PHYSICAL REVIEW B VOLUME 12, NUMBER 1 1 JULY 1975

Classical limit of the Heisenberg model*

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(Received 14 October 1974)

The proper way to take the classical limit of the Heisenberg model is demonstrated. It is shown that a mixing of quantum-mechanical and classical formulas can give unphysical results. Some examples show the need for the proper way to take the classical limit. The validity of various conclusions concerning the temperature dependence of the spin-wave damping arrived at from the first few frequency moments is also discussed for the classical Heisenberg linear chain.

I. INTRODUCTION

Recent experiments have brought new interest into the study of Heisenberg models. The discovery of astonishingly sharp spin waves in both ferromagnetically[1] and antiferromagnetically[2,3] coupled one-dimensional linear chains has called for a microscopical explanation. Many theories are invoked to give an account of the spin waves,[4–12] and some utilize exact static results for the classical Heisenberg model.[8–12] This can be attained by taking a "classical" limit of the ordinary quantum-mechanical Heisenberg model.[13–22] In the one-dimensional case, all the classical static properties can, in principle, be calculated exactly.[12,13] It is thus very tempting to base dynamical theories for quantum-mechanical Heisenberg linear chains on the static classical quantities. However, in doing this it is important to have the precise connection between the classical and quantum-mechanical models. One reason is that apparent contradictions may show up, if the precise connection is not held clear. Another, more important reason is that a mixing of classical and quantum-mechanical results may give rise to completely unphysical results. To be fully consistent, one should of course confine oneself to a completely classical calculation. But this naturally raises the question, to which extent the classical model describes the quantum-mechanical one. It is well known, e.g., that the specific heat of the classical model does not go to zero with temperature, which gives rise to a logarithmic singularity in the entropy. This is an unphysical feature and means that the classical model is a poor approximation to the quantum-mechanical model at low temperatures, when thermodynamic properties are of interest. When dynamics is considered, the problem is more involved. The quantum corrections to the classical dynamics have been the subject of some recent papers.[21,22]

The aim of this paper is to first give a very simpleminded and straightforward derivation of the classical limiting procedure. We will not go into fundamental questions concerning, e.g., the classical angular momentum in relation to the quantum-mechanical one, or the existence of the thermodynamic limit in the classical case, and its connection to the quantum-mechanical thermodynamic limit. Such subtleties seem to be sufficiently investigated[14,15] that we can restrict ourselves to a clarifying demonstration only. The demonstration reveals the importance of taking the basic dynamical equation into account, because otherwise the specification of the limit procedure is incomplete. The result is not original, but the derivation gives the proper detailed background for the discussion in Sec. III, where first the danger in improper mixing of classical and quantum-mechanical results is clarified, and then some mystifying statements from the literature are enlightened through the use of the proper classical limit. Section IV, finally, discusses spin-wave damping in classical linear Heisenberg chains, using exact static spin-correlation functions.

II. CLASSICAL LIMIT

The classical Heisenberg model is given by the Hamiltonian

$$H_{\rm cl} = -\frac{1}{2}\sum_{\vec{\rm R}\vec{\rm R}'} J_{\rm cl}(\vec{\rm R}-\vec{\rm R}')\,\vec{\rm M}(\vec{\rm R})\cdot\vec{\rm M}(\vec{\rm R}')\,, \tag{1}$$

where $\vec{\rm M}(\vec{\rm R})$ is a classical angular-momentum vector of length m at the lattice site $\vec{\rm R}$, $J_{\rm cl}(\vec{\rm R}-\vec{\rm R}')$ is the classical quantity corresponding to the quantum-mechanical exchange integral, and the sum runs over all pairs of lattice points. By definition, $J_{\rm cl}(\vec{0})$ equals zero. Furthermore, $J_{\rm cl}(\vec{\rm R})$ is taken to be nonzero only for nearest-neighboring lattice sites.

The classical angular-momentum vectors satisfy the relations

$$\vec{\rm M}(\vec{\rm R})\cdot\vec{\rm M}(\vec{\rm R}) = m^2 \tag{2}$$

and

$$[M^x(\vec{\rm R}), M^y(\vec{\rm R}')] = 0\,, \tag{3}$$

where the square bracket denotes a commutator.

