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Quantum theory of planar kinks in a finite easy plane ferromagnetic chain

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Abstract. An outline of a quantum approach to multi-kink profiles as coherent states in a ferromagnetic chain is given. Relying on the continuum and harmonic approximation the influence of the out-of-plane fluctuations on the stability and dynamics of multi-kink structures in a finite chain is studied and compared with the stability and dynamics of single-kink profiles in an infinite chain. Even in the harmonic approximation, very few modes are diagonal. The multi-kink structure does not exhibit a 'zero-frequency' Goldstone mode. This is a consequence of the out-of-plane fluctuations.

1. Introduction

Kink-like profiles, that can be described by the sine-Gordon equation, have received much attention during the last decade, especially in their relation to the non-linear excitations of one-dimensional ferromagnets with an easy plane. The properties of the kinks rely on the mapping (Mikeska 1978) of the magnetic chain on the sine-Gordon system and the thermodynamical and response functions of the sine-Gordon system. These functions can be calculated classically (Currie *et al* 1980) using transfer matrices and are simulated for the classical model (Schneider and Stoll 1980). The heat capacity data of CsNiF₃ (Ramirez and Wolf 1982) and [C₆H₁₁NH₃]CuBr₃ (referred to as CHAB) (Kopinga *et al* 1984b, Tinus *et al* 1985) have been interpreted in terms of the sine-Gordon model, at least in a certain temperature and external field range. The inverse spin-lattice relaxation time, which is proportional to the soliton density (Goto 1983, Benner *et al* 1984, Kopinga *et al* 1984a), and neutron scattering measurements of the central peak (Kjems and Steiner 1978, Kakurai *et al* 1984) have also been interpreted in terms of this model. This interpretation yields a renormalisation of the so-called soliton rest energy. However, there has always been some controversy about this interpretation as stated by several authors (Loveluck *et al* 1981, Reiter 1981, Pini and Rettori 1984, Chui and Ma 1983). Therefore, it is not obvious that the data actually support evidence for the presence of this particular kind of kink in these experimental systems.

The mapping of the easy plane ferromagnet on the sine-Gordon model assumes an extreme anisotropy which is, as such, not present in the real system. Investigations of the influence of the lack of extreme anisotropy have led to the prediction of instabilities at a critical magnetic field (Kumar 1982, Magyari and Thomas 1982).

However, the measurement of the inverse spin-lattice relaxation time (Benner *et al* 1984) shows a characteristic Arrhenius law with the renormalised soliton rest energy as an activation energy and does not show any marked deviation from this behaviour at the predicted critical field.

One of the crucial approximations in the mapping of the easy plane ferromagnetic chain on the sine-Gordon model is that the spin dynamics arise from a classical vector, obeying Poisson brackets analogous to the spin commutation relations. It has been conjectured that a considerable part of the deviation between the observed value of the soliton activation energy and the calculated soliton energy in a classical model is of quantum nature. Calculations made by Maki (1981) on the basis of the quantum sine-Gordon model and Mikeska (1982) on the basis of a more general quantum model predicted a reduction to the soliton rest energy. In these approaches the most important corrections to the soliton energy come from the zero-point quantum fluctuations and from normal ordering. Both calculations rely on methods used for the quantisation of classical field theories (Dashen *et al* 1975).

In the present calculation we will neglect this aspect of the problem. In relation to some experimental observations, it is found that the quantum sine-Gordon model is not superior to the 'classical' sine-Gordon model (Fowler *et al* 1984). Furthermore, for an antiferromagnetic chain it is shown (Wright *et al* 1985) that the renormalisation crucial to obtain the reduction of the soliton energy leads also to a reduction of the linear excitations of the system. It is necessary to take the out-of-plane fluctuations, which are neglected in the quantum sine-Gordon model, into account in order to obtain agreement with the measured values of the energy of the linear excitations (Heilmann *et al* 1981). Both arguments suggest that it is more important to consider the out-of-plane fluctuations on the same level as the in-plane fluctuations than to take the renormalisations due to differences in zero-point quantum fluctuations and normal ordering into account.

In this paper, we study the quantum fluctuations around a coherent state for an easy plane ferromagnet relying on well established quantum methods. Instead of using a semiclassical theory to obtain the kinks in the system, we have performed a canonical transformation that allows the introduction of site-dependent quantisation axes (Moussa and Villain 1976, 1977, Barnes 1981, Fischer and Heber 1985) in the easy plane. The transformed Hamiltonian is then calculated and the continuum approximation is made. The static sine-Gordon equation turns out to be the stationarity condition for the transformed Hamiltonian. Using a general solution of this equation the harmonic part of the Hamiltonian is further analysed: first we give a short review of the possible solutions of the static sine-Gordon equation. For the infinite chain with a single kink the harmonic spectrum is calculated. For the multi-kink solutions on a finite support we do not calculate the complete spectrum, which is analogous to the bandstructure of a one-dimensional model, but we solve the eigenvalue problem in some special points and indicate the differences between the single-kink and multi-kink profiles. In the last section we discuss the method of calculation and give the conclusions.

2. Quantum theory of kinks and their fluctuation

In this section, we will briefly indicate how the spin algebra can be simplified at the expense of complicating the Hamiltonian. We will then introduce a canonical transformation which allows us to describe a profile in the spin chain as a coherent state.

Subsequently we will discuss the linear excitations of the chain relying on the harmonic and continuum approximation for the quantum fields.

2.1. The Villain representation

We assume that the ferromagnetic chain can be described by the following Hamiltonian:

$$H = -J\sum_n \mathbf{S}_n^z \mathbf{S}_{n+1}^z + A\sum_n (\mathbf{S}_n^z)^2 - J\sum_n \frac{1}{2} (\mathbf{S}_n^+ \mathbf{S}_{n+1}^- + \mathbf{S}_{n+1}^+ \mathbf{S}_n^-) - g\mu_B H \sum_n \frac{1}{2} (\mathbf{S}_n^+ + \mathbf{S}_n^-). \quad (1)$$

The single-ion anisotropy originates from the term proportional to the constant A . It is commonly employed to induce an energetically favourable easy XY plane. The external magnetic field H introduces an additional anisotropy in this plane. Single-ion anisotropy, which is typical for CsNiF_3 , is not the only mechanism that can introduce an easy plane in the system. For CHAB the XY character of the Hamiltonian originates from the exchange anisotropy. Our calculations are performed for a system with single-ion anisotropy. The methods, however, are equally well applicable to a system with exchange anisotropy, but require somewhat more elaborate calculations.

