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Soliton dynamics in the uniaxially anisotropic quantum ferromagnetic chain

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Abstract. The energy–momentum dispersion relation for a pulse-type non-linear excitation of a uniaxially anisotropic quantum ferromagnetic chain is derived using the spin-coherent representation and a continuum description. A physical interpretation is given for the spectrum obtained.

1. Introduction

The subject of solitons in low-dimensional magnets has attracted considerable attention in recent years. Solitons have been experimentally observed at low temperatures as non-linear elementary excitations (Kjems and Steiner 1978, Kopinga *et al* 1984). The Heisenberg model—a *quantum lattice* Hamiltonian—is customarily used for the description of these systems. The model may be isotropic, or it may contain uniaxial/easy-plane/exchange anisotropy terms depending upon the magnetic system under consideration. A detailed study of spin dynamics in all these models is of considerable interest.

Solitons are entities that commonly arise as exact solutions of certain special non-linear partial differential equations describing classical dynamics in a continuum. It must be noted, however, that the underlying system giving rise to these excitations could be quantum-mechanical and discrete, as in the present problem. This transition from the *quantum lattice* description to a *classical continuous* one must be properly formulated (Makhankov *et al* 1987). Pioneering work on the continuum dynamics of the classical isotropic Heisenberg chain was carried out (Tjon and Wright 1977) essentially by the formal substitution of the spin operators in the Hamiltonian by classical vectors. (This is a good approximation for large spin values, $S \to \infty$.) Their analysis showed that the isotropic model supports pulse-type solitons. The energy–momentum dispersion relation was also determined. More recently it has been shown (Balakrishnan and Bishop 1985) that, starting with the quantum spin-operator evolution equation (valid for all spin values) for the isotropic model, and writing down the continuum version of the corresponding evolution equation for the diagonal matrix elements in the spin-coherent

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representation, the classical continuum equation given by Tjon and Wright (1977) is obtained. The coherent-state description represents a more rigorous derivation of the correspondence with the classical solutions since it takes into account the quantum character of the spin operators.

In this paper, we apply the spin-coherent-state formalism to the case of a quantum chain with uniaxial anisotropy. When the spins are considered to be classical vectors, the evolution equation can be solved exactly, irrespective of the magnitude of the anisotropy, to give pulse solitary-wave solutions for the spin evolution equation (Long and Bishop 1979). Subsequently the energy–momentum dispersion relation was derived for the single-ion anisotropy case (Sasada 1982) by adopting the variational method used (Tjon and Wright 1977) for the isotropic classical case. In our present formalism, we start with the evolution equation of the quantum spin-flip operator and use spin-coherent states to establish the correspondence with the classical solutions. We do not consider easy-plane and exchange anisotropies in this paper. It is known that for these cases, in contrast to the uniaxial case, one cannot find *exact* time-dependent solutions to the classical evolution equation, owing to the anisotropy. Such solutions can be found only within special approximations (Mikeska 1978, Kapor *et al* 1986), although exact *static* kinks exist for both types of anisotropy (Frahm and Hołyst 1989).

In contrast to the classical formalism in which the spins are treated as classical variables, the spin value S is expected to play a significant role in the quantum formalism. For instance, for $S=\frac{1}{2}$ a single-ion anisotropy term such as $A\,\Sigma_i(S_i^z)^2$ plays no role at all in the quantum formalism because of the operator identity $(S_i^z)^2=\frac{1}{4}$, whereas in a classical formalism it gives a non-vanishing contribution (Makhankov *et al* 1987, Sasada 1982). Furthermore, the spin value S appears as a mere scale factor in the expressions of the various physical quantities in the *classical* case, and does not affect the functional form of the dispersion relation. However, it is reasonable to expect that the dependence on S will be non-trivial when quantum effects are included. The conclusions based on the spin-coherent formalism (Balakrishnan and Bishop 1985) lend support to this. The aim of the generalised coherent-state formalism is *not* to derive conclusions regarding the underlying *discrete* quantum Heisenberg chain, based on continuum results, since distinct discrete models (integrable/non-integrable) could lead to the same continuum model (Papanicolaou 1987). Also 'topological' terms, which have been suggested as sources of distinctions between spectra for integral and half-odd-integral S (Haldane 1985) in *antiferromagnetic* chains, may be inadequately treated. Our motivation is to obtain information about the dynamics of the parameters describing the quantum state of the *continuum* system. Spin-coherent states provide an ideal framework for the study of solitons, which are in a sense coherent 'classical' entities, as discussed earlier in this section.

2. The anisotropic model and the evolution equations

Consider a one-dimensional magnetic system described by the Hamiltonian

$$H=-J\sum_i \boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1}-A\sum_i (S_i^z)^2-g\mu_{\mathrm{B}}B_3\sum_i S_i^z \tag{2.1}$$

characterised by an exchange energy $J>0$ and a single-ion, uniaxial anisotropy parameter $A>0$. Here B_3 is the external field along the $\hat{z}$ axis and $g\mu_{\mathrm{B}}$ is the magnetic moment.

The non-linear excitations of this system have been studied by considering the spins to be classical vectors and by using the continuum approximation, to obtain pulse-type solitary-wave solutions (Long and Bishop 1979). Treating the spins as quantum-mechanical operators, the evolution equation of the spin-raising operator S_j^+ at the site j is given by

$$i\hbar \frac{dS_j^+}{dt} = [S_j^+, H]$$

$$= -JS_j^z(S_{j-1}^+ + S_{j+1}^+) + J(S_{j-1}^z + S_{j+1}^z)S_j^+ + A(S_j^z S_j^+ + S_j^+ S_j^z) + g\mu_B B_3 S_j^+ \tag{2.2}$$

where $[S_i^\alpha, S_j^\beta] = i\varepsilon_{\alpha\beta\gamma} S_j^\gamma \delta_{ij}$ has been used.

The advantages of using a spin-coherent representation (Radcliffe 1971) to describe spin dynamics arising from non-linear evolution equations for spin operators has been discussed elsewhere in the context of the isotropic Heisenberg model (Balakrishnan and Bishop 1985). Here, we summarise some of the salient features of the representation.