The corresponding quantum-mechanical Heisenberg Hamiltonian is

$$H_{\mathrm{QM}} = -\frac{1}{2}\sum_{\vec{R}\vec{R}'} \hbar^2 J(\vec{R}-\vec{R}')\vec{S}(\vec{R})\cdot\vec{S}(\vec{R}') , \tag{4}$$

where $J(\vec{R})$ is the exchange integral, and the spin operator $\vec{S}(\vec{R})$ at lattice site $\vec{R}$ satisfies

$$\vec{S}(\vec{R})\cdot\vec{S}(\vec{R}) = S(S+1) , \tag{5}$$

and

$$[S^x(\vec{R}), S^y(\vec{R}')] = iS^z(\vec{R})\delta_{\vec{R},\vec{R}'} , \tag{6}$$

and cyclic permutations of Eq. (6).

The quantity $\hbar\vec{S}(\vec{R})$ is the quantum-mechanical angular momentum corresponding to $\vec{M}(\vec{R})$.[14] Note that in the quantum-mechanical case the thermodynamic functions and all the static correlation functions are completely determined at any temperature T by the three quantities S, $\hbar^2 J$, and $\beta = 1/k_B T$.

To see the connection to the classical Heisenberg model, we introduce

$$\vec{s}_{\mathrm{op}}(\vec{R}) = [S(S+1)]^{-1/2} m\vec{S}(\vec{R}) \tag{7}$$

into Eqs. (4)–(6), and get

$$H_{\mathrm{QM}} = -\frac{1}{2}\frac{S(S+1)}{m^2}\sum_{\vec{R}\vec{R}'} \hbar^2 J(\vec{R}-\vec{R}')\vec{s}_{\mathrm{op}}(\vec{R})\cdot\vec{s}_{\mathrm{op}}(\vec{R}') , \tag{8}$$

$$\vec{s}_{\mathrm{op}}(\vec{R})\cdot\vec{s}_{\mathrm{op}}(\vec{R}) = m^2 , \tag{9}$$

and

$$[s^x_{\mathrm{op}}(\vec{R}), s^y_{\mathrm{op}}(\vec{R}')] = im[S(S+1)]^{-1/2} s^z_{\mathrm{op}}(\vec{R})\delta_{\vec{R},\vec{R}'} . \tag{10}$$

Comparison of the last two equations with Eqs. (2)–(3) yields that when $S\to\infty$, the operator $\vec{s}_{\mathrm{op}}(\vec{R})$ tends to the classical angular momentum $\vec{M}(\vec{R})$. The Hamiltonians become identical if $S\to\infty$ and $\hbar\to 0$ such that

$$\hbar^2 S(S+1)J/m^2 \to J_{\mathrm{cl}} . \tag{11}$$

A complementary prescription for obtaining the classical limit appears, when also the basic dynamical equation is taken into account.

The Heisenberg equation of motion for the time-dependent spin operator $\vec{s}_{\mathrm{op}}(\vec{R}t)$ can by the use of Eq. (7) be written

$$\frac{\partial\vec{s}_{\mathrm{op}}(\vec{R}t)}{\partial t} = -\sum_{\vec{R}'} \hbar J(\vec{R}-\vec{R}')m^{-1}[S(S+1)]^{1/2} \times\vec{s}_{\mathrm{op}}(\vec{R}'t)\times\vec{s}_{\mathrm{op}}(\vec{R}t) , \tag{12}$$

and this should be compared with the classical equation of motion[23]

$$\frac{\partial\vec{M}(\vec{R}t)}{\partial t} = -\sum_{\vec{R}'} J_{\mathrm{cl}}(\vec{R}-\vec{R}')\vec{M}(\vec{R}'t)\times\vec{M}(\vec{R}t) . \tag{13}$$

The subsidiary condition for obtaining the classical limit reads

$$\hbar[S(S+1)]^{1/2} J m^{-1} \to J_{\mathrm{cl}} , \tag{14}$$

when $S\to\infty$, $\hbar\to 0$.

