DEPARTMENT OF PHYSICS, UNIVERSITY OF JYVÄSKYLÄ
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BY
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for the Degree of
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April 1980

Preface

This work has been carried out during the years 1978-1980 at Nordita in Copenhagen, Denmark, and at the Department of Physics, University of Jyväskylä, Finland. I wish to express my thanks to these institutes for the excellent working conditions provided for me.

It is a pleasure for me to express my sincere gratitude to Professor A. Luther, who guided me into this field of research. For an especially enjoyable co-operation I am indebted to Professor R. Bullough, as well as to my other coworkers, Dr. P. Bak, Professor V. Pokrovsky and Dr. M.J. Rice. I also want to extend my thanks to the staffs of the both institutes.

I am indebted to Professor P.O. Lipas for his careful and critical reading of the manuscript. My thanks also go to Miss T. Tuominen, who carefully typed this thesis, to Mr. T. Näränen, who skillfully finished the drawing and to Mr. K. Hillebrand, M.Sc., for his help in computing.

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To my wife and daughter I owe a great depth of gratitude for their support and unfailable forbearance.

Jyväskylä, August 1980

Jussi Timonen

DYNAMICS AND STATISTICAL MECHANICS OF NON-LINEAR SYSTEMS

Abstract

The exact partition function of the sine-Gordon field is calculated. This provides a complete thermal description of the system; as an example we have calculated the thermal densities of the soliton excitations.

In the overlayers of adsorbed atoms the coupling of the displacement field of the atoms to the strain imposed on it is shown to preserve the continuous nature of the commensurate-incommensurate transition, with a shift in the transition temperature. The coupling is shown to produce a very inhomogeneous strain. The inclusion of thermal fluctuations in the transition is shown to produce a square-root dependence of the observed misfit parameters on the temperature (pressure).

It is also shown that a crystalline order is established in the commensurate phase, but there is no true long-range order in the incommensurate phase.

We present a theoretical model which predicts an insulator-to-metal transition in doped trans-polyacetylene. An inhomogeneous charge distribution in the polyacetylene fibrils with a localisation depth of 5 Å gives the experimentally observed critical dopant concentration of $y_* \approx 1$ %.

We present a thorough non-linear analysis of the one-dimensional magnetic materials $CsNiF_3$ and $(CH_3)_4NMnCl_3$ (TMMC). The neutron scattering data on $CsNiF_3$ are interpreted as the first observation of a breather soliton. We give an argument which indicates that $CsNiF_3$ is a quantum sine-Gordon system with a substantial quantum correction to the kink mass. The results are extended to TMMC.

Contents

1. INTRODUCTION

A large part of physics has traditionally been restricted to considerations only of small amplitude phenomena around the ground state of the system in question. Although some solutions to non-linear differential equations were obtained[1,2] more than a hundred years ago, as a peculiar class of particular solutions they were supposed to be a rare phenomenon. And the first observation [3] in 1834 of a non-linear water wave was not generally appreciated.

In fact, there was a generally accepted hypothesis that the presence of non-linearities in a system always leads to the sharing of the energy among all the linearized modes of the system. The failure of the attempts[4,5] to verify this hypothesis numerically in one dimension can be regarded as the starting point for the new developments in the treatment of non-linearities. The word "soliton" was introduced by Zabusky and Kruskal[5] for the particle-like solutions to the Korteweg - de Vries equation they found numerically. This work led Gardner, Greene, Kruskal and Miura[6] to the construction of the inverse scattering method for solving exactly the Korteweg - de Vries equation; later on the same method has been extended to a whole class of non-linear differential equations[7]. An important step was the discovery by Zakharov and Faddeev[8] that the spectral transform of the inverse scattering method is in fact a canonical transformation to variables of an action-angle type.

