Singularities and Catastrophes in the Dynamics of One-Dimensional Systems

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Dynamical correlation functions at low temperature for one-dimensional systems that involve the decay of a single elementary excitation into three others show logarithmic singularities at the frequency of the original excitation, as well as discontinuities that become sharper as the temperature is lowered. The discontinuities are the result of an elementary catastrophe that occurs as the phase space available for the decay varies with frequency. They should be observable, for instance, as dramatic changes in the out-of-plane spin-wave linewidth in $CsNiF_3$ as a function of temperature and wave vector.

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The appearance of $(\omega-\omega_0)^{-1/2}$ singularities in the frequency response of one-dimensional systems, that arise when one elementary excitation decays into two others, is a well-known phenomenon. It will be shown here that there are characteristic $|\ln(\omega-\omega_0)|$ divergences when an excitation decays into three others. Furthermore, there is a discontinuity in the low-temperature spectral density associated with these processes, as a region of phase space becomes inaccessible for decay. The contribution of this region is nearly constant until the frequency is reached at which it becomes inaccessible, even though its phase-space volume is approaching zero. This is an example of an elementary catastrophe,[1] in the mathematic sense. Three-excitation decay processes will occur generically, but to be easily observable the two-excitation process must be absent, as otherwise it may be expected to be dominant. One system for which these processes are distinguishable is the easy-plane ferromagnet. In this case, the linewidth for the out-of-plane fluctuation is entirely due to three-spin-wave decay. For concreteness, this system will be used for this discussion. One remarkable consequence of the existence of the catastrophe is that there would be a sudden, large drop in the linewidth as the temperature was raised, followed by a further increase.

The dynamical correlation function of any spin system can be represented, with standard techniques, in the form[2]

$$S(q,\omega)\equiv\int_0^\infty e^{i\omega t}\langle S_q^a(t)S_{-q}^a\rangle dt$$
$$=i\langle S_q^a S_{-q}^a\rangle\{\omega-\omega_q^{2,a}/[\omega+\gamma_q^a(\omega)]\}^{-1}, \quad (1)$$

where $\omega_q^{2,a}$ is the second moment. $\gamma_q^a(\omega)$ is the spin-current damping rate, and is the central object of the theory to be presented. For the Hamiltonian

$$H=-J\sum_i \mathbf{S}_i\cdot\mathbf{S}_{i+1}+D\sum_i(S_i^z)^2, \quad (2)$$

which is appropriate to $CsNiF_3$, the second moment is, for the classical system, at low temperature[3]

$$\omega_q^{2,z}=\omega_q^2(1-\kappa a/r)(1-\kappa a), \quad (3)$$

where $\omega_q=S[(J_0-J_q)(J_0-J_q+2D)]^{1/2}$, $J_q=2J\cos qa$, $r=[D/J(D/J+2)]^{1/2}$, and κ is the inverse coherence length $kT/2JS^2a$ for the spin component perpendicular to the hard z axis. a is the lattice parameter, henceforth set equal to 1.

The coherence length of the classical system diverges as $T\rightarrow 0$, leading to the existence of well-defined excitations, at the frequency ω_q, and the vanishing of $\gamma_q^a(\omega)$. As a consequence it is possible to obtain the leading terms in a temperature expansion of $\gamma_q^a(\omega)$ exactly from spin-wave theory. The quantum corrections in $CsNiF_3$, that result in a finite linewidth of the excitations at $T=0$, are small,[4] and do not invalidate the theory for the description of that material. Furthermore, the singularity and catastrophe are present for the quantum case as well, since they are produced by a density of states, and it does not matter whether the matrix elements are calculated classically or not.