The spin-coherent states $|\mu_j\rangle$ at a site j are defined as follows:

$$|\mu_j\rangle = (1 + |\mu_j|^2)^{-S} \exp(\mu_j S_j^-)|0\rangle_j \tag{2.3}$$

where μ_j is a complex quantity, $|0\rangle_j$ is the ground state with $S_j^z|0\rangle_j = S|0\rangle_j$ and S_j^- is the spin-lowering operator. The states (2.3) are normalised, non-orthogonal and over-complete. Parametrising μ_j in terms of angle variables θ_j and φ_j as

$$\mu_j = \tan(\theta_j/2) \exp(i\varphi_j) \tag{2.4}$$

equation (2.3) becomes

$$|\theta_j, \varphi_j\rangle = [\cos(\tfrac{1}{2}\theta_j)]^{2S} \exp[\tan(\tfrac{1}{2}\theta_j) \exp(i\varphi_j) S_j^-]|0\rangle_j. \tag{2.5}$$

The completeness relation is

$$\frac{(2S+1)}{\pi} \int \frac{d^2\mu_j}{(1 + |\mu_j|^2)^2} |\mu_j\rangle\langle\mu_j|$$

$$= \frac{(2S+1)}{4\pi} \int_0^{2\pi} d\varphi_j \int_0^{\pi} d\theta_j \sin\theta_j |\theta_j, \varphi_j\rangle\langle\theta_j, \varphi_j| = 1. \tag{2.6a}$$

The non-orthogonality relation is

$$\langle\mu_i|\mu_j\rangle = (1 + \mu_i^* \mu_j)^{2S}(1 + |\mu_i|^2)^S(1 + |\mu_j|^2)^S$$

$$= \{\cos(\tfrac{1}{2}\theta_i)\cos(\tfrac{1}{2}\theta_j) + \sin(\tfrac{1}{2}\theta_i)\sin(\tfrac{1}{2}\theta_j)\exp[i(\varphi_i - \varphi_j)]\}^{2S}. \tag{2.6b}$$

The expectation values of the single-site operators are calculated to be just the classical expressions:

$$\langle\theta_j, \varphi_j|S_j^+|\theta_j, \varphi_j\rangle = S \sin\theta_j \exp(i\varphi_j) \tag{2.7}$$

$$\langle\theta_j, \varphi_j|S_j^z|\theta_j, \varphi_j\rangle = S\cos\theta_j. \tag{2.8}$$

Thus θ_j and φ_j represent the polar and azimuthal angles of a classical vector $\mathbf{S}$.

However, the correspondence with the classical expressions does not hold in general for the expectation value of the product of spin operators at the same site. For instance, using equations (2.5) and (2.6) it may be shown that (Lieb 1973)

$$\langle\theta_j, \varphi_j|(S_j^z)^2|\theta_j, \varphi_j\rangle = S(S-\tfrac{1}{2})\cos^2\theta_j + \tfrac{1}{2}S. \tag{2.9}$$

Similarly,

$$\langle\theta_j, \varphi_j|S_j^z S_j^+ + S_j^+ S_j^z|\theta_j, \varphi_j\rangle = 2S(S-\tfrac{1}{2})\sin\theta_j\cos\theta_j\exp(\mathrm{i}\varphi_j). \tag{2.10}$$

On the other hand, if one treats the spins as classical vectors, the expressions corresponding to equations (2.9) and (2.10) are, respectively,

$$(S_j^z)^2 = S^2\cos^2\theta_j \tag{2.11}$$

and

$$S_j^z S_j^+ + S_j^+ S_j^z = 2S^2\sin\theta_j\cos\theta_j\exp(\mathrm{i}\varphi_j). \tag{2.12}$$

For a system of N spins, the spin-coherent states are the direct product states

$$|\Omega\rangle = \bigotimes_{n=1}^{N}|\theta_n, \varphi_n\rangle. \tag{2.13}$$

Taking the diagonal matrix elements of the operator evolution equation (2.2) using the direct-product representation given in equation (2.13), we obtain the following coupled non-linear differential difference equations for the c-numbers θ_j and φ_j:

$$\begin{aligned}\hbar\sin\theta_j\,\mathrm{d}\varphi_j/\mathrm{d}t = {}& JS\cos\theta_j[\sin\theta_{j+1}\cos(\varphi_{j+1}-\varphi_j)\\ &+\sin\theta_{j-1}\cos(\varphi_{j-1}-\varphi_j)] - JS\sin\theta_j(\cos\theta_{j+1}+\cos\theta_{j-1})\\ &- g\mu_B B_3\sin\theta_j - A\eta(S)\sin\theta_j\cos\theta_j\end{aligned} \tag{2.14}$$

and

$$\hbar\,\mathrm{d}\theta_j/\mathrm{d}t = JS\sin\theta_{j+1}\sin(\varphi_j-\varphi_{j+1}) + JS\sin\theta_{j-1}\sin(\varphi_j-\varphi_{j-1}). \tag{2.15}$$

In deriving equations (2.14) and (2.15) we have made use of equations (2.7), (2.8) and (2.10), and the property that the states at a site are normalised to unity. In equation (2.14),

$$\eta(S) = (2S-1). \tag{2.16}$$

Thus for the case $S=\frac{1}{2}$, the anisotropy term involving A vanishes identically in the evolution equations (Makhanov *et al* 1987).

This is to be expected in any quantum formalism since the anisotropy term $A\,\Sigma_i(S_i^z)^2$ in the Hamiltonian (2.1) contributes just a constant for the case $S=\frac{1}{2}$, owing to the operator identity $(S_i^z)^2=\frac{1}{4}$. Equations derived (for the easy-plane case) by taking the spins to be classical variables (Wysin *et al* 1984) have the same form as equations (2.14) and (2.15) except that $\eta(S)$ is replaced by $2S$, $A\to -A$ and $\theta\to(\pi/2-\theta)$. Hence, classically for all S (including $S=\frac{1}{2}$) the anisotropy term makes a finite contribution. For $S\gg 1$, the quantum equation reduces to the classical one, a desirable feature.