The strong non-linearity in the equations of motion generated by (1) are introduced by the spin algebra. In order to transfer the non-linear behaviour from the spin algebra to the Hamiltonian a more convenient operator representation of this algebra is chosen. Among the many possibilities (Mead and Papanicolaou 1983) we have chosen the representation proposed by Villain (1974) and analysed more recently by Haldane (1983). In this representation the Hamiltonian transforms to the following expression:

$$H = -J[S(S+1)]\sum_n [\cos(\Phi_n - \Phi_{n+1}) + g\mu_B H / \{J[S(S+1)]^{1/2}\} \cos(\Phi_n)] \\ - J\sum_n \mathbf{S}_n^z \mathbf{S}_{n+1}^z - J\sum_n \frac{1}{2} \mathbf{S}_n^z [\cos(\Phi_n - \Phi_{n+1}) + \cos(\Phi_{n-1} - \Phi_n)] \\ + g\mu_B H / \{J[S(S+1)]^{1/2}\} \cos(\Phi_n) - 2A/J] \mathbf{S}_n^z + \text{higher-order terms.} \quad (2)$$

For a derivation of the higher-order terms in equation (2) we refer to Wright *et al* (1985). From the calculation of these authors the higher-order terms can be obtained to the sixth order in \mathbf{S}^z by a simple transformation of their expression. It should be noted that \mathbf{S}_n^z and Φ_n will be treated as canonical adjoint operators with the approximative commutation relation:

$$[\Phi_n, \mathbf{S}_m^z] = i\delta_{nm} \quad (3)$$

instead of operators with the following correct Weyl relation:

$$F(\mathbf{S}_n^z) \exp(\pm i\Phi_n) = \exp(\pm i\Phi_n) F(\mathbf{S}_n^z \pm 1) \quad (4)$$

where $F(x)$ is an arbitrary function of x . In this respect, we wish to remark that (3) is invariant under the rescaling of Φ_n and \mathbf{S}_n^z used in the quantum sine-Gordon model while (4) does not exhibit this scaling property.

2.2. A canonical transformation

The non-linear excitations of (2) are usually studied in a semiclassical approach: one considers (2) as a classical system, one obtains the non-linear solutions and then the small oscillations around these solutions are quantised. This procedure is equivalent to the functional integration approach (Dashen *et al* 1975) and has served as a basis for most quantum calculations on this system and related systems (Maki 1981, Mikeska 1982, Fogedby *et al* 1985). Recent studies of Klaunder and Daubechies (1984) and

Mead and Papanicolaou (1982) have shown how one can use spin coherent states to obtain functional integrals for quantum spin systems directly, without invoking a 'classical' counterpart of the system. Because there is a close relationship between coherent states and the canonical transformations of the displaced oscillator type, we will use such transformations to introduce a site-dependent function φ_n into the Hamiltonian (2) by displacing the operator Φ_n via the canonical transformation with the following generator:

$$U = i\sum_n S_n^z \varphi_n. \tag{5a}$$

The operator Φ_n transforms then as follows:

$$\exp(-U)\Phi_n \exp(U) = \Phi_n - \varphi_n. \tag{5b}$$

This result is directly obtained from the Weyl relation. Before the transformation the operator Φ_n is related to an angle which reference is the X axis for all the sites of the chain. The introduction of φ_n gives the Φ_n operator a site-dependent reference axis rotated over the angle φ_n for that site. The transformation (5) introduces a site-dependent quantisation axis into the description of the chain.

The transformed Hamiltonian can be decomposed as a sum of terms containing a definite number of operators as indicated by the superscript of H

$$\exp(-U)H \exp(U) = H^0 + H^1 + H^2 + H^3 + H^4 + \dots \tag{6}$$

The first three terms in this decomposition are given below.

$$H^0 = -J[S(S+1)]\sum_n (\cos(\varphi_n - \varphi_{n+1}) + g\mu_B H / \{J[S(S+1)]^{1/2}\} \cos(\varphi_n)) \tag{7}$$

$$H^1 = -J[S(S+1)]\sum_n \Phi_n (\sin(\varphi_n - \varphi_{n+1}) - \sin(\varphi_{n-1} - \varphi_n) + g\mu_B H / \{J[S(S+1)]^{1/2}\} \sin(\varphi_n)) \tag{8}$$

$$H^2 = J[S(S+1)]\sum_n \frac{1}{2}(\Phi_n)^2 (\cos(\varphi_n - \varphi_{n+1}) + \cos(\varphi_{n-1} - \varphi_n) + g\mu_B H / \{J[S(S+1)]^{1/2}\} \cos(\varphi_n)) - \Phi_n \Phi_{n+1} \cos(\varphi_n - \varphi_{n+1}) + J\sum_n \frac{1}{2}(S_n^z)^2 (\cos(\varphi_n - \varphi_{n+1}) + \cos(\varphi_{n-1} - \varphi_n) + g\mu_B H / \{J[S(S+1)]^{1/2}\} \cos(\varphi_n) + 2A/J) - S_n^z S_{n+1}^z. \tag{9}$$

It is seen that H^1 becomes identically zero if φ_n satisfies the following difference equation

$$\sin(\varphi_n - \varphi_{n+1}) - \sin(\varphi_{n-1} - \varphi_n) + g\mu_B H / \{J[S(S+1)]^{1/2}\} \sin(\varphi_n) = 0. \tag{10}$$

In the continuum approximation, the equation equivalent to (10) leads to the static part of the sine-Gordon equation

$$\varphi''(x) = m^2 \sin(\varphi(x)) \tag{11}$$

where " denotes the second derivative with respect to x and m is given by the well known expression

$$m^2 = g\mu_B H / \{Ja^2[S(S+1)]^{1/2}\} \tag{12}$$

where a is the distance between the magnetic ions. The Hamiltonian H^1 (8) can be interpreted as that part of the energy operator which expresses the energy due to the site-dependent force applied on the in-plane spin component via the angle operator Φ_n . For a solution of (10) this force is zero and therefore the solutions of (10) can be used to classify the metastable states of the total Hamiltonian. As we shall see further the spectrum of H^2 will also be important for each of these solutions, because the stability of the coherent state depends on it.