Combining Eqs. (11) and (14), we find that the prescription for taking the classical limit properly is

$$S\to\infty , \ \hbar\to 0 , \ J\to J_{\mathrm{cl}} ,$$

subject to the condition

$$\hbar[S(S+1)]^{1/2}\to m .$$

We note that this makes the right-hand side of Eq. (10) tend towards zero.

III. ILLUSTRATIVE EXAMPLES

A. Mixing of the quantum-mechanical and classical models

It may readily be demonstrated that an insertion of exact results for the classical Heisenberg model into exact equations for the quantum mechanical model can give unphysical results. We consider the quantity

$$C(\vec{q}t) = [NS(S+1)]^{-1}\langle\vec{S}_{\vec{q}}(t)\cdot\vec{S}_{-\vec{q}}(0)\rangle , \tag{15}$$

where $\vec{S}_{\vec{q}}(t)$ is the spatial Fourier transform of $\vec{S}(\vec{R}t)$, N is the number of lattice points, and the angular brackets denote thermal average. From Eqs. (4), (6), and (12) it is straightforward to derive

$$i\left.\frac{\partial C(\vec{q}t)}{\partial t}\right|_{t=0} = \frac{\hbar}{N}\sum_{\vec{q}'}^{\text{zone}} [J(\vec{q}') - J(\vec{q}-\vec{q}')]\, C(\vec{q}'0) \tag{16}$$

and

$$-\left.\frac{\partial^2 C(\vec{q}t)}{\partial t^2}\right|_{t=0} = \frac{\hbar^2}{N^2}\sum_{\vec{q}'\vec{q}''}^{\text{zone}} [J(\vec{q}') - J(\vec{q}-\vec{q}')][J(\vec{q}'') - J(\vec{q}+\vec{q}'')][NS(S+1)]^{-1}\left\langle S^x_{\vec{q}'} S^y_{\vec{q}-\vec{q}'} S^x_{\vec{q}''} S^y_{-\vec{q}-\vec{q}''} + \begin{pmatrix} x\to y \\ y\to z\end{pmatrix} + \begin{pmatrix} x\to z \\ y\to x\end{pmatrix}\right\rangle , \tag{17}$$

where $J(\vec{q})$ is the spatial Fourier transform of $J(\vec{R})$, and the sums run over the N points in the first Brillouin zone. The spin correlation functions in the right-hand sides of Eqs. (16) and (17) cannot be calculated exactly, except for the classical linear Heisenberg chain. For this we have, e.g.,

$$C_{\mathrm{cl}}(q0) \equiv (Nm^2)^{-1}\langle\vec{M}_{\vec{q}}(0)\cdot\vec{M}_{-\vec{q}}(0)\rangle$$

$$= (1 - u_{\text{cl}}^2)/(1 + u_{\text{cl}}^2 - 2u_{\text{cl}} \cos qa) \;, \tag{18}$$

where a is the lattice spacing, and

$$u_{\text{cl}} = \coth(\beta m^2 J_{\text{cl}}) - (\beta m^2 J_{\text{cl}})^{-1} \;. \tag{19}$$

We insert the classical results into Eqs. (16) and (17) with the transcription $m^2 J_{\text{cl}} \to \hbar^2 JS(S+1)$ [cf. Eq. (11)], and find the approximate relations

$$i \left.\frac{\partial C(qt)}{\partial t}\right|_{t=0} = 2\hbar Ju(1 - \cos qa) \tag{20}$$

and

$$-\left.\frac{\partial^2 C(qt)}{\partial t^2}\right|_{t=0} = 4Ju(1 - \cos qa)/\beta \;, \tag{21}$$

where

$$u = \coth[\beta\hbar^2 S(S+1)J] - [\beta\hbar^2 S(S+1)J]^{-1} \;. \tag{22}$$

We now consider the difference

$$\Delta^2 \equiv -\left.\frac{\partial^2 C(qt)}{\partial t^2}\right|_{t=0} \Big/ C(q0) - \left(i \left.\frac{\partial C(qt)}{\partial t}\right|_{t=0} \Big/ C(q0) \right)^2 \;, \tag{23}$$