In the continuum approximation, equations (2.14) and (2.15) reduce to

$$h\sin\theta\left(\frac{\partial\varphi}{\partial t}\right) = JSa^2\frac{\partial^2\theta}{\partial x^2} - JS^2\sin\theta\cos\theta\left(\frac{\partial\varphi}{\partial x}\right)^2 - A\eta(S)\sin\theta\cos\theta - g\mu_B B_3\sin\theta \tag{2.17}$$

and

$$\hbar\frac{\partial\theta}{\partial t}=-JSa^2\sin\theta\frac{\partial^2\varphi}{\partial x^2}-2JSa^2\cos\theta\left(\frac{\partial\theta}{\partial x}\right)\left(\frac{\partial\varphi}{\partial x}\right). \tag{2.18}$$

Defining $\cos\theta = p$ and writing $\varphi = q$, equations (2.17) and (2.18) become

$$\hbar\frac{\partial q}{\partial t}=-JSa^2\left[p(1-p^2)^{-2}\left(\frac{\partial p}{\partial x}\right)^2+(1-p^2)^{-1}\frac{\partial^2 p}{\partial x^2}+p\left(\frac{\partial q}{\partial x}\right)^2\right]-A\eta(S)p-g\mu_B B_3 \tag{2.19}$$

and

$$\hbar\frac{\partial p}{\partial t}=JSa^2\left[(1-p^2)\frac{\partial^2 q}{\partial x^2}-2p\left(\frac{\partial p}{\partial x}\right)\left(\frac{\partial q}{\partial x}\right)\right]. \tag{2.20}$$

We seek solitary-wave solutions of equations (2.19) and (2.20) of the form

$$q = q(u) + \Omega_1 t \qquad p = p(u) \tag{2.21}$$

where

$$u = (x - vt)/a. \tag{2.22}$$

Then equations (2.19) and (2.20) reduce to

$$V\frac{dq}{du} = p(1-p^2)^{-2}\left(\frac{dp}{du}\right)^2 + (1-p^2)^{-1}\frac{d^2p}{du^2} + p\left(\frac{dq}{du}\right)^2 + \tau_Q p + (\Omega_3 + \omega) \tag{2.23}$$

and

$$V\frac{dp}{du} = -(1-p^2)\frac{d^2q}{du^2} + 2p\left(\frac{dp}{du}\right)\left(\frac{dq}{du}\right) = -\frac{d}{du}\left((1-p^2)\frac{dq}{du}\right) \tag{2.24}$$

where

$$V = v/JSa\hbar^{-1} \qquad \tau_Q = A\eta(S)/JS$$
$$\Omega_3 = g\mu_B B_3/JS \qquad \omega = \hbar\Omega_1/JS. \tag{2.25}$$

Equation (2.24) is integrated to give

$$(dq/du) = V(p_0 - p)(1-p^2)^{-1} \tag{2.26}$$

where p_0 is an integration constant. Substituting equation (2.26) in equation (2.23) and using the identity

$$2\left[p(1-p^2)^{-2}\left(\frac{dp}{du}\right)^2 + (1-p^2)^{-1}\frac{d^2p}{du^2}\right]\frac{dp}{du} = -\frac{d}{du}\left[(p^2-1)^{-1}\left(\frac{dp}{du}\right)^2\right] \tag{2.27}$$

in the resulting equation yields after some algebra

$$(dp/du)^2 = F(p) \tag{2.28}$$

where

$$F(p) = 2\Omega p(p^2-1) + \tau_Q p^2(p^2-1) - V^2(1 + p_0^2 - 2pp_0) - p_1(p^2-1). \tag{2.29}$$

In equation (2.29), $\Omega = \Omega_3 + \omega$ and p_1 is an integration constant. Setting $p = (1 - 2s)$ so that $s = \sin^2(\theta/2)$, we get

$$(u - u_0) = -2\int ds/[F(s)]^{1/2} \tag{2.30}$$

where

$$F(s) = -V^2(1 - p_0^2)^2 + 4s(p_1 - 2\Omega - \tau_Q - p_0V^2) + 4s^2(6\Omega + 5\tau_Q - p_1) - 16s^3(\Omega + 2\tau_Q) + 16s^4\tau_Q. \tag{2.31}$$

Pulse-type solutions of equation (2.30) may be determined by choosing integration constants p_0 and p_1 such that the constant and linear terms in $F(s)$ vanish: $p_0 = 1$ and $p_1 = V^2 + \tau_Q + 2\Omega$. Then equation (2.30) yields

$$s = \sin^2(\theta/2) = 2K_Q^2/[(\Omega + 2\tau_Q) + (\Omega^2 + \tau_QV^2)^{1/2}\cosh(2K_Q\zeta)] \tag{2.32}$$

where

$$\zeta = (u - u_0) \qquad \text{and} \qquad K_Q^2 = (\Omega + \tau_Q - \tfrac{1}{4}V^2) \geqslant 0. \tag{2.33}$$

From equation (2.26),

$$(d\varphi/du) = V/2\cos^2(\theta/2). \tag{2.34}$$

Substituting equation (2.32) in (2.34) and integrating leads to

$$\varphi = \varphi_0 + \frac{V}{2}\zeta + \Omega_1 t + \tan^{-1}\left[\left(\frac{(\Omega^2 + \tau_QV^2)^{1/2} + (\Omega - \frac{1}{2}V^2)}{(\Omega^2 + \tau_QV^2)^{1/2} - (\Omega - \frac{1}{2}V^2)}\right)^{1/2}\tanh(K_Q\zeta)\right]. \tag{2.35}$$

The classical solutions are identical to those given in equations (2.32) and (2.35) except that τ_Q is replaced by $\tau_{cl} = 2A/J$, the corresponding classical expression for a given S (See equations (2.25) and (2.16)).

In what follows explicit calculations for the conserved quantities, namely the energy E, the linear momentum P and the angular momentum M, will be given for the case $S = 1$. This provides an illustrative example, since as demonstrated for the isotropic model (Balakrishnan and Bishop 1985) the behaviour of the dispersion relation for other S values will be qualitatively similar. For the anisotropic case, however, $S = \frac{1}{2}$ is a notable exception, as discussed in the previous section.

The exact classical dispersion relation can be derived analytically. By comparing it with the dispersion relation derived using the spin-coherent representation, we will show that quantum effects play an important role in the dynamics of those solitons with *small widths*. This is as expected, since the uncertainty in the momentum would be large for a 'thin' soliton, and its momentum consequently would differ appreciably from the corresponding classical value. Our results will show a departure from the classical dispersion relation for the small-width solitons. In contrast, for solitons with large widths, the quantum effects are physically expected to be negligible and our formalism confirms that the dispersion relation is practically identical to the classical one.