For the in-plane function, $\gamma_q^\perp(\omega)$ is due to two spin-wave decay processes, and has been discussed elsewhere.[5] For the out-of-plane function it can be shown that[6]

$$\gamma_q^{z\,\prime\prime}(\omega)=\frac{\pi(kT)^2}{8S^2}\sum_{q_1q_2q_3}\{(\Gamma_{123}^+)^2[\delta(\omega-\omega_1+\omega_2+\omega_3)+\delta(\omega+\omega_1-\omega_2-\omega_3)]$$
$$+\tfrac{1}{3}(\Gamma_{123}^-)^2[\delta(\omega-\omega_1-\omega_2-\omega_3)+\delta(\omega+\omega_1+\omega_2+\omega_3)]\}$$
$$\times[(1-\cos q_1+\bar{D})(1-\cos q_2+\bar{D})(1-\cos q_3+\bar{D})]^{-1}\delta(q-q_1-q_2-q_3), \quad (4)$$

where $\bar{D}=D/J$.

The vertex functions $\Gamma^\pm$ are trigonometric functions of the arguments that can be obtained from the equations of motion and do not have any bearing on my conclusion. I will omit an explicit expression for them for brevity here.

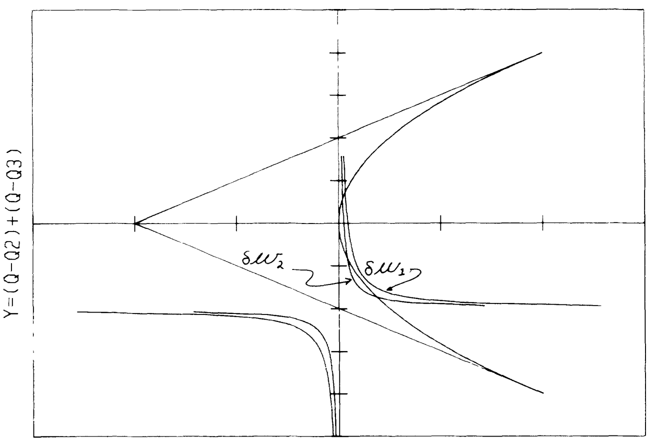

FIG. 1. The image of a small square domain about the point $q_1=q$, $q_2=q$, $q_3=q$ under the transformation given in the text. The hyperbolas are the locus of points for which the argument of the δ function vanishes, for different value of $\delta\omega$. The parabola $y^2=4x$ is a locus of singularities of the density of states. $\delta\omega_1 > \delta\omega_2$.

A general three-excitation decay process will contain the four-frequency δ functions shown. To evaluate the spin-wave damping at low temperature, one would naively expect to calculate $\gamma_q^z(\omega_q)$. However, the second δ function leads to an integral that is logarithmically divergent at ω_q, so that to calculate the damping, one must use the fact that the resonance is shifted because of the temperature dependence of $\omega_q^{2,z}$. One then obtains a finite damping. The existence of this divergence does not depend upon any particular detail of the dispersion relation, although at the q value where $\partial^2\omega_q/\partial q^2=0$, the divergence is even stronger.

The region of phase space leading to the divergence is the region near $q_1=-q$, $q_2=q_1$, $q_3=q$, and corresponds to a process in which the existing spin wave absorbs one of nearly opposite momentum and decays into two of nearly the same momentum. In this region, with $q_1=-q-\rho-\Delta$, $q_2=q+\rho$, $q_3=q+\Delta$, $\omega=\omega_q+\delta\omega$, we find that the argument of the δ function becomes

$$\delta\omega+\alpha\rho\Delta+\beta(\rho^2\Delta+\Delta^2\rho), \tag{5}$$

where $\alpha=\partial^2\omega/\partial q^2|_q$ and $\beta=\frac{1}{2}\,\partial^3\omega/\partial q^3|_q$. The divergence is due to the vanishing of the linear term in Δ and ρ, since $\partial\omega/\partial q|_{-q}=-\partial\omega/\partial q|_q$. As long as $\alpha\neq 0$, the singularity as $\delta\omega\to 0$ will be determined by the term $\alpha\rho\Delta$ in (5), and may easily be seen to be logarithmic. The higher-order term has an important effect at $\alpha=0$ and as one moves away from the singularity, for any q, and leads to a catastrophe occurring in the evaluation of the integral.

