constantinou 48, GR-116 35 Athens, Greece

(Received 11 December 1995; revised manuscript received 2 April 1996)

We calculate the thermodynamic properties of the spin-S, isotropic ferromagnetic chain with nearest-neighbor logarithmic interactions, in an external magnetic field. The calculation is performed via the transfer integral method ($S=\infty$) and via the interacting soliton-gas scheme (any S). The results indicate scaling behavior of the field-dependent part of the free energy; the scaling function appears to be spin independent. [S0163-1829(96)08629-8]

I. INTRODUCTION

The Ishimori-Haldane-Faddeev[1–3] ferromagnet (IHFF), a one-dimensional, classical lattice model of spins with logarithmic nearest-neighbor interactions, is of considerable theoretical interest due to its exceptional property of complete integrability. The model's soliton-dominated dynamics has made possible the development[4] of an essentially exact, (semiclassical), ''soliton-gas'' approach to its thermodynamics. Numerical[5] and analytical[4] results have already been reported in the zero-field case. A further feature which makes the model particularly interesting from the viewpoint of fundamental condensed-matter physics is that, at low temperatures, the leading-order asymptotic behavior is identical with that of the isotropic Heisenberg ferromagnet (IHF),[5] a key model for the understanding of magnetism.

In this work, we report the results of extensive numerical investigations based on the soliton approach to the thermodynamics of the IHFF in the case of low temperatures T, nonvanishing magnetic field h, and arbitrary spin S; the general theory of the interacting gas of nontopological magnetic solitons, and its analytical application to selected, zero-field, limiting cases has been presented in Ref. 4, which will be referred to as I in this work. In the classical limit, $S\rightarrow\infty$, we also perform a leading-order test of the validity of the soliton approach by comparison with exact values, which we obtain by an accurate numerical implementation of the transfer-integral (TI) method.[6]

Both approaches, soliton and TI, reveal the scaling behavior of the field-dependent part of thermodynamic quantities: in the immediate vicinity of the ''critical'' point ($T=0,\ h=0$), dependence on the temperature and the magnetic field enters only in the combination h/T^2. Moreover, in the soliton approach, the scaling function which describes the dependence of the field-dependent part of the free energy on the reduced variable h/T^2, appears to be independent of the value S of the spin. It should be noted that similar scaling behavior has been recently reported for the magnetization of the IHF.[7]

The paper is organized as follows: Section II presents the results obtained by the numerical solution of the TI-eigenvalue problem, introduces, and verifies a scaling Ansatz appropriate to the ''critical'' regime ($h\rightarrow 0,\ T\rightarrow 0$). Section III presents the results of the low-temperature, field-dependent, soliton-based statistical mechanics, for both quantum [$S=\mathcal{O}(1)$], and classical ($S\rightarrow\infty$) cases. Concluding remarks are made in Sec. IV.

II. EXACT CLASSICAL (TI) THERMODYNAMICS

The dimensionless (I) classical IHFF model Hamiltonian

$$H/j=-2\sum_i \ln\left(\frac{1}{2}+\frac{\hat{S}_i\cdot\hat{S}_{i+1}}{2}\right)-h\sum_i (\hat{S}_i^z-1), \quad (2.1)$$

describes a chain of unit spins $\hat{S}_i$ placed in an external field h along the z axis; energies and magnetic fields are measured in units of the exchange constant j.

The thermodynamic properties of the classical IHFF can be expressed[6,8] in terms of the largest eigenvalue Λ_{00} of the integral equation

$$\int_{-1}^{1}dx'\left|\frac{x+x'}{2}\right|^{2\beta}e^{\kappa(x+x')/2}P_{2\beta}^{0}\left(\frac{1+xx'}{|x+x'|}\right)\psi_{l0}(x')=\Lambda_{l0}\psi_{l0}(x), \quad (2.2)$$

where $\beta=j/k_BT$, $\kappa=\beta h$, and P_ν^m is the Legendre function. Equation (2.2) is the analog of Eq. (21) in Ref. 6 for the IHF. It has been examined by Weber[9] in the two special cases which are analytically tractable, i.e., (i) $\kappa=0$ and (ii) $\beta=0$. Here, we quote the result for case (i), which will be useful below:

$$\Lambda_{00}(\beta,\kappa=0)=\frac{1}{2\beta+1}. \quad (2.3)$$

We have numerically solved (2.2) in the low-temperature regime $\beta\gg 1$, by the method of 32-point Gaussian integration.[6] The accuracy of the method can be checked in the two special cases (i) and (ii) (cf. above), and is typically of $\mathcal{O}(10^{-11})$.