2.3. The Hamiltonian in the continuum approximation

In the remainder of the paper, we will use the continuum approximation. Making this approximation clearly restricts the possible solutions of (10): only those solutions where φ_n changes smoothly over a large number of cells are taken into account. As shown in a recent paper by Etrich *et al* (1985) on an equivalent classical model the influence of the lattice is important because (10) also has other types of solutions and the discreteness of the lattice influences their stability. This restricts our approach to phenomena that vary slowly along the chain. A further analysis of this point will be given in the discussion.

Introducing dimensionless units $y = mx$, H^0 and H^2 in the continuum approximation are as follows:

$$H^0 = -N\{JS(S+1) + g\mu_B H[S(S+1)]^{1/2}\} + JS(S+1)ma \int dy [\frac{1}{2}(\varphi')^2 + 2 \sin^2(\varphi/2)] \tag{13}$$

$$H^2 = JS(S+1)ma \int dy [\frac{1}{2}(\Phi)^2 + \frac{1}{2}\Phi^2 \cos(\varphi)] + Jma \int dy [\frac{1}{2}(\mathbf{S}')^2 + \frac{1}{2}\mathbf{S}^2(\cos(\varphi) - (\varphi')^2 + \delta)]. \tag{14}$$

The $\varphi(y)$ denoted by φ in the equations is now a solution of the dimensionless static sine-Gordon equation obtained from (11) by changing units. N is the number of magnetic sites in the chain, the first term of (13) is the classical ground state and the second term expresses the energy needed to shift the operator Φ over an angle φ all over the chain. Requiring that H^0 is extreme is equivalent to (10) being satisfied. The anisotropy term in (14) is given by $\delta = 2A/Jm^2a^2$. We have denoted the continuum counterpart of the operator S_n^z by S . The integrals extend over the complete chain length. For the derivation of (14) it is assumed that the fields vanish in the endpoints. In the same approximation the higher-order terms are

$$H^3 = JS(S+1)ma \frac{1}{3!} \int dy [\Phi^3 \sin(\varphi)] + Jma \int dy [S\Phi S\varphi'] \tag{15}$$

$$H^4 = -JS(S+1)ma \frac{1}{4!} \int dy [\Phi^4 \cos(\varphi)] - Jma \int dy [S(\frac{1}{2}(\Phi)^2 + \frac{1}{4}\Phi^2 \cos(\varphi))S] - Jma/S(S+1) \int dy [S(\frac{1}{4}(\mathbf{S}')^2 - \frac{1}{8}\mathbf{S}^2 \cos(\varphi))S]. \tag{16}$$

Before we discuss the excitations generated by H^2 it should be mentioned that if S and Φ are written in creation and annihilation operators and we put H^3 and H^4 in normal order, this procedure would give rise to additional terms in H^1 coming from H^3 , in H^2 coming from H^4 and so on. As explained in the introduction we will not consider this procedure which leads to a self-consistent calculation or to diagrammatic expansions of the relevant quantities.

2.4. The harmonic spectrum

The harmonic part of the transformed Hamiltonian leads to the following coupled

equations for the quantum fields $\Phi(y)$ and $S(y)$:

$$\dot{\Phi}(y) = 2Jma\mathbf{H}_S S(y) \quad (17)$$

$$\dot{S}(y) = -2JS(S+1)ma\mathbf{H}_\Phi\Phi(y) \quad (18)$$

where the dot denotes the derivative with respect to time and

$$\mathbf{H}_S = \frac{1}{2}p^2 + \frac{1}{2}\delta + \frac{1}{2}[1 - (\varphi')^2 - 2\sin^2(\varphi/2)] \quad (19)$$

$$\mathbf{H}_\Phi = \frac{1}{2}p^2 + \frac{1}{2}[1 - 2\sin^2(\varphi/2)] \quad (20)$$

where p^2 is minus the second derivative with respect to the variable y .

Let us consider the propagator

$$\mathbf{D}(yt, y_0t_0) = i\theta(t-t_0)\langle[\Phi(y, t), \Phi(y_0, t_0)]\rangle \quad (21)$$

which describes the in-plane fluctuations of the system in the presence of a coherent state characterised by φ . The harmonic approximation for \mathbf{D} follows then from the equations of motion (17) and (18):

$$\ddot{\mathbf{D}}(yt, y_0t_0) = 2Jma\mathbf{H}_S\delta(y-y_0)\delta(t-t_0) - (2Jma)^2S(S+1)\mathbf{H}_S\mathbf{H}_\Phi\mathbf{D}(yt, y_0t_0). \quad (22)$$

It is important to realise that \mathbf{H}_S and \mathbf{H}_Φ do not commute *a priori*. Indeed, for an arbitrary solution φ of the static sine-Gordon equation (11), the commutator is

$$[\mathbf{H}_S, \mathbf{H}_\Phi] = -2[(\varphi')^2 + \varphi'\varphi'']. \quad (23)$$

If commutator (23) is different from zero, there is no set of eigenfunctions which is common to both Hamiltonian operators (19) and (20). Therefore, no complete set with appropriate quantum numbers can be found which diagonalises both. If one expands the $\Phi(y)$ field in a complete set belonging to one of the two Hamiltonian operators, it then follows from (22) that these fluctuations will decay. They have a self-energy, even in the harmonic approximation, with an imaginary part indicating the lifetime of the excitation. In order that the solution of the sine-Gordon equation (11) has the meaning of a coherent state in the quantum system the spectrum of $\mathbf{H}_S\mathbf{H}_\Phi$ has to be non-negative. Indeed, if it has a negative part it means that the quantum fluctuations grow in time and will destroy the coherence of the state. The non-negative spectrum of $\mathbf{H}_S\mathbf{H}_\Phi$, however, is not sufficient to always ensure the coherence as we shall see in the next section.

3. Static solutions and their quantum fluctuations

The spectrum of H^2 (14) is important for the stability of the coherent states. Before we study the quantum fluctuations resulting from H^2 it is useful to mention briefly the solutions of (11) which have been studied by many authors (Scott 1969). Once the solutions are given we derive the operators \mathbf{H}_S and \mathbf{H}_Φ which govern the quantum fluctuation around the profile. How the spectrum of \mathbf{H}_S and \mathbf{H}_Φ influences the stability and coherence of the profile will be shown first for the infinite chain solution of (11). After that we discuss the coherence and stability of the solutions of (11) which are subjected to the periodic boundary conditions appropriate for a chain with a finite length L .