I consider a small region $|\Delta|\le q_0$, $|\rho|\le q_0$, $q_0\ll\pi$, about the point in phase space at which the singularity occurs. Let $\rho\Delta=x$, $\rho+\Delta=y$. Then this domain maps (twice) onto the region shown in Fig. 1, and the locus of points for which the δ function vanishes is given by the hyperbola in Fig. 1. The other terms in the integral in (4) can all be evaluated at $\Delta=\rho=0$, and so to a good first approximation, the frequency dependence of $\gamma_q^z(\omega)$ is determined by

$$\int\delta(\delta\omega+\alpha\rho\Delta+\beta(\rho\Delta^2+\rho^2\Delta)) =\int dx\,dy\frac{\delta(\delta\omega+\alpha x+\beta xy)}{(y^2-4x)^{1/2}}. \tag{6}$$

Doing the integral over y, we obtain for the integral in (6)

$$\sum_i\int_{x_a^i}^{x_b^i}\frac{dx}{[(\delta\omega+\alpha x)^2-4\beta^2x^3]^{1/2}}, \tag{7}$$

where x_a^i and x_b^i are the beginnings and ends of intervals corresponding to the intersection of the hyperbola $\delta\omega+\alpha x+\beta xy=0$ with the boundaries of the domain shown in Fig. 1. Those intersections corresponding to the parabola $y^2=4x$ [$\rho=\Delta$ in the original variables] are singularities in the integral in (7). As I have drawn it, there are three such points, corresponding to the three roots x_1,x_2,x_3 of the polynomial $(\delta\omega+\alpha x)^2-4\beta^2x^3$, but one can see that as $\delta\omega$ is increased, a value is reached at which two of the roots x_2 and x_3 coalesce to a single root, and then the entire branch no longer contributes to the integral. It is easy to see that the contribution of the branch is finite up to value of $\delta\omega$ at which it vanishes, since

$$\lim_{x_2\to x_3}\int_{x_2}^{x_3}\frac{dx}{[(x-x_1)(x-x_2)(x_3-x)]^{1/2}}\to\frac{1}{(x_2-x_1)^{1/2}}\int_{x_2}^{x_3}\frac{dx}{[(x-x_2)(x_3-x)]^{1/2}}=\frac{\pi}{(x_2-x_1)^{1/2}}. \tag{8}$$

There is, therefore, a discontinuity in $\gamma_q^z(\omega)$, as well as a singularity. The singular contribution to $\gamma_q(\omega)$ is shown in Fig. 2, as a function of $\delta\omega/\omega_q$, calculated numerically directly from Eq. (4), for a value of $\bar{D}=0.21$, appropriate to $CsNiF_3$. The discontinuity occurs at $-\delta\omega=\alpha^3/27\beta^2$ and is of magnitude $\pi\sqrt{3}/\alpha$. There is also a discontinuity at the value $q=0.5\pi$, since α is not quite zero there, but it is too close to $\delta\omega=0$ to appear in the graph. The position of the zero of α is insensitive to $\bar{D}$, for small values of $\bar{D}$.

It is clear from the above discussion that the phenomenon I am discussing is quite generally present in 1D systems. It should be observable in $CsNiF_3$.[7] In Fig. 3 the out-of-plane linewidth is given as a function of wave vector in $CsNiF_3$. This is calculated by the evaluation of $\gamma_q(\omega)$ at $\omega=(\omega_q^{2,z})^{1/2}$, the shifted spin-wave frequency, for several temperatures corresponding to the values of

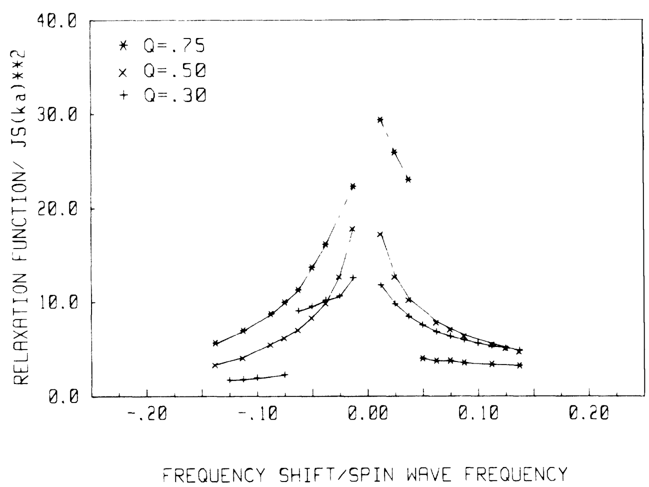

FIG. 2. The singular part of $\gamma_q^z(\omega)$ as a function of ω/ω_q, for several q values. The position of the discontinuity is determined by $\delta\omega = a^3/27b^2$.