3. Classical soliton dispersion relation

When the spins are treated as classical variables, the derivation of the soliton dispersion relation proceeds as follows. In the continuum approximation, the Hamiltonian (2.1) yields the following expression for the total energy (on subtracting the ground-state energy):

$$E_{cl} = JS^2 \int_{-\infty}^{+\infty} [\tfrac{1}{2}(d\theta/du)^2 + \tfrac{1}{2}\sin^2\theta(d\varphi/du)^2 + 2(\Omega_3 + \tau_{cl})\sin^2(\theta/2) - 2\tau_{cl}\sin^4(\theta/2)]\, du \tag{3.1}$$

where

$$\tau_{cl} = 2A/J.$$

We have

$$(d\theta/du)^2 = \operatorname{cosec}^2\theta(dp/du)^2.$$

Using equations (2.26) and (2.28) in equation (3.1) gives

$$E_{cl}=2JS^2\int_{-\infty}^{+\infty} du[(2\Omega_3+\omega+2\tau_{cl})\sin^2(\theta/2)-4\tau_{cl}\sin^4(\theta/2)]. \tag{3.2}$$

The total angular momentum is given by

$$M_{cl}=S\int_{-\infty}^{+\infty} du(1-\cos\theta). \tag{3.3}$$

Finally, the total momentum is given by (Tjon and Wright 1977, Long and Bishop 1979)

$$P_{cl} = \int_{-\infty}^{+\infty} du \left(S_x \frac{dS_y}{du} - S_y \frac{dS_x}{du}\right) \Big/ (S + S_z). \tag{3.4}$$

Equivalently,

$$P_{cl} = S\int_{-\infty}^{+\infty} (1-\cos\theta)\left(\frac{d\varphi}{du}\right) du = SV\int_{-\infty}^{+\infty} \tan^2\left(\frac{\theta}{2}\right) du \tag{3.5}$$

where equation (2.34) has been used.

For pulse solitary-wave solutions in the classical case, the expression for $\sin^2(\theta/2)$ is as in equation (2.32) with τ_Q replaced by τ_{cl}. Thus we calculate (Gradshteyn and Ryzhik 1980)

$$\int_{-\infty}^{+\infty} \sin^2(\theta/2)\, du = (2/\tau_{cl}^{1/2})\tanh^{-1}\chi_{cl} \tag{3.6}$$

$$\int_{-\infty}^{+\infty} \sin^4(\theta/2)\, du = [(\Omega + 2\tau_{cl})/\tau_{cl}^{3/2}]\tanh^{-1}\chi_{cl} - K_{cl}/\tau_{cl} \tag{3.7}$$

to find E_{cl} and M_{cl}. Here,

$$\chi_{cl} = \left(\frac{(\Omega + 2\tau_{cl}) - (\Omega^2 + \tau_{cl}V^2)^{1/2}}{(\Omega + 2\tau_{cl}) + (\Omega^2 + \tau_{cl}V^2)^{1/2}}\right)^{1/2} \tag{3.8}$$

and

$$K_{cl}^2 = \Omega + \tau_{cl} - \tfrac{1}{4}V^2 \geq 0. \tag{3.9}$$

Finally

$$\int_{-\infty}^{+\infty} \tan^2(\theta/2)\, \mathrm{d}u = (4/V) \sin^{-1} \eta_{\mathrm{cl}} \tag{3.10}$$

where

$$\eta_{\mathrm{cl}} = \{[(\Omega^2 + \tau_{\mathrm{cl}} V^2)^{1/2} + (\Omega - \tfrac{1}{2}V^2)]/2(\Omega^2 + \tau_{\mathrm{cl}} V^2)^{1/2}\}^{1/2}. \tag{3.11}$$

In evaluating equations (3.6), (3.7) and (3.10), the condition

$$V^2 \leqslant 4(\Omega + \tau_{\mathrm{cl}}) \tag{3.12}$$

has been used. Using these results, equations (3.2), (3.3) and (3.5) become, respectively,

$$E_{\mathrm{cl}} = 4JS^2[(\Omega_3/\tau_{\mathrm{cl}}^{1/2}) \tanh^{-1} \chi_{\mathrm{cl}} + K_{\mathrm{cl}}] \tag{3.13}$$

$$M_{\mathrm{cl}} = (4S/\tau_{\mathrm{cl}}^{1/2}) \tanh^{-1} \chi_{\mathrm{cl}} \tag{3.14}$$

and

$$P_{\mathrm{cl}} = 4S \sin^{-1} \eta_{\mathrm{cl}} \tag{3.15}$$

giving

$$P_{\mathrm{cl}} = 2S \cos^{-1}[(\tfrac{1}{2}V^2 - \Omega)/(\Omega^2 + \tau_{\mathrm{cl}} V^2)^{1/2}]. \tag{3.16}$$

Using equation (3.14) in (3.13) we get

$$E_{\mathrm{cl}} = J[M_{\mathrm{cl}} S\Omega_3 + 4S^2(\Omega + \tau_{\mathrm{cl}} - \tfrac{1}{4}V^2)^{1/2}]. \tag{3.17}$$

Defining

$$\beta = (\Omega^2 + \tau_{\mathrm{cl}} V^2)^{1/2}/(\Omega + 2\tau_{\mathrm{cl}}) \tag{3.18}$$

we have from equations (3.8) and (3.14).

$$\tanh^2(M_{\mathrm{cl}} \tau_{\mathrm{cl}}^{1/2}/4S) = (1 - \beta)/(1 + \beta). \tag{3.19}$$

Thus

$$\sinh(M_{\mathrm{cl}} \tau_{\mathrm{cl}}^{1/2}/2S) = (1 - \beta^2)^{1/2}/\beta. \tag{3.20}$$

Using equations (3.16) and (3.20) we have

$$\cos(P_{\mathrm{cl}}/2S)/\sinh(M\tau_{\mathrm{cl}}^{1/2}/2S) = (\tfrac{1}{2}V^2 - \Omega)/(\Omega + 2\tau_{\mathrm{cl}})(1 - \beta^2)^{1/2}. \tag{3.21}$$

Equations (3.20) and (3.21) combine to give

$$[\cosh(M\tau_{\mathrm{cl}}^{1/2}/2S) - \cos(P_{\mathrm{cl}}/2S)]/\sinh(M\tau_{\mathrm{cl}}^{1/2}/2S) = (\Omega + \tau_{\mathrm{cl}} - \tfrac{1}{4}V^2)^{1/2}/\tau_{\mathrm{cl}}^{1/2}. \tag{3.22}$$

Substituting equation (3.22) in equation (3.17) yields the classical dispersion relation

$$E_{\mathrm{cl}} = JM_{\mathrm{cl}} S\Omega_3 + 4JS^2[\tau_{\mathrm{cl}}^{1/2}/\sinh(M_{\mathrm{cl}}\tau_{\mathrm{cl}}^{1/2}/2S)] \times [\cosh(M_{\mathrm{cl}}\tau_{\mathrm{cl}}^{1/2}/2S) - \cos(P_{\mathrm{cl}}/2S)] \tag{3.23}$$

where $0 \leqslant P_{\mathrm{cl}} \leqslant 2\pi S$.