which on using Eqs. (20)–(21) and the transcribed Eq. (18) becomes

$$\Delta^2 = 4Ju\beta^{-1}(1 - \cos qa)\,(1 + u^2 - 2u \cos qa)(1 - u^2)^{-1}[1 - \beta\hbar^2 Ju(1 - \cos qa)\,(1 + u^2 - 2u\cos qa)\,(1 - u^2)^{-1}] \;. \tag{24}$$

For a nonzero q the square bracket in Eq. (24) becomes negative, when T is less than a temperature of the order $\hbar^2 J[S(S+1)]^{1/2}/k_B$.

However, Δ^2 is nothing but the mean square deviation in the frequency with the temporal Fourier transform $C(q\omega)$ as the (unnormalized) distribution;

$$\Delta^2 = \frac{\int \omega^2 C(q\omega)\, d\omega}{\int C(q\omega)\, d\omega} - \left(\frac{\int \omega C(q\omega)\, d\omega}{\int C(q\omega)\, d\omega}\right)^2 \;. \tag{25}$$

As $C(q\omega)$ is non-negative, Δ^2 must be non-negative. The unphysical negative value obtained from Eq. (24) is due to the fact that we have used the classical forms for the static spin correlation functions in an otherwise quantum-mechanical calculation. This means that a mixing of quantum-mechanical and classical equations must be made with great care. We note that in the proper classical limit the unphysical behavior disappears, as is seen from

$$\Delta_{\text{cl}}^2 = 4J_{\text{cl}} u_{\text{cl}}(1 - \cos qa) \times (1 + u_{\text{cl}}^2 - 2u_{\text{cl}} \cos qa)/\beta(1 - u_{\text{cl}}^2) \;, \tag{26}$$

which is non-negative.

Some physical insight into the occurrence of the negative mean square deviation in frequency can be gained from a consideration of a linear harmonic lattice. For this system approximations similar to those used above yield the same unphysical result. For the linear harmonic lattice the defect is due to the neglect of the quantum-mechanical zero-point fluctuations in the use of classical results. The classical structure factor, which has a form similar to Eq. (18) but with a different definition of u_{cl}, tends to zero with T at a finite q. This is not the case for the quantum-mechanical structure factor due to zero-point fluctuations. A too small structure factor will enhance the magnitude of the second term in the mean square deviation in frequency relative to the first [cf. Eq. (25)]. Thus the mixing of quantum-mechanical and classical formulas leads to a negative mean square deviation in frequency at low enough temperature.

For the linear Heisenberg chain the situation must be similar. When we use the classical spin pair correlation function we neglect quantum-mechanical fluctuations and they are important. These fluctuations are of purely quantum-mechanical origin, and are not connected with the large thermal fluctuations, which exist in the classical model as well, and in both models are sufficiently large to prevent a magnetic transition at any finite temperature.

Mathematically the negativeness of Δ^2 is due to the fact that the approximative Eq. (21) is a fully classical result, whereas Eq. (20) is the quantum-mechanical result to order $\hbar$. The classical correlation function is even in t, and thus its first derivative vanishes at $t = 0$. This does not happen in Eq. (20) unless $\hbar$ is set to zero, i.e., the proper classical limit is taken.

B. Spin waves and the classical correlation function

In Ref. 10 it is stated that undamped spin-waves seem to be incompatible with the exact classical correlation function. It is reminded that for the antiferromagnetic chain at low temperatures

$$C_{\text{cl}}(q, 0) \propto (K^2 + q^{*2})^{-1} \;, \tag{27}$$

where

$$q^* = \pi/a - q$$

and

$$K = (1 - u_{\text{cl}})/a u_{\text{cl}}^{1/2} \;.$$

Thus for nonzero temperatures $C_{\mathrm{cl}}(\pi/a, 0)$ is finite.