The calculation demands exact knowledge of the Legendre function of high order and large values of the argument (including infinity, from the $x'=-x$ contribution). We have made use of the limiting property

0163-1829/96/54(6)/4033(5)/$10.00

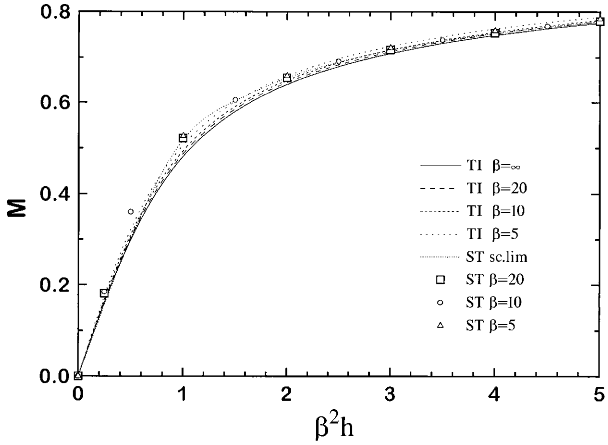

FIG. 1. Average magnetization per site vs $\beta^2 h$ of the IHFF for β = 5, 10, and 20 obtained via the TI and ST models. The TI $\beta=\infty$ curves are obtained by extrapolation of the finite β results. The ST ''scaling limit'' curve is obtained by the process described in the caption of Fig. 7.

$$\lim_{z\to\infty}\widetilde{P}_\nu(z)\equiv z^{-\nu}P_\nu(z)=\frac{\Gamma(\nu+\frac{1}{2})}{\Gamma(\nu+1)\Gamma(\frac{1}{2})}. \tag{2.4}$$

For finite values of the argument $z>1$, we have evaluated $\widetilde{P}_\nu(z)$ by direct integration of the ordinary differential equation

$$(1-z^2)\frac{d^2\widetilde{P}}{dz^2}+2\left[\frac{\nu}{z}-(\nu+1)z\right]\frac{d\widetilde{P}}{dz}+\frac{\nu(\nu-1)}{z^2}\widetilde{P}=0 \tag{2.5}$$

in the interval $1\leqslant z<\infty$, subject to the initial conditions $\widetilde{P}(1)=1$, and $\widetilde{P}'(1)=\nu(\nu-1)/2$.

At low temperatures, we will use a scaling ansatz for the free energy. Some properties of the scaling function which enters the ansatz, as well as the crucial ''critical exponents'' can be deduced exactly from the limiting behavior ($h\to 0$ and $h\to\infty$) as follows:

The free energy per site can be separated into field-independent and field-dependent parts

$$f(\beta,h)\equiv f_0(\beta)+\delta f(\beta,h), \tag{2.6}$$

where $\beta f_0=-\ln[\Lambda_{00}(\beta,\kappa=0)]=\ln(2\beta+1)$. For the field-dependent part we make the scaling ansatz

$$\delta f(\beta,h)\sim-\beta^\sigma g(\beta^\tau h), \tag{2.7}$$

where $g(0)=0$ by definition. The various thermodynamic functions can now be expressed in terms of the scaling function g. The magnetization per site is given by

$$m\sim\beta^{\sigma+\tau}g'(\beta^\tau h), \tag{2.8}$$

and the isothermal susceptibility by

$$\chi\sim\beta^{\sigma+2\tau}g''(\beta^\tau h). \tag{2.9}$$

From the known zero-field asymptotic behavior of the susceptibility,[9] $\chi\to 2/3\beta^2$, we deduce that $\sigma+2\tau=2$ and $g''(0)=2/3$. The vanishing long-range order at all finite temperatures implies $g'(0)=0$, and the saturation magnetization at high magnetic fields and at all temperatures demands $g'(\infty)=1$ and $\tau=-\sigma$ (= 2, cf. above). Thus g is a function of $x=\beta^2 h$.