This classical spectrum agrees with that obtained using a variational method (Sasada 1982). It is similar in form to the *exact* excitation spectrum of the spin-$\frac{1}{2}$ quantum discrete (Heisenberg–Ising) exchange anisotropic model (Johnson and McCoy 1972) derived using the Bethe *ansatz* method. The $M = 1$ soliton spectrum coincides with the magnon spectrum and $M = 2, 3, \ldots$ semiclassical solitons (in the continuum model) may be identified with multi-magnon bound states. Such a correspondence also exists for the isotropic model (Jevicki and Papanicolaou 1979).

Our formalism will show that the effect of quantum fluctuations is to destroy this correspondence in the case of narrow-width solitons with energy higher than a certain critical energy. However, it is still possible to identify low-energy solitons with magnon bound states.

4. Soliton dispersion relation using spin-coherent representation

First we calculate the expressions E_Q, M_Q and P_Q for the total energy, angular momentum and momentum, respectively, by defining them as usual to be diagonal matrix elements in the spin-coherent basis. E_Q is calculated from the Hamiltonian (2.1) and $M_Q = \langle \Sigma_i (S - S_i^z) \rangle$. Note that both these are expressed as *discrete sums* over lattice sites. Using equation (2.13) and the continuum approximation yields expressions for E_Q and M_Q that are identical to the classical expressions (3.2) and (3.3), leading respectively to (3.13) and (3.14), with τ_{cl} ($=2A/J$) replaced by $\tau_Q = \tau_{cl}(S - \frac{1}{2})/S$. This is because, except for the anisotropy term in the Hamiltonian, all other terms occur as single spin operators at a site, so that the classical values are obtained (see equations (2.7) and (2.8)). Thus we have (for $S \neq \frac{1}{2}$)

$$E_Q = 4JS^2[(\Omega_3 M_Q/4S) + K_Q] \tag{4.1}$$

$$M_Q = (4S/\tau_Q^{1/2}) \tanh^{-1} \chi_Q \tag{4.2}$$

where χ_Q is defined as in equation (3.8) (with τ_{cl} replaced by τ_Q) and K_Q is given in equation (2.33). (It must be mentioned that in the figure captions, the symbol τ has been used to denote τ_{cl} for the classical spectrum and τ_Q for the quantum spectrum.)

Determining P_Q, however, is not so straightforward, as has already been emphasised in the context of the isotropic model (Balakrishnan and Bishop 1985). In contrast to E and M it is not obvious how to construct a total momentum operator as a *discrete sum* over sites of products of spin operators defined at each site, so as to use equation (2.13) to find its diagonal matrix elements. We shall return to this problem subsequently. Note that the translation operator $\hat{T}$ can be defined as

$$\hat{T} = \exp(-\mathrm{i}\hat{P}a/\hbar) \tag{4.3}$$

so that

$$P_Q = \langle \hat{P} \rangle = (\mathrm{i}\hbar/a)\langle \log \hat{T} \rangle. \tag{4.4}$$

However, finding $\langle \log \hat{T} \rangle$ is not an easy task, although it is possible to construct $\hat{T}$ in terms of the trace of the product of $(2S + 1)$-dimensional matrices. It is straightforward to calculate $\langle \hat{T} \rangle$ in the coherent-state basis (Haldane 1986):

$$\langle \hat{T} \rangle = \prod_n \langle \theta_n, \varphi_n | \hat{T} | \theta_n, \varphi_n \rangle = \prod_n \langle \theta_n, \varphi_n | \theta_{n-1}, \varphi_{n-1} \rangle. \tag{4.5}$$

Using equation (2.6*b*), one obtains

$$\langle \hat{T} \rangle = \prod_n (\alpha_n^* \alpha_{n-1} + \beta_n^* \beta_{n-1})^{2S} = \exp\left(2S \sum_n \log(\alpha_n^* \alpha_{n-1} + \beta_n^* \beta_{n-1})\right) \tag{4.6}$$

where $\alpha_n = \cos(\frac{1}{2}\theta_n)$ and $\beta_n = \sin(\frac{1}{2}\theta_n) \exp(\mathrm{i}\varphi_n)$. Using the continuum approximation, which assumes $\Gamma \gg a$ ($\Gamma = 2aK_Q^{-1}$ being the width of the soliton; see § 5), we have

$$\alpha_{n-1} \to \alpha(x) - a(\partial\alpha/\partial x) + O(a^2). \tag{4.7}$$

After some algebra equation (4.6) reduces to

$$\langle \hat{T} \rangle = \exp\left[\mathrm{i}S \int \mathrm{d}u(\cos\theta - 1)\left(\frac{\partial\varphi}{\partial u}\right)\right]. \tag{4.8}$$

From the solutions (2.32)–(2.35) and expression (3.5) for P_{cl}, it is clear that

$$\langle \hat{T} \rangle = \exp(-\mathrm{i}\tilde{P}a/\hbar) = T_{\mathrm{S}} \tag{4.9}$$

where $\tilde{P}$ is given by an expression identical to the classical expression (3.16), with τ_{cl} replaced by τ_{Q}. From equation (4.9)

$$\tilde{P} = (\mathrm{i}\hbar/a)\log\langle \hat{T} \rangle. \tag{4.10}$$

It has been proved (Haldane 1986) that $\log\langle \hat{T} \rangle = \langle \log \hat{T} \rangle$ in the continuum model, so that comparing equations (4.4) and (4.10) it is concluded that $P_{\mathrm{Q}} = \tilde{P}$. This in turn implies that quantum corrections to the classical dispersion relation are absent in a continuum model in the spin-coherent basis. However, as has been discussed in detail elsewhere (Balakrishnan and Bishop 1989), this proof is valid only for limitingly low-energy solitons with width $\Gamma \rightarrow \infty$. As is well known, the minimum width of a soliton is finite and fixed by the parameters of the given magnetic system. For the continuum approximation to be justified, we must only ensure that $\Gamma_{\min} \gtrsim a$, the lattice constant a remaining finite. It is then shown that $P_{\mathrm{Q}} \neq \tilde{P}$ for solitons with width less than a certain critical width. The difficulties encountered in calculating P_{Q} from $\langle \log \hat{T} \rangle$ have also been discussed.