The entrance of solitons into condensed matter physics began with the work of Krumhansl and Schrieffer[9]. They introduced the idea that any (non-linear) system is to be described in terms of non-linear soliton-like excitations and ordinary small-amplitude

oscillations. These together form the non-linear "normal modes" of the system. In this connection the "soliton" is to be understood to mean a localized, finite energy solution to the equation governing the excitations of the system, with the remarkable additional property that each soliton in collision with another excitation appears to pass through it with essentially no interaction. It should be noted that soliton solutions are frequently singular points of linear perturbation theory and cannot be reached by any finite-order perturbation expansion. This fact motivated the attempts to build the non-linear modes into a starting model and only then consider small further perturbations[10].

This kind of approach has now been applied in almost every branch of condensed matter physics[11,12]. In many cases, however, non-linearities do not play any major role, and new striking phenomena are not to be expected there. Perhaps the most important results so far are the discovery of non-linear spin excitations (see section 3.3) and a kind of configurational picture[11,12] given in certain cases by the solitonic approach, and related to domain wall phenomena of various kinds (see section 3.1).

One of the major efforts has been the calculation of statistical mechanics of non-linear systems in terms of all the modes, including especially the non-linear ones[11,12]. This also forms a part of the present thesis. All the exactly soluble non-linear models except the Toda lattice are continuum models, and the statistical mechanics needed is that of non-linear classical fields. This means that we have to apply the method of functional integration. One of the questions under discussion has been how we are to include the residual interaction of the excitations of completely integrable Hamiltonian

systems found in configuration space[11,12]. We consider[13] the case of the sine-Gordon field and base our calculation on the full separability of the Hamiltonian under the spectral transform. The result is a description of the statistical mechanics of the system in terms of each mode separately, including the breather mode. This calculation is reviewed in chapter 2.

The other part of the thesis deals first with non-linear ground states in surface layers of adsorbed atoms[14,15] and in charge-density wave systems[14], and secondly with non-linear excitations in charge-density waves[16] and in quasi-one-dimensional spin systems[12,17].

In reference 14 we consider the coupling between the order parameter and elastic degrees of freedom (strain) near the commensurate-incommensurate transition. We find that the transition remains a second-order transition and that the strain follows the spatial modulation of the order parameter. In reference 15 we consider the effect of thermal fluctuations on the transition and find a square-root behaviour of the phase gradient as a function of pressure. Furthermore, we show in the appendix that a crystalline order is established in the commensurate phase, but there is no true long-range order in the incommensurate phase although large regions of a regular "soliton lattice" nature can occur near the transition. "Soliton lattice" means here a succession of one type of domain wall. These results form the contents of section 3.1.

In reference 16 we present a model of the insulator-to-metal transition in doped polyacetylene. The extra charge carriers are assumed to go into localized states at the centre of the band gap; these states accompany local soliton-like deformations in the dimerized ground state of the polyacetylene chains. We find that the transition

is driven by an overlapping of these localized states. We also stress the likelihood of the inhomogeneous charge distribution in the polyacetylene fibrils. The analysis is reviewed in section 3.2.

In references 13 and 17 we consider non-linear spin excitations in the quasi-one-dimensional magnetic materials $CsNiF_3$ and $(CH_3)_4NMnCl_3$ (TMMC). We first justify, in the classical and continuum limits, the transformation of the appropriate spin Hamiltonian to a sine-Gordon form. We then calculate the dynamic correlation function for non-linear excitations of each kind including the breather excitation, and compare the results with the existing neutron scattering data on $CsNiF_3$. We find that $CsNiF_3$ cannot be considered as a pure classical sine-Gordon system within the current interpretation of the experimental data. If there is a restriction on the largest breather sizes, breather contributions explain almost all of the available data. We also evaluate the quantum corrections to the energies of the excitations, find them sizable and discuss their effects on the observable properties. We stress the need for a quantal analysis of the system. We also show the results of a similar kind of analysis of the TMMC compound and comment some qualitative features which should be found in the planned neutron-scattering experiments. The review of this part of the work is presented in section 3.3.