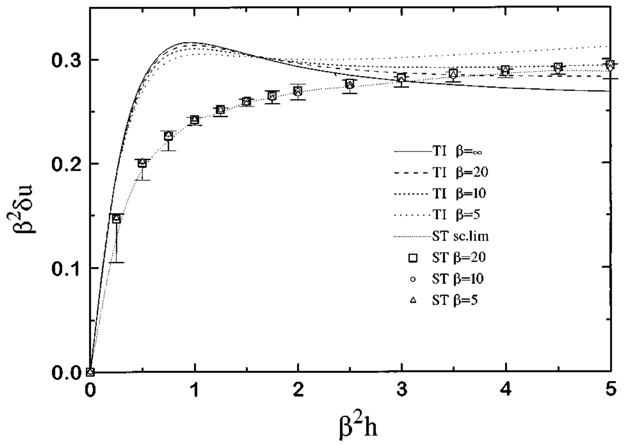

FIG. 2. Same as Fig. 1, for the field-dependent part of the average energy per site.

In terms of g, the field-dependent part δu, of the internal energy is given by

$$\beta^2\delta u\sim g(x)-2xg'(x)+x. \tag{2.10}$$

The curves in Figs. 1–3 summarize our low-temperature TI results for the magnetization, energy, and susceptibility, respectively. The onset of scaling behavior is somewhat slower in the case of the energy, probably because it involves the (presumably stronger) corrections to scaling in the function $g(x)$ itself, rather than its derivative. Our numerical results suggest a finite value of $G_\infty\equiv\lim_{x\to\infty}[g(x)-2g'(x)x+x]\sim 0.25$.

III. SOLITON THERMODYNAMICS

The theory of soliton-based thermodynamics (ST) of the IHFF has been presented in I. It is formulated in terms of a two-dimensional nonlinear integral equation for the quasiparticle energy and is in principle exact, since it incorporates all phase-shift interactions between solitons. At low temperatures, it is possible to use approximate expressions for the

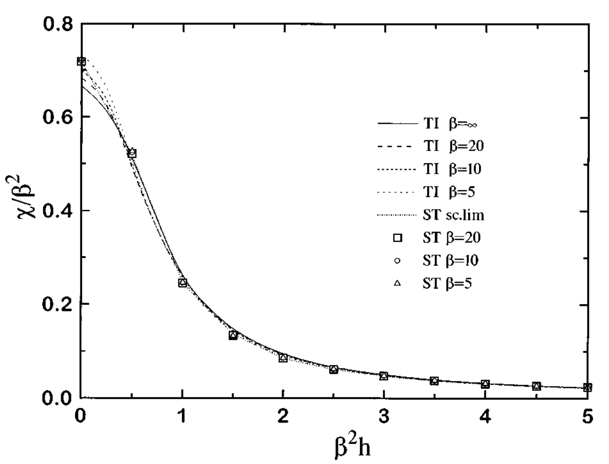

FIG. 3. Same as Fig. 1, for the isothermal susceptibility.

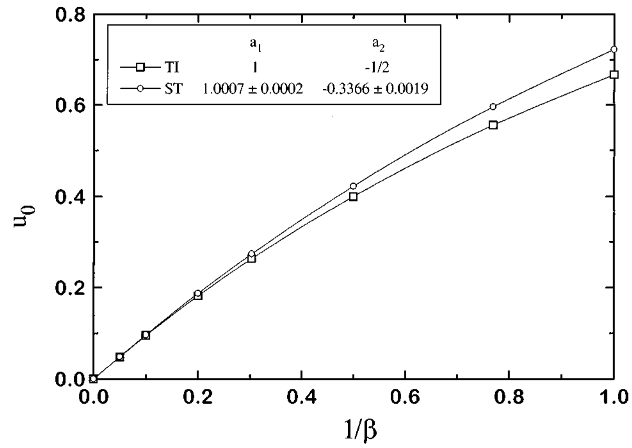

FIG. 4. Energy vs temperature for zero field. Both TI and ST asymptotically tend to $1/\beta$. Terms of $O(T^2)$ differ in the prefactor.

phase shifts and reduce the problem to the one-dimensional integral equation (4.2) of I [or the equivalent ordinary differential equation, (4.3), which is solved numerically in this work].