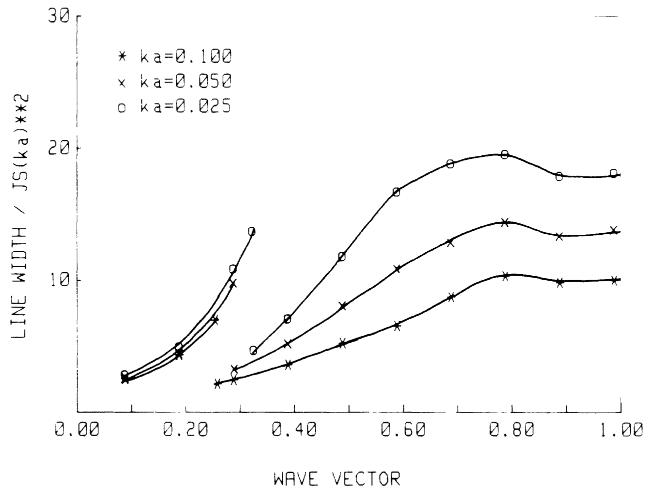

FIG. 3. The out-of-plane linewidth as a function of temperature ($\kappa a = kT/2JS^2$) and wave vector in a classical easy-plane ferromagnet with a value of $D/J = 0.21$, corresponding to $CsNiF_3$. The points are calculated from the theory. The solid line is a guide to the eye.

κa shown. The temperature dependence of the linewidth is then $T^2 \ln T$. For a given temperature, as q increases from zero, α decreases and eventually the criterion $|\delta\omega| \geq |\alpha^3/27\beta^2|$ is exceeded, leading to the drop in the linewidth. As the temperature is lowered, $\delta\omega$ becomes smaller, and q must be closer to the value of approximately 0.5π at which a vanishes. The discontinuity also becomes larger. At the value $\kappa a = 0.1$, which corresponds to about 8 K in $CsNiF_3$, the linewidth is 0.13 meV (full width at half maximum), before it drops at $q = 0.3\pi/a$, which is within the capability of existing spectrometers to resolve, although existing measurements have not done so.[7-9] By way of comparison, the full width for the in-plane fluctuations, at this wave vector, is accurately given by the isotropic value[5] $4(\kappa a)JS\sin q$, and is considerably larger, 0.61 meV. One would expect the linewidths for the in-plane and out-of-plane fluctuations to become comparable at the crossover temperature, which corresponds to $\kappa a = (2D)^{1/2}/J \simeq 0.65$, although the present results are restricted to temperatures considerably below that, and cannot simply be extrapolated. The observed discontinuity will be smoothed by finite-temperature corrections to (4), primarily by replacement of the δ function with a Lorentzian of width proportional to kT. This should lead to the drop occurring over a region of wave vector of width of order κ, which would still leave it easily observable. Given the small ratio of interchain exchange to intrachain exchange, $J'/J \simeq 10^{-2}$, the small dispersion in the spin-wave frequency with the out-of-chain wave vector will produce a negligible rounding compared with the finite-temperature correction, at temperatures at which the linewidth will be large enough to be measurable. I note that the quantum mechanical corrections to Eq. (4) do not affect the existence of, or the criterion for the location in phase space of, the catastrophe, although they can affect the magnitude of the observed discontinuity.

In conclusion, in one-dimensional systems that show well-defined excitations at low temperature, and for which a weak-coupling perturbation theory is valid, one can expect to find interesting anomalies in the physical response that correspond to the existence of a divergence and a catastrophe in the three excitation decay processes.

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