The thesis is based mainly on the new results presented in the appendix and the publications referred to above, and these are the following:

13) J. Timonen and R.K. Bullough

Solitons in physics: an application to spin waves in the one-dimensional ferromagnet $CsNiF_3$

to appear in Rencontre Interdisciplinaire des Problèmes Inverses, ed. P.C. Sabatier (Edition du Centre National de La Recherche Scientifique, Paris 1980)

14) Per Bak and Jussi Timonen

Coupling between phase solitons and strain near the commensurate-incommensurate transition

J. Phys. C 11 (1978) 4901

https://doi.org/10.1088/0022-3719/11/24/019

15) A. Luther, J. Timonen and V. Pokrovsky

Domain walls and the commensurate phase

in Phase Transitions in Surface Films, eds. J.G. Dash and J. Ruvalds (Plenum Publ. Corp., New York 1980) pp. 115-126

https://doi.org/10.1007/978-1-4613-3057-8_4

16) M.J. Rice and J. Timonen

Insulator-to-metal transition in doped polyacetylene

Phys. Lett. 73A (1979) 368

https://doi.org/10.1016/0375-9601(79)90563-2

17) J. Timonen and R.K. Bullough

Breather contributions to the dynamical form factors of the sine-Gordon systems $CsNiF_3$ and $(CH_3)_4NMnCl_3$ (TMMC)

Dept. of Physics, University of Jyväskylä, Research Report No. 9/1980, and to be published

https://doi.org/10.1016/0375-9601(81)90116-X

2. STATISTICAL MECHANICS OF THE SINE-GORDON FIELD

In dimensionless units the sine-Gordon field is described by the Hamiltonian

$$H = \gamma_0^{-1} \int \left[\frac{1}{2} \phi_x^{\,2} + \frac{1}{2} \phi_t^{\,2} + m^2(1 - \cos\phi) \right] dx, \tag{2.1}$$

where γ_0 is the coupling constant and m is the elementary mass. By ϕ_x we mean $\phi_x \equiv \frac{\partial \phi}{\partial x}$. The elementary excitations of this system are governed by the sine-Gordon equation

$$\phi_{xx} - \phi_{tt} = m^2 \sin\phi \,. \tag{2.2}$$

These are therefore[18] the kinks, antikinks, breathers and oscillatory wave, that is phonon-like, modes of this equation. Each of them has the soliton property: a solitary wave in collision with another appears to pass through it with essentially no interaction. A single kink solution describes a localized change of the field from zero to 2π ($2\pi \to 0$ for an antikink), and in the rest frame a single breather solution behaves like a standing wave modulated in space by a hyperbolic-secant envelope.

In thermal equilibrium kinks must be excited across the energy gap $M = 8m\gamma_0^{-1}$, but breathers of low enough energy in the breather band $0 \leq M_b \leq 2M$ can always be excited.

As Feynman first showed[19], the partition function Z can be expressed as a functional integral over the field. In the classical limit we get

$$Z = N \int \mathcal{D}\phi e^{-\beta H[\phi,\phi_x]}, \qquad (2.3)$$

where N is a normalising factor, $\mathcal{D}\phi$ is a formal notation for functional integration and $H[\phi,\phi_x]$ is given by eq. (2.1) without the time derivative. This integral can be calculated by the transfer integral technique[20] or by a perturbation expansion[21]. The weakness of the former method is the fact that it does not separate the contributions of the various modes. When calculating observable quantities like correlation functions we would like to know the thermal density of each mode separately[13]. The latter method is quite cumbersome and its use is limited to the simplest kinds of excitation and to low temperature expansions.