On the other hand, assuming sharp spin waves, it is found in a quantum-mechanical calculation[10] that

$$[NS^2]^{-1}\langle S_q^+ S_{-q}^-\rangle = 2J\hbar^2 S^2(1-\cos qa)\coth(\tfrac{1}{2}\beta\hbar\omega_q)/\hbar\omega_q\ , \tag{28}$$

where

$$\hbar\omega_q = 2J\hbar^2 S \sin qa\ . \tag{29}$$

Equation (28) diverges, when $q \to \pi/a$ at any temperature. Thus an incompatibility exists, and in Ref. 10 a wave-vector dependent renormalization of the spin-wave energy is invoked as a rescue.

But, as is easily seen, the incompatibility stems from the use of sharp spin waves at $q = \pi/a$, which is in contrast to what is expected. If we keep q away from π/a, we can show that the exact classical correlation function and the classical limit of the the spin-wave correlation function agree at low temperatures. For $q < \pi/a$ we find from Eqs. (18) and (19) (with u_{cl} changed to $-u_{\mathrm{cl}}$ for the antiferromagnet)

$$C_{\mathrm{cl}} \to (\beta m^2 J_{\mathrm{cl}})^{-1}(1+\cos qa)^{-1}\ , \tag{30}$$

when $T \to 0$. From Eqs. (28) and (29) we find in the classical limit $\hbar \to 0$, $S \to \infty$, $J \to J_{\mathrm{cl}}$, $\hbar[S(S+1)]^{1/2} \to m$ that

$$[NS^2]^{-1}\langle S_q^+ S_{-q}^-\rangle \to (\beta m^2 J_{\mathrm{cl}})^{-1}(1+\cos qa)^{-1}\ . \tag{31}$$

The right-hand sides of Eqs. (30) and (31) are identical, and thus there is no incompatibility at all for those wave vectors, where sharp spin waves can be expected.

The result in Sec. II also explains the apparent contradiction in Ref. 11. There $\hbar = 1$ and it is stated that the approximation

$$\coth(\tfrac{1}{2}\beta\omega) \to 2/\beta\omega \tag{32}$$

is exact for a classical system. This means that all relevant frequencies satisfy

$$\tfrac{1}{2}\beta\omega \ll 1\ . \tag{33}$$

But it is also stated that a classical system exhibits spin-waves, and that their frequencies satisfy

$$\tfrac{1}{2}\beta\omega \gtrsim 1\ , \tag{34}$$

contradicting Eq. (33).

The contradiction disappears if $\hbar$ is inserted and the classical limit is taken properly. Eq. (32) is then changed to

$$\hbar\coth(\tfrac{1}{2}\beta\hbar\omega) \to 2/\beta\omega\ , \tag{35}$$

which obviously is exact, when $\hbar \to 0$. On the other hand we find for spin-wave frequencies, using Eq. (29) and the classical limit,

$$\tfrac{1}{2}\beta\omega \sim \beta\hbar JS \to \beta m J_{\mathrm{cl}} \gtrsim m^{-1}\ , \tag{36}$$

being true for temperatures $T \lesssim J_{\mathrm{cl}} m^2/k_B$. Note that the quantity $\frac{1}{2}\beta\omega$ has the dimension inverse angular momentum, which is made explicit in Eq. (36).

IV. COMMENTS ON SPIN-WAVES DAMPING IN CLASSICAL LINEAR CHAINS

In this section we shall comment upon some earlier results concerning spin-wave damping and the range of wave vectors, where spin waves exist. These results are based on exact frequency moments for the classical linear Heisenberg chains.[8-12]