We consider the sequence of (semiclassically quantizable) versions of the Hamiltonian (2.1) [cf. Eq. (2.1) of I]; the spin

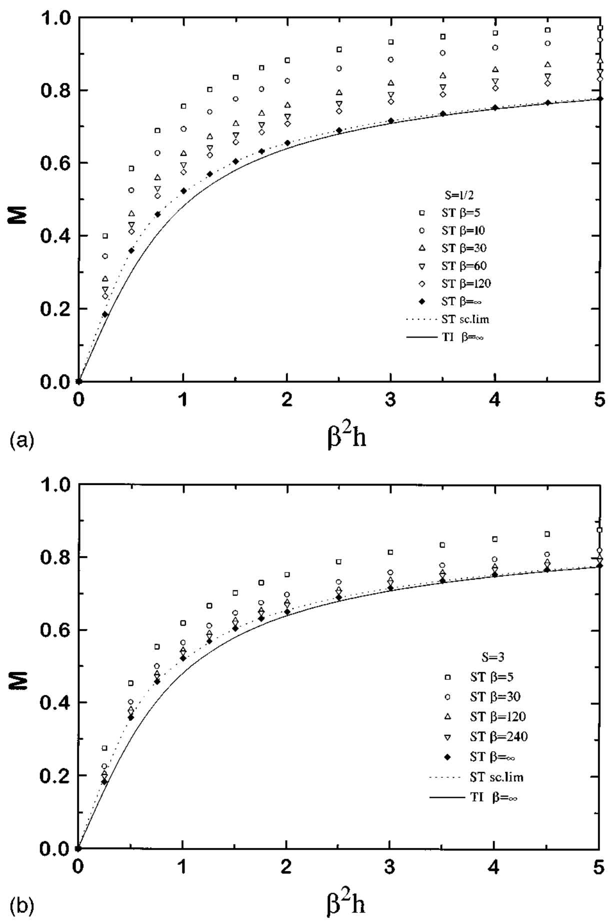

FIG. 5. The magnetization per site for the semiclassical $S=1/2$ IHFF (a) and $S=3$ (b), in the low-temperature regime. The solid diamonds are obtained by extrapolating the finite β curves to $\beta=\infty$. Also shown are the limiting scaling curves of Fig. 1, both for ST and TI.

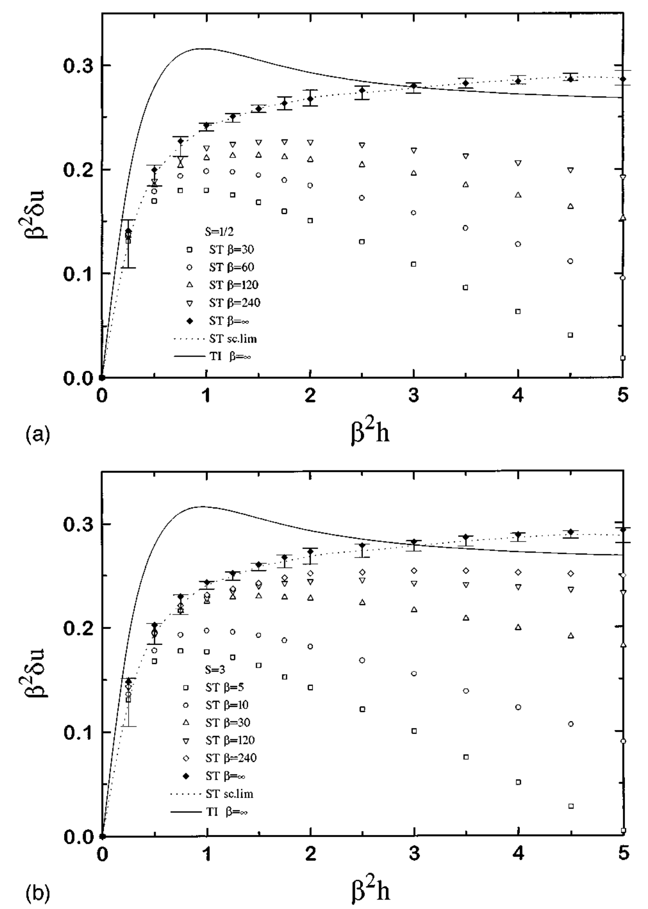

FIG. 6. Same as in Fig. 5 for the field-dependent part of the energy.

vectors have length S, the physical exchange constant is $J_S=j/S^2$, and the magnetic field $h_S=h/S$. The sequence thus constructed approaches (2.1) in the classical limit, $S\to\infty$, $\hbar\to 0$, $\hbar S\to$const.[8]

The following limiting cases provide us some guidance on what to expect: (i) If the soliton description is correct, classical ST should agree with TI thermodynamics.[10] (ii) Since the IHFF has the same low-T asymptotic behavior as the IHF,[5] the (classical-like) behavior for the susceptibility obtained by the numerical solution of the $S=1/2$ Bethe ansatz for the IHF,[11,12] should be recovered here as well. In fact, as will be seen below, this turns out to be a special case of a more general scaling behavior, which holds near $T=0$ (cf. Sec. II) and is independent of the value of S.