In view of this, the *ansatz* proposed for $\hat{P}$ (Balakrishnan and Bishop 1985) provides a useful alternative. It is obtained by first discretising the classical continuum expression in equation (3.4), then using the corresponding principle to replace the spin vectors by the corresponding operators at various sites, and finally symmetrising the resulting expression to make it Hermitian. Although the expectation value of this *ansatz* in the continuum approximation may not exactly coincide with that obtained from an exact calculation of equation (4.4) (if feasible), we do expect that it will manifest the qualitative features of the soliton dispersion relation that arise essentially due to quantum effects. The expression used is

$$\hat{P} = (\hbar/2a)\sum_{n} \{(S_n^x S_{n+1}^y - S_{n+1}^x S_n^y)[S^{1/2}(S+1)^{1/2} + S_n^z]^{-1} + \mathrm{HC}\} \tag{4.11}$$

where HC stands for Hermitian conjugate. Calculating diagonal elements of $\hat{P}$ in the spin-coherent basis and passing to the continuum description gives, for $S = 1$.

$$P_{\mathrm{Q}}(S=1) = \langle \hat{P} \rangle = (\hbar/2\sqrt{2}\,a)\int_{-\infty}^{+\infty} (3 - \sqrt{2}\cos\theta)\sin^2\theta\left(\frac{\mathrm{d}\varphi}{\mathrm{d}u}\right)\mathrm{d}u. \tag{4.12}$$

Using equation (2.26) in equation (4.12) leads to

$$P_{\mathrm{Q}}(S=1) = \frac{\hbar V}{\sqrt{2}\,a}\left((3-\sqrt{2})\int_{-\infty}^{+\infty}\sin^2(\theta/2)\,\mathrm{d}u + 2\sqrt{2}\int_{-\infty}^{+\infty}\sin^4(\theta/2)\,\mathrm{d}u\right). \tag{4.13}$$

Finally, substituting equations (3.6) and (3.7) in equation (4.13) yields (for $B_3 = 0$)

$$P_{\mathrm{Q}}(S=1) = (\hbar V/a)\{\tfrac{1}{4}M_{\mathrm{Q}}[3\sqrt{2} + 2(\omega/\tau_{\mathrm{Q}}) + 2] - 2\tau_{\mathrm{Q}}^{-1}(\omega + \tau_{\mathrm{Q}} - \tfrac{1}{4}V^2)^{1/2}\}. \tag{4.14}$$

Combining equations (4.1) and (4.2) we get (for $B_3 = 0$)

$$E_{\mathrm{Q}} = 4J(\omega + \tau_{\mathrm{Q}} - \tfrac{1}{4}V^2)^{1/2}. \tag{4.15}$$

Equations (4.14) and (4.15) will be used to plot E_{Q} versus P_{Q} for a fixed value of the total angular momentum M_{Q}.

Define

$$C = (\omega^2 + \tau_Q V^2)^{1/2}/(\omega + 2\tau_Q). \tag{4.16}$$

From equations (4.2) and (3.8),

$$M_Q = 4S\tau_Q^{-1/2} \tanh^{-1} [(1 - C)/(1 + C)]^{1/2}. \tag{4.17}$$

Hence fixing M_Q implies fixing the parameter C, so that equation (4.16) leads to

$$V^2 = \tau_Q^{-1}[2C\tau_Q - (1 - C)\omega][2C\tau_Q + (1 + C)\omega]. \tag{4.18}$$

Since $\tau_Q > 0$, the condition $V^2 \geqslant 0$ shows that the internal frequency of the soliton satisfies the inequality

$$\omega_{\min} \leqslant \omega \leqslant \omega_{\max} \tag{4.19}$$

where

$$\omega_{\min} = -2C\tau_Q/(1 + C) = -\tau_Q[1 - \tanh^2(M_Q\tau_Q^{1/2}/4)] \tag{4.20a}$$

and

$$\omega_{\max} = 2C\tau_Q/(1 - C) = \tau_Q/\sinh^2(M_Q\tau_Q^{1/2}/4). \tag{4.20b}$$

From equation (4.17), we have $0 \leqslant C \leqslant 1$, since M_Q is real. The constraint $V^2 < 4(\omega + \tau_Q)$ (see equation (2.33) with $\Omega = \omega$) is automatically satisfied for $C < 1$.

For $\tau_Q \rightarrow 0$, equations (4.20) lead to $\omega_{\min} \rightarrow 0$ and $\omega_{\max} \rightarrow (16/M^2)$, as required for the isotropic case. Also, $V = 0$ when $\omega = \omega_{\min}$ and $\omega = \omega_{\max}$ for all τ_Q. From equation (4.18), setting $(\mathrm{d}V/\mathrm{d}\omega) = 0$, we see that the maximum velocity V_S and the corresponding frequency ω_S are given as

$$V_S = 2C\tau_Q^{1/2}(1 - C^2)^{-1/2} = 2\tau_Q^{1/2}/\sinh(M_Q\tau_Q^{1/2}/2S) \tag{4.21}$$

$$\omega_S = 2C^2\tau_Q/(1 - C^2) = 2\tau_Q/\sinh^2(M_Q\tau_Q^{1/2}/2S) \tag{4.22}$$

yielding the soliton energy

$$E_S = 4JS^2\tau_Q^{1/2}(1 - C)^{-1/2} = 4JS^2\tau_Q^{1/2} \tanh(M_Q\tau_Q^{1/2}/2S). \tag{4.23}$$

5. Results and discussion

For a fixed value of C (i.e. fixed M_Q—see equation (4.17)), values of ω lying in the range given in equation (4.19) are considered and the corresponding values of V^2 are determined from equation (4.18). Equation (4.14) determines P_Q. The dependences of P_Q on ω and V are given in figures 1 and 2, respectively. Figure 3 gives the plot of E_Q versus P_Q (for fixed M_Q) in the absence of an external field. The corresponding classical plot of E_{cl} versus P_{cl} is also given in the same figure for comparison. The energy gap in both spectra (for $P \rightarrow 0$) appears due to the coupling of M to an effective magnetic field arising from the anisotropy term A, and vanishes for $\tau \rightarrow 0$ (the classical plot is given for illustration in figure 3). The corresponding quantum plot studied earlier (Balakrishnan and Bishop 1985) has not been included in the figure.