For the evaluation of the partition function we suggest the following procedure, which is efficient within the whole class of completely integrable Hamiltonian systems. We start with the Hamiltonian form[22] for the propagator G,

$$G(y,y_0:t) = \int_{\phi=y_0}^{\phi=y} \mathcal{D}p\,\mathcal{D}\phi \exp\left\{\frac{i}{\hbar}\int_0^t \left[p\dot{\phi} - H[p,\phi]\right] dt'\right\}, \qquad (2.4)$$

which we have written in the single-particle case for notational simplicity; p is the momentum conjugate to ϕ. The integral in the exponent in (2.4) is recognised as the classical action. It is easy to show by an integration over p that this propagator takes the familiar Feynman form when the Hamiltonian is quadratic in the momentum variable, $H = p^2/2m + V(\phi)$. The partition function of the system described by H can be calculated in the usual way:

$$Z = \mathrm{Tr}\ \bar{G}(y,y_0) = \int_{-\infty}^{\infty} dy\ \bar{G}(y,y) \ ,$$

$$\bar{G}(y,y_0) = \int\int_{\phi=y_0}^{\phi=y} \mathcal{D}p\mathcal{D}\phi \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} [H[p,\phi] - ip\dot{\phi}]\, d\tau\right\}. \qquad (2.5)$$

We are interested in the classical partition function, i.e. the limit of vanishing $\hbar$. In this limit the "time" derivative $\dot{\phi}$ in eq. (2.5) vanishes because in the partition function we integrate over closed paths, $\phi(\beta\hbar) = \phi(0)$. Therefore, the classical partition function is

$$Z = \int\int \mathcal{D}p\mathcal{D}\phi\, e^{-\beta H[p,\phi]} \ , \qquad (2.6)$$

which is intuitively an evident result. In the case of the sine-Gordon field the Hamiltonian $H[p,\phi]$ is given by eq. (2.1) when ϕ_t is replaced by p.

The form (2.6) for the partition function is attractive because it deals with canonical invariants. A canonical transformation leaves the phase space invariant, and if it provides a diagonalisation of the Hamiltonian the integrals in eq. (2.6) are greatly simplified. The spectral transform of the inverse scattering method provides[7,18] a canonical transformation which diagonalises the sine-Gordon Hamiltonian (2.1), and its diagonal form is

$$H = \sum_{i=1}^{K} (M^2 + p_i^2)^{\frac{1}{2}} + \sum_{i=1}^{\bar{K}} (M^2 + p_i^2)^{\frac{1}{2}} + \sum_{j=1}^{K_b} (4M^2\sin^2\theta_j + p_j^2)^{\frac{1}{2}} +$$

$$+ \int_0^{\infty} (m^2 + p^2)^{\frac{1}{2}}\, \rho(p)dp \ , \qquad (2.7)$$

where M is the kink mass $M = 8\gamma_0^{-1}m$, and K, $\bar{K}$, and K_b are the numbers of kinks, antikinks and breathers, respectively; the continuous part of the spectrum describes the small oscillations of the field. Only momenta appear in the Hamiltonian (2.7) which is thus in the action-angle form. Notice that the momentum density $\rho(p)$ of the small oscillations appears as a canonical momentum, and the momentum $4\gamma_0^{-1}\theta_j$ is related to the internal oscillation of the breather. The phase spaces are $\mathbb{R} \times \mathbb{R}$ for the kinks, antikinks and the centre-of-mass motions of the breathers, $[0,2\pi]\times[0,\infty)$ for the small oscillations, and $[0,8\pi]\times[0,2\pi\gamma_0^{-1}]$ for the internal oscillations of the breathers.

Because of the canonically invariant nature of eq. (2.6) we can calculate the partition function of the sine-Gordon field starting from the Hamiltonian (2.7), which provides a natural definition for a canonical ensemble that can then be extended to a grand canonical one. A corresponding definition is not possible in the case of the original Hamiltonian (2.1), and this fact actually plagues all the transfer integral calculations[20] based on it. Another thing worth noting here is the definition of an elementary excitation in the two cases. For example, single kink solutions are elementary excitations in the configuration space of the Hamiltonian (2.1). They do not belong to the diagonal states of the system and feel a residual interaction which appears[7,18,24] as phase shifts in mutual collisions. However, these phase shifts are built into the excitations of the diagonal Hamiltonian (2.7), and in this sense its excitations are different from the single-soliton states of eq. (2.1). The thermal properties of a system should not, of course, depend on the definition of the elementary excitations.