3.1. The solutions of the static sine-Gordon equation

A way to classify the solutions of (11) is to consider the first integral

$$(\varphi')^2 = 4\sin^2(\varphi/2) + c \quad (24)$$

(c is an integration constant) that can take all real values greater than -4 . If an analogy with the pendulum (Scott 1969) is made then the solutions for which c is negative correspond to oscillations (thus the spatial evolution of φ will be a turn to the left followed by a turn to the right and so on) and the solutions for which c is positive correspond to rotations (thus the spatial evolution of φ will be a turn to the right over 2π followed by the same turn). The solutions with c negative will not be considered because it is known that they are unstable against small fluctuations (Giachetti *et al* 1984). For c positive (24) can be integrated giving

$$\pm(y - y_0) = k[F(\varphi^0/2 + \pi/2, k) - F(\varphi/2 + \pi/2, k)] \tag{25}$$

where F is the elliptic integral of the first kind and k is the modulus, y_0 is an integration constant and φ^0 is the value of φ in y_0 . The periodicity of F is $2K$, where K is the complete elliptic integral of the first kind (Abramowitz and Stegun 1964) and k is related to c for $c > 0$ by

$$k = 1/(1 + c/4)^{1/2}. \tag{26}$$

The solution (25) is periodic in the variable y with a period of $2kK$. If a chain of length $L = Na$ contains n kinks then the number of kinks is equal to the chain length divided by the kink length (i.e. the period of the solution in the variable $x = y/m$)

$$n = mL/2kK. \tag{27}$$

The kink density (being the number of links divided by the number of magnetic ions) is easily derived from (27) and is inversely proportional to the kink period $2kK$. Because K is a monotonic function of k we have plotted in figure 1 the kink density times $(ma)^{-1}$, which is a universal quantity in our approach, in terms of the modulus k . It is seen that for $k = 1$, the period of the kink becomes infinite, leading to zero

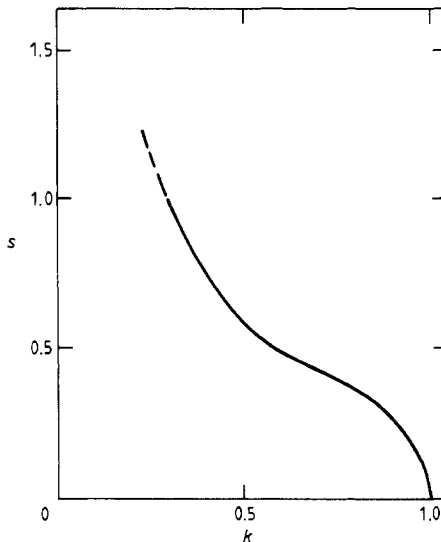


Figure 1. The period of an array of kinks is in a unique way related to its modulus k . The number of kinks (n) plotted against the number of magnetic sites (N) is the kink density n/N . In the figure the kink density s is expressed in units $(ma)^{-1}$ and the modulus k is given as a function of this dimensionless quantity. The low density limit corresponds to $k = 1$, i.e. one kink in an infinite chain.

density, or equivalently to one kink in an infinite chain. We will refer to this situation as the low density limit. For k a few per cent smaller than 1 the density rapidly increases. In the remainder of the paper we will use the modulus k as a measure for the kink density. For $k = 1$ ($c = 0$) solution (25) reduces to the well known single-kink solution:

$$\varphi = 4 \tan^{-1} \exp[\pm (y - y_0)]. \quad (28)$$

For a general k we obtain the following relation

$$\sin^2(\varphi/2) = \text{cn}^2(z) = 1 - \text{sn}^2(z) \quad (29)$$

where sn and cn are respectively the sine and cosine amplitude function. Together with dn they are the three basic Jacobian elliptic functions. Their argument z is related to y by

$$z = (y - y_0)/k - F(\varphi^0/2 + \pi/2, k). \quad (30)$$

Using the solution (25) together with (26) and (27) and imposing the boundary condition that the chain will contain an integer number of kinks the energy per kink of the static structure follows from H^0 . Figure 2 shows this energy as a function of the modulus k . This energy is of course identical to the energy of sine-Gordon kinks (Giachetti *et al* 1984, Sutherland 1973, Gupta and Sutherland 1976) provided one uses the correct parametrisation. The solutions of (11) are now characterised by the modulus k , which is directly related to the kink density. The question of whether for all densities or for the corresponding moduli a profile can be found which is stable has to be considered next.

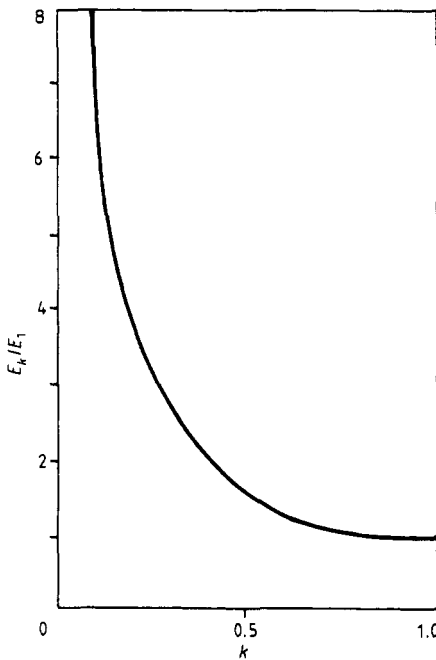


Figure 2. The energy E_k of a kink divided by the energy E_1 of a kink in the low density limit ($k = 1$) is given as a function of the kink modulus k .