In the case of vanishing magnetic field, the ST energy u_0 is shown in Fig. 4. It is in good agreement, to leading order in T, with the TI predictions, i.e., $u_0\sim a_1/\beta+a_2/\beta^2$, where $a_1=1$. Since the soliton density is equal to 1/2 (I), the meaning of this result is that every soliton contributes an average of $2/\beta$ to the energy, in agreement with the equipartition theorem. This result is not trivial; the fact that (asymptotic) equipartition can be recovered within the soliton picture, demonstrates that the complexity of the (dense) classical soliton gas can be captured by the approximation of pairwise interacting solitons. The discrepancy which occurs at higher order (a_2^{ST} differs significantly from the TI value of

$-1/2$) does not imply a fundamental limitation of soliton theory; it is a consequence of the approximate phase shifts which were used in obtaining Eq. (4.3) in I, and which limit our ability to describe soliton-soliton interactions beyond the leading order in the temperature.

For nonzero magnetic fields, we have performed ST calculations for various sequences of S. In the classical limit, $S\to\infty$, results are represented by the points in Figs. 1–3, for the magnetization, energy, and susceptibility, respectively. In the case of the magnetization, agreement between ST and TI is satisfactory, with the exception of a small region around $\beta^2 h \leqslant 1$. A similar agreement is observed in the case of the susceptibility (Fig. 3), which further yields $g''_{\mathrm{ST}}(0)=0.72$, in fair accord with the TI value 2/3. Agreement is less satisfactory in the case of the energy. In particular: (i) Our soliton calculation in the classical limit, fails to account for the bump which appears in the TI results around $\beta^2 h \sim 0.9$. However, the property of asymptotic scaling (as $\beta\to\infty$) *per se*, is verified, even though the details of the ST and TI scaling functions differ. (ii) We note the discrepancy between the limiting values of $G_\infty^{\mathrm{ST}}=0.30$ and $G_\infty^{\mathrm{TI}}=0.25$. Although numerical accuracy is a serious issue (the values of energy differences δu approach the numerical accuracy as the temperature is lowered), we believe that both deficiencies, in view of the fact that they occur also at higher, numerically more reliable, temperatures, are more likely to reflect the approximations made in the soliton phase shifts (cf. above) rather than any limitations of the numerical procedure.

In the quantun cases $S=1/2$ and 3, ST results are shown in Figs. 5 (magnetization) and 6 (energy), respectively. We note two important features of leading-order asymptotics: (i) It appears that in the limit $\beta\to\infty$, scaling behavior prevails, i.e., thermodynamic quantities depend on the reduced variable $\beta^2 h$. (ii) The limiting scaling function seems to be universal, i.e., independent of S. Both features can be clearly demonstrated by the details shown in Fig. 7. At a given value of $\beta^2 h$, the extrapolations $\beta\to\infty$ lead to the same asymptotic result, independently of the value of S. Deviations from exact scaling behavior are of course stronger in the quantum cases but, ultimately, classical and quantum cases approach a common scaling limit (shown in Figs. 1–3, 5, and 6).