A very simple-minded way to describe spin waves in the *ferromagnetic* case is to make an *ansatz* for the frequency distribution $C(q, \omega)$ containing two symmetrically placed Gaussian-shaped peaks. The two parameters in the *ansatz* are determined from two known frequency moments. If the second and fourth moments are used, the peak width, i.e., the spin-wave damping, comes out proportional to the square root of the temperature;

$$\Gamma(q, T) \propto T^{1/2}\ . \tag{37}$$

The spectral function found in this way contains no central peak, not even for small wave vectors, in contrast to what is expected. More elaborate theories take this into account, in that they predict a single diffusion peak at long wavelengths. For wave vectors larger than a certain critical value q_c one obtains two spin-waves peaks with a width proportional either to the temperature,[11,12]

$$\Gamma(q, T) \propto T\ , \tag{38}$$

or to the temperature raised to the three-halves power[9]:

$$\Gamma(q, T) \propto T^{3/2}\ . \tag{39}$$

The temperature dependence for q_c is either linear[11]

$$q_c \propto T \tag{40}$$

or of the form[9,12]

$$q_c \propto T^{1/2}\ . \tag{41}$$

The results in Eqs. (37)–(41) are confusingly different. The reason for the differences is of course that any procedure based only on static quantities to determine dynamical properties must include an *a priori* assumption concerning the shape of the spectral function. This assumption is often hidden in the mathematical approximations, which makes it difficult to judge the validity of the results. At present we do not know which of the results in Eqs. (37)–(41) are most correct.

The same comments can be made for the *antiferromagnetic* case. Here, too, one finds very different results for the width of the spin-wave peaks depending on the particular choice of procedure.

The above results show the necessity of having proper justifications for one's scheme of extracting dynamics from the low-order frequency moments. Evidently, more attention has to be paid to this point.

ACKNOWLEDGMENTS

I gratefully acknowledge valuable support and numerous suggestions from Professor A. Sjölander. I also thank Professor M. Blume for clarifying discussions, and Professor A. Sjölander, Professor K. S. Singwi, and Professor M. Blume for critically reading an earlier version of the manuscript.

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*Work supported by the Swedish Council for Atomic Research.

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[1] M. Steiner, Int. J. Magn. 5, 95 (1973).

[2] R. J. Birgeneau, R. Dingle, M. T. Hutchings, G. Shirane, and S. L. Holt, Phys. Rev. Lett. 26, 718 (1971).

[3] M. T. Hutchings, G. Shirane, R. J. Birgeneau, and S. L. Holt, Phys. Rev. B 5, 1999 (1972).

[4] S. A. Scales and H. A. Gersch, Phys. Rev. Lett. 28, 917 (1972).

[5] J. Kondo and K. Yamaji, Prog. Theor. Phys. 47, 807 (1972).

[6] E. Rhodes and S. A. Scales, Phys. Rev. B 8, 1994 (1973).

[7] K. Tomita and K. Kawasaki, Prog. Theor. Phys. 49, 1848 (1973).

[8] S. W. Lovesey and R. A. Meserve, Phys. Rev. Lett. 28, 614 (1972).

[9] S. W. Lovesey, J. Phys. C 7, 2008 (1974).

[10] P. M. Richards, Phys. Rev. Lett. 27, 1800 (1971).

[11] F. B. McLean and M. Blume, Phys. Rev. B 7, 1149 (1973).

[12] K. Tomita and H. Mashiyama, Prog. Theor. Phys. 48, 1133 (1972).

[13] M. E. Fisher, Am. J. Phys. 32, 343 (1964).

[14] P. W. Atkins and J. C. Dobson, Proc. R. Soc. Lond. A 321, 321 (1971).

[15] E. H. Lieb, Commun. Math. Phys. 31, 327 (1973).

[16] M. E. Harrigan and G. L. Jones, Phys. Rev. B 7, 4897 (1973).

[17] E. D. Siggia and M. Blume (private communication).

[18] P. D. Loly, Ann. Phys. (N.Y.) 56, 40 (1970).

[19] P. D. Loly and P. Mikusik, Phys. Rev. B 1, 3204 (1970).

[20] A. B. Harris, D. Kumar, B. I. Halperin, and P. C. Hohenberg, Phys. Rev. B 3, 961 (1971).

[21] Y. I. Chang, G. C. Summerfield, and D. M. Kaplan, Phys. Rev. B 3, 3052 (1971).

[22] Y. I. Chang and G. C. Summerfield, Phys. Rev. B 4, 4023 (1971).

[23] See, e.g., H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, Mass., 1959), Chap. 8.