3.2. The harmonic spectrum

The operator H_Φ (20) can be written in terms of the sine amplitude function of modulus k

$$H_\Phi = -(1/2k^2)[d^2/dz^2 + k^2(1 - 2 \operatorname{sn}^2(z))]. \tag{31}$$

This is the linear operator of a generalised Lamé equation with index 1 (Whittaker and Watson 1935). Imposing periodic boundary conditions on the solutions of

$$H_\Phi \Psi = e_\Phi \Psi \tag{32}$$

the spectrum e_Φ has been calculated by Sutherland (1973). It has two branches, separated by a gap at the first Brillouin zone. It should be noted that this zone is induced by the periodic array of kinks. For all the values of the modulus k given by (27) the spectrum of e_Φ is non-negative. The operator H_S can also be written in terms of the sine amplitude function

$$H_S = -(1/2k^2)[d^2/dz^2 + k^2 + 4 - \delta k^2 - 6k^2 \operatorname{sn}^2(z)]. \tag{33}$$

This is again the linear operator of a generalised Lamé equation (with index 2 now). The spectrum e_S generated by the eigenvalue problem

$$H_S \Psi = e_S \Psi \tag{34}$$

is not known analytically for arbitrary k . It can be calculated because the eigenfunctions are known. In figure 3 we have plotted one period of φ and the corresponding potentials V_Φ and V_S for the same period. (In V_Φ and V_S the line indicates the lowest eigenvalue of (32) and (34). The calculation of this eigenvalue is performed at the end of this section.) Before we discuss the general case ($k \neq 1$) we consider the low density limit ($k = 1$).

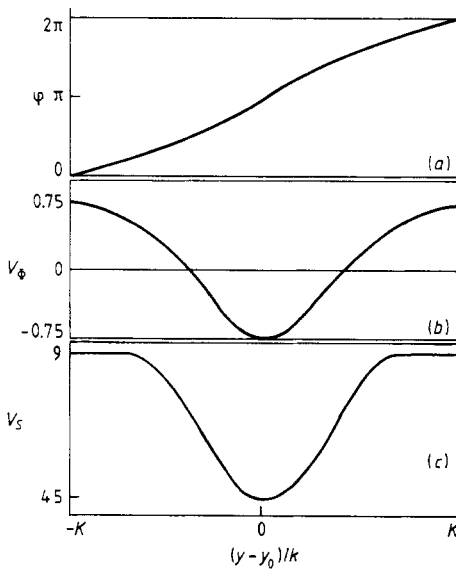


Figure 3. For the modulus $k = 0.707$ and $\delta = 7$ is shown (a) the profile of a kink (i.e. one period of the array) (b) the potential V_Φ for the in-plane fluctuations, and (c) the potential V_S for the out-of-plane fluctuations.

3.2.1. *The spectrum for a single (k = 1) kink.* The H_Φ and H_S transform to expressions which are familiar from the classical stability analysis of the problem (Magyari and Thomas 1982, 1983, 1984, Kumar 1982, Liebmann *et al* 1983) and also from the study of the thermodynamical properties of the classical spin chain in which out-of-plane components are taken into account (Fogedby *et al* 1983, 1984, 1985),

$$H_{\Phi_1} = \frac{1}{2}p^2 + \frac{1}{2}(1 - 2 \operatorname{sech}^2(y)) \tag{35}$$

$$H_{S_1} = \frac{1}{2}p^2 + \frac{1}{2}(1 + \delta - 6 \operatorname{sech}^2(y)). \tag{36}$$

The eigenspectrum of (35) is well known: it has a bound state with eigenvalue zero and a wavefunction proportional to $\operatorname{sech}(y)$ and a continuum starting at $\frac{1}{2}$. The eigenfunctions and the spectrum of H_S are also well known (Wada and Schrieffer 1978, Wada and Ishiuchi 1982). The Hamiltonian (36) has two bound states, the translation mode and the tilting mode (denoted by the index 0, 1) with eigenvalue $(\delta - 3)/2$ and $\delta/2$ and with wavefunction $\operatorname{sech}^2(y)$ and $\operatorname{sech}(y) \tanh(y)$. The continuum of (36) starts at $\frac{1}{2}(1 + \delta)$ and the wavefunctions are denoted by their wavenumber k (not to be confused with the modulus k which is equal to 1 in this context).

Our quantum treatment of the fields Φ and S relies on the quantum numbers ($i = 0, 1, k, \dots$) of the complete set of eigenfunctions $\Psi_i(y)$ of (36). Their completeness relation can be used to represent the Dirac delta function which originates from the continuum limit of (3). This leads to the following representation of the quantum fields

$$\Phi(y) = q_0\Psi_0(y) + q_1\Psi_1(y) + \sum_k q_k\Psi_k(y) \tag{37}$$

$$S(y) = p_0\Psi_0(y) + p_1\Psi_1(y) + \sum_k p_k\Psi^*k(y). \tag{38}$$

The p_i and q_i now have the usual commutation relations. In terms of these new operators H^2 takes the following form

$$\begin{aligned} H^2 = & Jma[(\delta - 3)\frac{1}{2}p_0^2 + \delta/2p_1^2 + \frac{1}{2}\sum_k p_k(1 + \delta + k^2)p_k^*] \\ & + JmaS(S + 1)[\frac{4}{5}q_1^2 + \frac{1}{2}\sum_k q_k(1 + k^2)q_k^* \\ & + \frac{1}{2}q_1\sum_k g_{1k} + \frac{1}{2}\sum_{kk'} q_k g_{kk'} q_k^*] \end{aligned} \tag{39}$$

where

$$\begin{aligned} g_{1k} = & \langle \Psi_1, H_\Phi \Psi_k \rangle = -\delta k/2[3\pi(1 + k^2)(4 + k^2)]^{1/2} \\ & \operatorname{sech}(\pi k/2)(8/15 + 83/80k^2) \end{aligned} \tag{40}$$

and

$$\begin{aligned} g_{kk'} = & \frac{1}{4}(1 + \delta + k^2)(k - k') \operatorname{cosech}[\pi(k - k')/2] \\ & \times \{ \frac{34}{5} - 3kk' + k^2k'^2 + (k - k')^2[\frac{11}{2} + \frac{1}{2}(k^2 + k'^2) - kk'] \\ & + \frac{9}{4}(k - k')^4 \} / [(1 + k^2)(1 + k'^2)(4 + k^2)(4 + k'^2)]. \end{aligned} \tag{41}$$

Considering the part of the propagator (22) which describes the correlation between the q_0 operator part of the $\Phi(y)$ field one obtains after Fourier transformation

$$D_{00}(\omega) = -Jma(\delta - 3)/\omega^2. \tag{42}$$

This is precisely the response one should expect for a free particle with a mass proportional to $1/(\delta - 3)$. This analogy is only meaningful for δ larger than 3, which is the high anisotropy and/or low magnetic field case. In this case p_0 is a conserved quantity, which can be interpreted as the momentum of the kink. It should be realised

that the fact that q_0 is cyclic is due to the special relation between the wavefunction Ψ_0 and the bound-state wavefunction of H_{ϕ_1} . Indeed Ψ_0 is proportional to the square of the bound-state wavefunction $\text{sech}(y)$. Within this interpretation $Jma(\delta - 3)\frac{1}{2}p_0^2$ represents the kinetic energy of the kink. If δ is smaller than 3 the kink can lower its energy by taking a finite value for p_0 . This means that within the harmonic approximation the expectation value of the $S(y)$ field is no longer zero. In appendix 1 we will come back to this question. Further we will discuss the case $\delta > 3$.