Writing the soliton solution in equation (2.32) as

$$\sin^2(\theta/2) = 2K_Q^2/\{[(\Omega + 2\tau_Q) - (\Omega^2 + \tau_Q V^2)^{1/2}] + 2(\Omega^2 + \tau_Q V^2)^{1/2} \cosh^2 K_Q\zeta\} \tag{5.1}$$

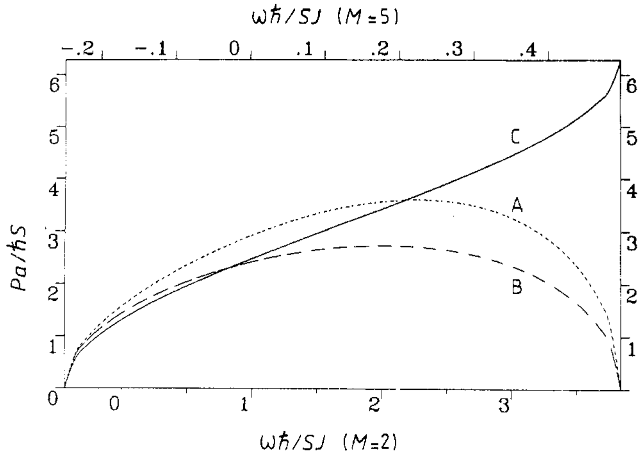

Figure 1. The quantum momentum (units of $\hbar a^{-1}$) versus soliton internal frequency ω (units of $J\hbar^{-1}$) for $S = 1$, $\tau = 0.5$, $M/S\hbar = 2$ and 5 respectively. A schematic classical plot ($S = \infty$) is also shown. Curves: A, $S = 1$, $\tau = 0.5$, $M/S\hbar = 2$; B, $S = 1$, $\tau = 0.5$, $M/S\hbar = 5$; C, $S = \infty$, $\tau = 0.5$.

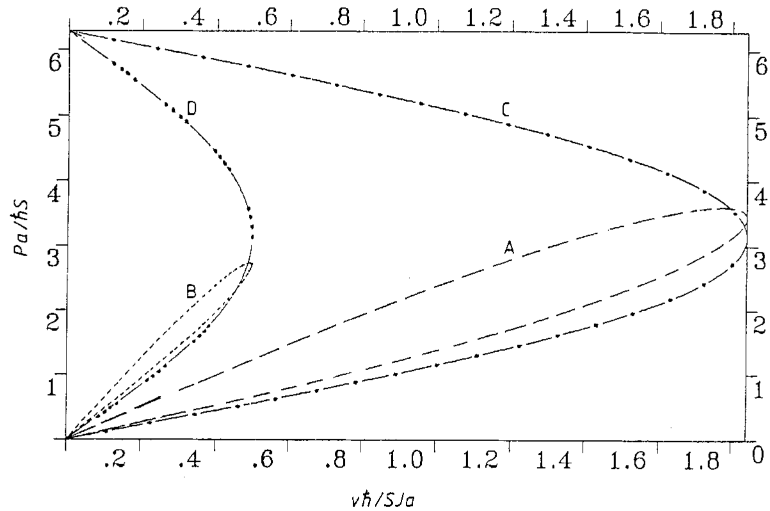

Figure 2. The quantum momentum (units of $\hbar a^{-1}$) versus soliton velocity v (units of $Ja\hbar^{-1}$) for $S = 1$, $\tau = 0.5$, $M/S\hbar = 2$ and 5 respectively. The corresponding classical plots ($S = \infty$) are also shown. Curves: A, $S = 1$, $\tau = 0.5$, $M/S\hbar = 2$; B, $S = 1$, $\tau = 0.5$, $M/S\hbar = 5$; C, $S = \infty$, $\tau = 0.5$, $M/Sh = 2$; D, $S = \infty$, $\tau = 0.5$, $M/S\hbar = 5$.

it is easily verified that as $\tau_Q \rightarrow 0$, the usual soliton solution for the isotropic model (Fogedby 1980) is obtained:

$$\sin^2(\theta/2) = (K_0^2/\Omega)\,\mathrm{sech}^2(K_0\zeta). \tag{5.2}$$

Here $K_0 = (\Omega - \frac{1}{4}V^2)^{1/2}$. Two different definitions for the soliton width Γ have been used for the isotropic model, viz. $\Gamma = a/K_0$ (Fogedby 1980) and $\Gamma = 2a/K_0$ (Haldane 1982). Using the latter definition, Haldane determined the condition to be satisfied by M for

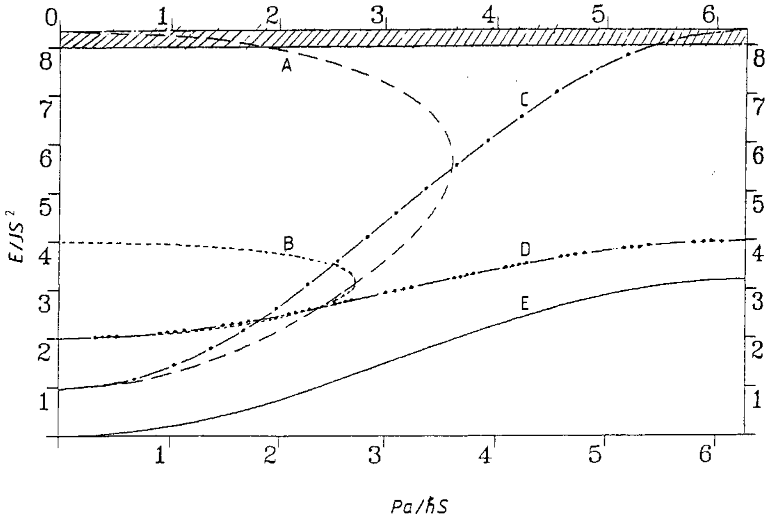

Figure 3. The classical and quantum soliton spectra: the energy E (units of JS^2) versus momentum P (units of $\hbar a^{-1}$) for $S = 1$, $\tau = 0.5$, $M/S\hbar = 2$ and 5 respectively. The gapless classical spectrum for the isotropic case $\tau = 0$ is also shown for $M/S\hbar = 5$. The hatched area is the part of the spectrum for $M/S\hbar = 2$ for which the continuum criterion $\Gamma_Q \gtrsim a$ is not satisfied. Curves: A, $S = 1$, $\tau = 0.5$, $M/S\hbar = 2$; B, $S = 1$, $\tau = 0.5$, $M/S\hbar = 5$; C, $S = \infty$, $\tau = 0.5$, $M/S\hbar = 2$; D, $S = \infty$, $\tau = 0.5$, $M/S\hbar = 5$; E, $S = \infty$, $\tau = 0$, $M/S\hbar = 5$.