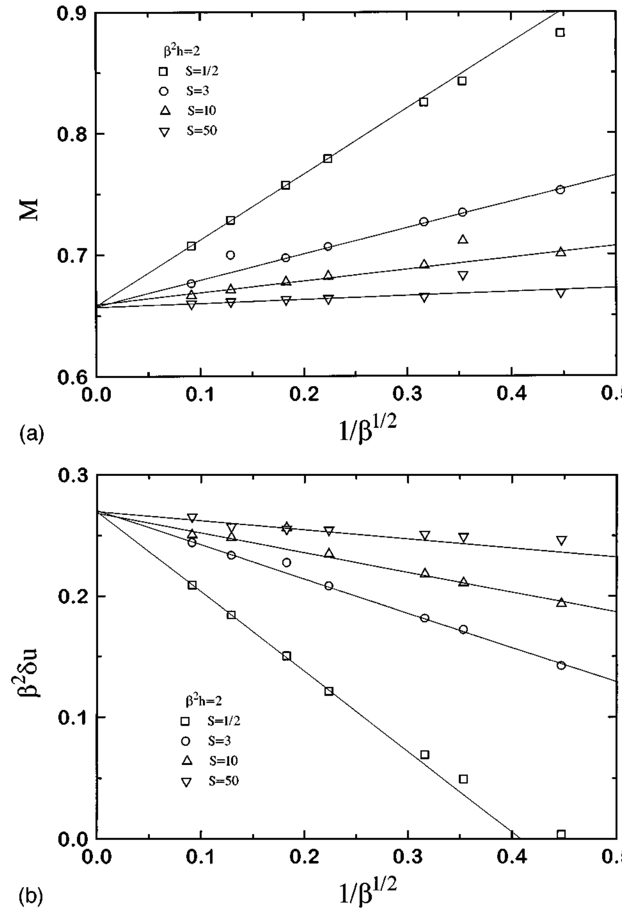

FIG. 7. (a) The magnetization per site vs the square root of the temperature for various values of S, as computed in the soliton gas approach; note that the extrapolated value, in the limit $\beta\to\infty$, is independent of S. (b) Same as (a) for the field-dependent part of the energy (multiplied by β^2). The points obtained by repeated application of this extrapolation procedure for various values of $\beta^2 h$, produce the ''ST scaling limit'' curve referred to in the other figures.

IV. CONCLUDING REMARKS

We have presented extensive TI and ST results for the field-dependent thermodynamic properties of the IHFF chain in the low-temperature regime. Our findings suggest that the same thermodynamic scaling function describes the leading-order asymptotics of both classical and quantum chains. The results presented here extend those of Ref. 7, which were restricted to the magnetization (of the asymptotically equivalent Heisenberg model). In addition, the soliton-theoretical calculation provides a computationally traceable link between soliton dynamics (as expressed by the phase shifts) and thermodynamic scaling near a ''critical point.''

Our classical ST calculations exhibit significant systematic deviations from exact TI results. These limitations presumably reflect the approximate phase shifts used in reducing the two-dimensional integral equation (3.4) of Ref. 4 to a numerically tractable one-dimensional form. Pending a (presently) computationally prohibitive exact implementation of the full interacting soliton-gas scheme, we have still been able to draw valuable conclusions about the existence of an S-independent, $T\to 0$, scaling limit of thermodynamics near zero temperature, along with acceptable estimates of the (high- and very low-field) limits of the scaling function.

[1] Y. Ishimori, J. Phys. Soc. Jpn. **51**, 3417 (1982).
[2] F.D.M. Haldane, J. Phys. C. **15**, L1309 (1982).
[3] L.D. Faddeev, in *Recent Advances in Field Theory and Statistical Mechanics*, Proceedings of the Les Houches Summer School, 1982, edited by J.B. Zuber and R. Stora (North-Holland, Amsterdam, 1984).
[4] N. Theodorakopoulos, Phys. Rev. B **52**, 9507 (1995).
[5] N. Theodorakopoulos and N.C. Bacalis, Phys. Rev. Lett. **67**, 3018(1991).
[6] M. Blume, P. Heller, and N.A. Lurie, Phys. Rev. B **11**, 4483 (1975).
[7] H. Nakamura and M. Takahashi, J. Phys. Soc. Jpn. **63** 2563 (1994).
[8] M.E. Fisher, Am. J. Phys. **32**, 343 (1964).
[9] R. Weber, Doctoral Dissertation, Universität Basel, 1988.
[10] The dependence of ST on the value of S is singular in the limit $S\rightarrow\infty$. We have not been able to absorb this singularity and produce a classical ST equation. Thus our classical results are obtained by a (stable) extrapolation of high-$S(>20)$ semiclassical values to $S=\infty$.
[11] P. Schlottmann, Phys. Rev. Lett. **54**, 2131 (1985); Phys. Rev. B **33**, 4880 (1986).
[12] M. Takahashi and M. Yamada, J. Phys. Soc. Jpn. **54**, 2808 (1985).