The autocorrelations of the q_1 and also of the q_k parts can be calculated. To second order in the non-diagonal interaction coefficients one obtains for the tilting mode:

$$D_{11}(\omega) = -Jma\delta/[\omega^2 - (2Jma)^2 S(S+1)(\frac{4}{5}\delta + \Sigma_{11}(\omega))] \tag{43}$$

where the self-energy (in the indicated approximation) is given by

$$\Sigma_{11}(\omega) = \Sigma_k |g_{1k}|^2 / \{[\omega/2Jma\sqrt{S(S+1)}]^2 - e_k(e_k + g_k)\} \tag{44}$$

and

$$e_k = \frac{1}{2}(1 + \delta + k^2) \tag{45a}$$

$$g_k = 2/\pi(\frac{4}{5} + 3k^2 + k^4)/(4 + 5k^2 + k^4). \tag{45b}$$

The propagator $D_{kk}(\omega)$ takes an analogous form, with two self-energies, one for the decay into the tilting mode and another for the decay into a k' mode. This calculation shows that the spectrum of $H_{\phi_1}H_{S_1}$ is non-negative. Therefore the quantum fluctuation does not destroy the coherence of the $k = 1$ kink. The lower bound of this spectrum is given by

$$(\Psi, H_{\phi_1}H_{S_1}\Psi) \geq 0 \tag{46}$$

where Ψ is a square integrable function satisfying the boundary conditions. Taking for Ψ a linear combination of the three bound states of H_{ϕ_1} and H_{S_1} it is easy to show that (46) is satisfied for all values of δ . As explained in appendix 1 the kink can develop out-of-plane components to lower its energy when H_{S_1} has a negative eigenvalue. This analysis leads to the conclusion that for a single ($k = 1$) kink and for δ larger than 3 the profile can be described as a coherent state, which is free to move in the harmonic approximation.

3.2.2. The harmonic spectrum for the $k \neq 1$ solution. It is well known that the spatial derivative of the kink profile is a solution of the eigenvalue problem (32) with eigenvalue zero. For the sine-Gordon system this is a direct consequence of the Goldstone theorem. The derivative φ' is proportional to $\text{dn}(z)$. Direct verification shows that $\text{dn}(z)$ satisfies the generalised Lamé equation (31) and is a solution of (32) with $e_\phi = 0$. This function is even, it has periodicity $2K$ in the variable z and it is nodeless: it is the eigenfunction of H_{ϕ_k} with the lowest eigenvalue and as a consequence the spectrum of H_{ϕ_k} is non-negative. It is interesting to note that in the $k = 1$ limit $\text{dn}(z)$ as well as $\text{cn}(z)$ become equal to $\text{sech}(y)$ leading to the ground-state function of H_{ϕ_1} with zero eigenvalue. Direct verification shows that $\text{cn}(z)$ is a solution of (32) with eigenvalue $\frac{1}{2}(1 - k^2)/k^2$. Comparing this result with the exact calculation by Sutherland (1973) one sees that $\text{dn}(z)$ is the wavefunction of a state belonging to the middle of the Brillouin zone whereas $\text{cn}(z)$ is the wavefunction of a state that belongs to the same branch at the endpoint of the first Brillouin zone (the Brillouin zone introduced by the periodicity of the multi-kink profile). Knowing that the eigenfunctions of H_{S_k} are

combinations of elliptic functions it is possible to construct a nodeless wavefunction Ψ_0 for H_{Sk} :

$$H_{Sk}\Psi_0 = e_{S0}\Psi_0 \tag{47}$$

with

$$e_{S0} = \frac{1}{2}\{\delta - 1 - 2/k^2[(4k^4 - 13k^2 + 13)^{1/2} - 1]\}. \tag{48}$$

Ψ_0 is given in appendix 2. In figure 4 we show the region in the (δ, k) plane where e_{S0} is negative. The spectrum of the product operator $H_{Sk}H_{\Phi k}$ is related to e_{S0} as follows

$$\langle \Psi_0 H_{Sk} H_{\Phi k} \Psi_0 \rangle = e_{S0} \langle \Psi_0 H_{\Phi k} \Psi_0 \rangle. \tag{49}$$

Because the expectation value of $H_{\Phi k}$ is positive for $k \neq 1$ the spectrum of the operator $H_{Sk}H_{\Phi k}$ will have a negative part if e_{S0} is negative. For $k = 1$ one obtains for (48) the known result

$$e_{S0} = \frac{1}{2}(\delta - 3) \tag{50}$$

and Ψ_0 becomes $\text{sech}^2(y)$, the square of the eigenfunction of $H_{\Phi 1}$ with eigenvalue zero. Therefore (49) is no longer conclusive for the $k = 1$ case. Any eigenstate of H_{Sk} which is a product of two eigenstates of $H_{\Phi k}$ is an eigenstate of the product operator $H_{Sk}H_{\Phi k}$ and this eigenstate is diagonal in the harmonic approximation (it has no interactions with the other harmonic fluctuations). For $k = 1$ the wavefunction $\text{sech}^2(y)$ is directly connected with the diagonal kinetic energy operator in H^2 . For $k \neq 1$ the following wavefunction

$$\Psi_1 = N \text{cn}(z) \text{dn}(z) \tag{51}$$

is an eigenstate of H_{Sk} :

$$H_{Sk}\Psi_1 = \frac{1}{2}(\delta - 3/k^2)\Psi_1. \tag{52}$$

The state belongs to the end of the first Brillouin zone and is a product of eigenfunctions of $H_{\Phi k}$. This leads to

$$H_{Sk}H_{\Phi k}\Psi_1 = \frac{1}{2}(\delta - 3/k^2)\frac{1}{2}(1 - k^2)/k^2\Psi_1. \tag{53}$$

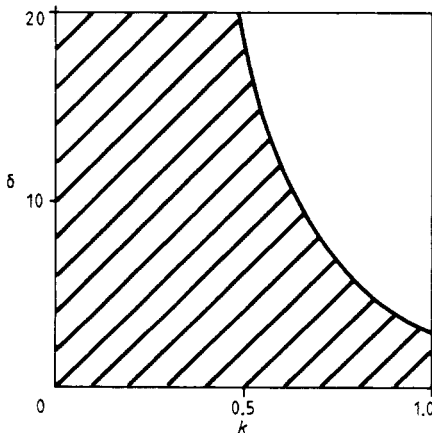


Figure 4. The lowest eigenvalue of H_{Sk} is shown as a function of δ and k . In the hatched region the eigenvalue is negative. For parameters belonging to the hatched region the multi-kink structure loses its coherence and is unstable.