the validity of the continuum approximation in that model. We will use its analogue to discuss the anisotropic case. Thus for $\tau_Q \neq 0$ we define from Equation (5.1)

$$\Gamma_Q = 2a/K_Q \tag{5.3}$$

where K_Q is given in equation (2.33). Using equations (4.15) and (5.3), we have

$$\Gamma_Q = (8JS^2/E_Q)a = 2a/(\omega + \tau_Q - \tfrac{1}{4}V^2)^{1/2}. \tag{5.4}$$

Note that similar expressions hold good for the classical case as well, as discussed in § 2 and §3. We will therefore drop the subscript Q in the following discussion.

If the continuum model is to describe the underlying discrete system (classical/quantum) self-consistently, we must require (Haldane 1982) $\Gamma \gtrsim a$ and the asymptotic soliton wavenumber (see equation (2.35)) $k_0 = \tfrac{1}{2}V \lesssim \pi$. The former implies a condition on the minimum soliton width, while the latter implies a condition on the maximum value of k_0. Let us discuss the soliton widths first.

Let Γ_{min} and Γ_{max} denote the minimum and maximum possible soliton widths. Using equations (4.17) to (4.20) in equation (5.4) we get

$$\Gamma_{min} = 2a/(\omega_{max} + \tau)^{1/2} = 2a\tau^{-1/2}\tanh(M\tau^{1/2}/4S) \tag{5.5}$$

and

$$\Gamma_{max} = 2a/(\omega_{min} + \tau)^{1/2} = 2a\tau^{-1/2}\coth(M\tau^{1/2}/4S). \tag{5.6}$$

For a given S, τ and M, we derive a quantitative criterion for M by demanding that the whole spectrum of solitons fulfils $\Gamma \gtrsim a$, i.e. $\Gamma_{min} \gtrsim a$. This yields

$$M \gtrsim 4S\tau^{-1/2}\tanh^{-1}(\tau^{1/2}/2). \tag{5.7}$$

For $\tau \to 0$, equation (5.7) reduces to

$$M \gtrsim 2S \tag{5.8}$$

as found earlier (Haldane 1982) ($\Gamma_{max} \to \infty$ as $\tau \to 0$). Equation (5.7) also implies the restriction $\tau < 4$. Furthermore, the condition $\Gamma \geqslant a$ combined with equation (5.4) gives $E_Q \leqslant 8JS^2$.

To satisfy the second 'continuum' condition $k_0 = V/2 \leqslant \pi$ for all solitons with fixed values of S, τ and M, we need $k_0^{max} \leqslant \pi$ or $V_S \leqslant 2\pi$. Equation (4.21) yields

$$\tau^{1/2}/\sinh(M\tau^{1/2}/2S) \leqslant \pi. \tag{5.9}$$

It is easy to verify that equation (5.9) implies a less restrictive condition on M than equation (5.7). In the limiting case $\tau \to 0$, equation (5.9) leads to $2S/M \leqslant \pi$, in agreement with the result for the isotropic case (Haldane 1982).

As an illustrative example, we take $S = 1$, $\tau = 0.5$. Equation (5.7) gives $M \geqslant 2.09$, while equation (5.9) leads to $M \geqslant 0.63$. Figure 3 gives E_Q versus P_Q for $M = 2$ and $M = 5$. Using equations (5.5) and (5.6) we get

$$\Gamma_{min} = 0.96a \qquad \Gamma_{max} = 8.33a \qquad \text{for } M = 2$$

$$\Gamma_{min} = 2a \qquad \Gamma_{max} = 3.99a \qquad \text{for } M = 5.$$

Thus for $M = 2$, only a very small part of the (classical and quantum) spectrum corresponding to $E > 8JS^2$ (see hatched portion in figure 3) does not meet the requirement $\Gamma_{min} \geqslant a$. For $M = 5$, this cut-off in energy does not affect the spectra. More generally, it is clear that, for $M \geqslant 2$, the full spectrum is physically relevant. In particular, both the upper and lower branches of the quantum spectrum must be considered. For very large values of M, $E_{cl} \to 4JS^2\tau^{1/2}$ (see equation (3.23)) for $0 \leqslant P_{cl} \leqslant 2\pi S$. For the quantum case, the separation between the upper and lower branches decreases as M increases.

Figure 2 shows that the maximum velocity corresponds approximately to the maximum momentum (for a given M) in the quantum case. Thus the energy E_S at which the upper branch begins can be evaluated from equation (4.23) to be $E_S = 5.48$ for $M = 2$ and $E_S = 2.99$ for $M = 5$ (compare with figure 3). Equation (5.4) shows that higher energy values correspond to high-amplitude, narrow-width solitons. The quantum correction $\langle \Delta P \rangle$ to the classical soliton momentum, which is vanishingly small for low-energy solitons with large widths, is expected to increase and become finite as the energy increases, essentially because of the effect of localisation caused by the smallness of the width. Since the maximum energy is the same for both classical and quantum models, this increase in $\langle \Delta P \rangle$ can be consistently accommodated only if the E_Q versus P_Q curve bends back, leading to the two branches in figure 3. Thus the inclusion of quantum effects leads to the existence of a maximum critical momentum (and velocity) above which the pulse-type excitations become unstable. We conclude by noting that there will be no restrictions on M such as in equations (5.7) and (5.9) if one is interested in studying quantum effects in a *continuum* spin model *per se*, without relating it to an underlying discrete chain.

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