In figure 5 we have plotted this eigenvalue as a function of the modulus k for a large δ value. The state with this eigenfunction (51) also becomes $\text{sech}^2(y)$ for k going to 1. Combining (49) and (53) it is found that the out-of-plane fluctuations introduce a gap in the spectrum. The lowest energy of a fluctuation around a profile is larger than zero, except in the $k = 1$ limit and at k_c : this is the modulus that corresponds with the critical density, where the multi-kink profile becomes unstable. This point will be clarified in the next section.

3.3. The coherence and dynamics of planar kinks

For the single kink ($k = 1$), one knows that for $\delta > 3$ the planar character is stable against the creation of out-of-plane components, because the eigenvalues of H_S are positive. The lowest eigenvalue of the product operator $H_S H_\Phi$ is zero so that this spectrum has no direct consequences for the coherence of the kink. For the ($k < 1$) multi-kink structure the stability and coherence analysis coincide: for almost all k values H_{S_k} and $H_{S_k} H_{\Phi_k}$ have the same sign. Figure 4 divides the δk plane into a region where stable multi-kink structures are possible (positive eigenvalues) and a region where the coherence is destroyed by quantum fluctuations.

The out-of-plane quantum fluctuations generated by H_{S_k} have a substantial influence on the spectrum of the harmonic modes in the presence of kinks. For $k \neq 1$ the lowest energy of these modes is no longer zero: the energy spectrum has a gap. This gap is proportional to expression (49) for the middle of the Brillouin zone. At the endpoint of the first Brillouin zone it is given by (53). The so-called Goldstone mode of zero frequency associated with the translational invariance of the system is no longer present: for exactly the same reasons as the magnon frequency in an anisotropic magnetic system with an external magnetic field has a gap for wavevector zero, the out-of-plane fluctuations induce a gap in the excitation spectrum around a multi-kink structure. The stability and dynamics of multi-kink structures are thus markedly different from the corresponding properties of a ($k = 1$) single kink.

The statistical properties of such multi-kink structures (Giachetti *et al* 1984), which are studied for the pure sine-Gordon system, give the impression that as far as the free energy is concerned the multi-kink structure appears as a relatively small perturbation to the single-kink contribution. In this respect we remark that the mean distance between two kinks can be estimated roughly using these statistical properties. However

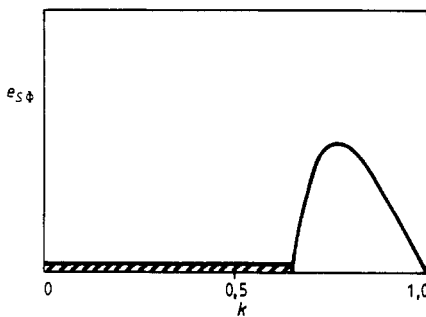


Figure 5. The eigenvalue $e_{S\Phi}$ of an exact eigenstate of $H_{S_k} H_{\Phi_k}$ is shown for $\delta = 7$ as a function of the modulus k . This eigenstate becomes the translation mode in the low density limit.

it cannot be excluded that the out-of-plane fluctuations also have a serious impact on the free energy.

It should be noted that the difference in dynamical behaviour is originated by the spatial dependence of the potential V_S (33). In the sine-Gordon system, the entire energy operator H_S (33) is a constant and then it is found that the thermodynamical properties, characterised by the kink density n_s , arising from the so-called ideal gas picture and those arising from a strongly correlated multi-kink picture (Hammer and Shrauner 1984, Giachetti *et al* 1984) are strikingly similar. As pointed out by Giachetti *et al* (1984) the correction due to the strongly correlated structure, i.e. the finite support, is of the same order of magnitude as the next order correction (in our formulation coming from H^3 and H^4) to the ideal gas picture (Sasaki 1983, Fischer and Heber 1985). We expect that the mean distance between two kinks still can be roughly estimated by the statistical properties of the sine-Gordon system. However it cannot be excluded that the out-of-plane fluctuations also have a serious impact on the free energy.

4. Discussion and conclusions

A crucial step in our calculation is the use of the Villain-Haldane representation, which corresponds to an operator expansion of the non-polynomial Hamiltonian in powers of $[S(S+1)]$. This expansion has been criticised by Mead and Papanicolaou (1982) for the ground state: it requires more terms in a $[S(S+1)]$ expansion than in a S^2 expansion. The difference in expansion parameters is related to the representation of the spin algebra, and it is known that one has to be careful in this respect, see e.g. Lindgard and Kowalski (1976). Indeed, if one considers the generator U (5) and if one uses the proposed expansion for $S(y)$ (38) one obtains

$$U = i\sum_j p_j a_j \quad (54)$$

where

$$a_j = \int dy \varphi(y) \Psi_j^*(y). \quad (55)$$

The quantity a_j is well defined for the bound states ($j=0, 1$), but due to the fact that $\varphi(y)$ takes a value different from zero at one of the boundaries, some regularisation procedure is necessary for the infinite chain. In our calculation we formally assumed that these coefficients are well defined. If one would try to calculate the transition probability between the state with a kink and a state with no kink, the numerical value of the coefficients would play a role. In order to obtain additional insight into this aspect, we have performed the same calculation using, like Swanson (1983), the Holstein-Primakoff transformation. In this case the generator is given by

$$U = (\pi/4)\sum_n \exp(i\varphi_n) S_n^- - \exp(-i\varphi_n) S_n^+. \quad (56)$$

The results of § 2 are recovered substituting $S(S+1)$ by S^2 . This means that whatever representations one chooses, at a certain external field, it will be more favourable for the kink to have out-of-plane components different from zero. For the finite chain the boundary conditions of $\Psi_j(z)$ ensure that (55) is always defined.

Another important point in our approach is the use of the continuum approximation. This approximation is legitimate if one can show that the solutions of the difference equation (10) are analytic functions of the site number. (10) can be written as a map, which has been studied (Aubry 1984). This map has, depending on the value of m , solutions with the required properties. A full analysis and exploitation of the solutions of (10) along these lines is out of the scope of this paper, but indicates that in these matters the continuum approximation has to be handled with care.

In the assumption that the Villain representation and the continuum approximation lead to reliable results, the main conclusions can be summarised as follows.

(i) A quantum mechanical treatment of the spin chain leads via a canonical transformation to the solutions of the static sine-Gordon equation as a tool to classify the excited states of the chain.

(ii) In the transformed Hamiltonian each of the excited states acts as a vacuum containing a number of kinks with accompanying in-plane and out-of-plane fluctuations.

(iii) The propagator of the in-plane fluctuations cannot be diagonalised in the harmonic approximation. This is a consequence of the out-of-plane potential V_S , which is usually considered to be constant.

(iv) The stability limit for the low anisotropy or high field, known from the classical approach, is recovered and manifests itself now as a change in sign of the energy of the translation mode in the low density limit.

(v) For increasing density, the translation mode becomes an oscillation, which can become soft signalling a density-dependent instability.

(vi) The periodic array introduces gaps in the fluctuation spectrum at the endpoints of the Brillouin zone associated with the periodicity of the kinks.

The model, which we consider, follows directly in the Villain representation and diverges considerably from the ideal gas picture (Currie *et al* 1980) which is a many-kink model based on single-kink properties of the low density limit. In our approach the kinks are interacting: this interaction requires that a chain consists of either kinks or anti-kinks. A mixture of both in the same chain is unstable at the level of the harmonic fluctuations. It also is the interaction which requires that the kinks go on a periodic array: a chain with kinks at random positions can lower its energy by adapting the distances between the kinks. As shown by Sutherland (1973) for the sine-Gordon model the cross section between the kink and the linear excitation is also minimal in this case for periodic structures. The effect of higher-order terms H^3, H^4, \dots , is not considered for $k < 1$. In the low density limit it is shown for similar models (Wada and Schrieffer 1978, Wada and Ishuichi 1982) that the ballistic behaviour found in the harmonic approximation where the kink momentum is a constant of motion is changed in diffusive behaviour by the higher-order terms.

The statistical mechanics needed to obtain an expression of the kink density as a function of temperature is not studied in this paper. However, if we assume that the out-of-plane components have only a minor effect on this relation, the sine-Gordon calculation (Giachetti *et al* 1984) can be used. Then it can be concluded that the kink density for a periodic structure as a function of temperature is very similar to the analogous expression of the ideal gas model, at least for moderate kink densities. Therefore it will be very difficult to make a distinction between a model in which kinks behave as if they are quasi-free or a model in which they are confined to a periodic array on the basis of the kink density only, because this quantity seems quite insensitive to the choice of the model.

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Appendix 1

The question of what happens when δ is almost equal or a little bit smaller than 3 will now be discussed. With one kink in the chain our analysis indicates that $S(y)$ is not zero on the average. Therefore it is better to restart the calculation, now with a more general canonical transformation that introduces a 'c number' s_j value to the j th lattice site. The generator of transformation, given in the Villain-Haldane representation, is

$$V = -i \sum_j \Phi_j s_j \quad (\text{A1.1})$$

with

$$\exp(-V) S_j^z \exp(V) = S_j^z - s_j. \quad (\text{A1.2})$$

Assuming that s_j is relatively small, we obtain to second order in s_j and in the continuum approximation the following expression for H^0 :

$$\begin{aligned} H^0 = & -N \{ JS(S+1) + g\mu_B H [S(S+1)]^{1/2} \} \\ & + JS(S+1) ma \int dy \left[\frac{1}{2} (\varphi')^2 + 2 \sin^2(\varphi/2) \right] \\ & + Jma \int dy \left[\frac{1}{2} (s')^2 + \frac{1}{2} s^2 (\cos(\varphi) - (\varphi')^2 + \delta) \right]. \end{aligned} \quad (\text{A1.3})$$

The extremalisation condition for H^0 , which is equivalent to the condition that H^1 is identically zero, is then

$$(1 - s^2) \varphi'' = \sin(\varphi) \quad (\text{A1.4})$$

and

$$-s'' + (1 - 2 \sin^2(\varphi/2) - (\varphi')^2 + \delta) s = 0. \quad (\text{A1.5})$$

Elementary bifurcation theory shows that a $s \neq 0$ solution exists for $\delta = 3$. For this value a non-trivial solution of (A1.5) is possible. The interpretation given to this phenomenon given in the semiclassical analysis is slightly different, because there s is strongly related to the classical velocity of the kink. In the quantum analysis it is found that for the one-kink system the shape of the kink has an out-of-plane component whose average is different from zero. Therefore a further analysis of the one-kink model firstly requires a precise calculation of the shape of the kink, because this shape determines the precise form of H_S and H_Φ . The spectrum of these operators will then determine the behaviour of the 'new' elementary excitations.

Appendix 2

The ground-state function of H_{Sk} can be constructed using the second derivative of

the square of the Jacobian elliptic function $\text{dn}(z)$:

$$\text{dn}^{2n}(z) = 6k^2 \text{sn}(z) \text{dn}^2(z) + (2 - 4k^2) \text{dn}^2(z) + 2(k^2 - 1). \quad (\text{A2.1})$$

Then we write

$$\Psi = N(\text{dn}^2(z) + \Omega(k)). \quad (\text{A2.2})$$

The constant $\Omega(k)$ is calculated in such a way that Ψ is an eigenfunction and N is the normalisation:

$$\Omega(k) = [(4k^4 - 13k^2 + 13)^{1/2} - 4 + 2k^2]/3. \quad (\text{A2.3})$$

This choice of Ω avoids nodes and Ψ belongs to the eigenvalue

$$\begin{aligned} & -(1/2k^2)\{\Psi'' + [k^2(1 - \delta) + 4 - 6k^2 \text{sn}^2(z)]\Psi\} \\ & = (1/2k^2)[k^2(1 - \delta) + 2 - 2(4k^4 - 13k^2 + 13)^{1/2}]\Psi. \end{aligned} \quad (\text{A2.4})$$

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