The partition function of a canonical ensemble is thus

$$Z = \int\int \mathcal{D}\rho\,\mathcal{D}Q \prod_{i=1}^{K} \frac{dp_i dq_i}{} \prod_{i=1}^{\bar{K}} \frac{dp_i dq_i}{2\pi} \prod_{j=1}^{K_b} \frac{dp_j dq_j d\theta_j d\Phi_j}{\pi^2 \gamma_0}\, e^{-\beta H} \quad , \tag{2.8}$$

in which H is given by eq. (2.7), and variables occur in canonically conjugated pairs. This factorizes into

$$Z = Z_{ph} Z_k Z_{\bar{k}} Z_b \quad , \tag{2.9}$$

where we have separate contributions from "phonons", kinks, antikinks and breathers. Each of these can be calculated exactly in the sense of functional integration.

We first calculate the soliton parts of the partition function. Since the Hamiltonian (2.7) depends only on the momenta, we can integrate immediately over the coordinates q_i, each of which gives a factor L, the length of the system, and L is infinite. We assume here that it is sufficient to carry the factors L in a formal way and scale them out at the end to find thermodynamic quantities as densities. We finally calculate the partition function of the grand canonical ensemble, where

$$Z_{k_j} = \sum_{K_i=0}^{\infty} \frac{1}{K_i!}\, e^{\beta \mu_{k_j} K_i}\, Z_{k_j}(K_i) \quad , \tag{2.10}$$

and find for the kinks (antikinks) and breathers

$$Z_k = \exp\left\{ e^{\beta \mu_k} LM\pi^{-1} K_1(M\beta) \right\} \quad , \tag{2.11a}$$

$$Z_b = \exp\{ e^{\beta\mu_b}\, 8LM\gamma_0^{-1} \left[I_0(M\beta)K_1(M\beta) - I_1(M\beta)K_0(M\beta) \right] \} , \qquad (2.11b)$$

where I_ν and K_ν denote modified Bessel functions[23], and the expression for $Z_{\bar{k}}$ is identical with eq. (2.11a).

Every thermal quantity associated with soliton excitations can now be calculated from the partition function (2.9) by using equations (2.11). In many applications the quantity of special interest is the density of each thermally excited species. The equilibrium densities n(T) per unit length are given by

$$n(T) = L^{-1} \frac{\partial}{\partial\mu} \left(\frac{\ln Z}{\beta}\right)_{\mu=0} . \qquad (2.12)$$

Thus we easily find

$$n_k(T) = n_{\bar{k}}(T) = \pi^{-1} M\, K_1(M\beta) \underset{\beta\to\infty}{\longrightarrow} \frac{M}{2\pi} \sqrt{\frac{2\pi}{M\beta}}\, e^{-M\beta} , \qquad (2.13a)$$

$$n_b(T) = 8M\gamma_0^{-1} \left[I_0(M\beta)K_1(M\beta) - I_1(M\beta)K_0(M\beta) \right]$$

$$\underset{\beta\to\infty}{\longrightarrow} 4M\gamma_0^{-1}(M\beta)^{-2} , \qquad (2.13b)$$

The "phonon" contribution to the partition function is

$$Z_{ph} = \int\!\!\int \mathcal{D}\rho\, \mathcal{D}Q\, \exp\{ -\beta \int_0^\infty (m^2 + p^2)\rho(p)\rho(p)dp \} . \qquad (2.14)$$

For this we find

$$Z_{ph} = \lim_{n\to\infty} (L/\pi\beta)^n (n!)^{-1} \left[mL/\sinh(mL) \right]^{1/2} , \qquad (2.15)$$

where L is again the length of the system. We have obtained exactly the same result for a field of harmonic oscillators described by the Hamiltonian

$$H = \frac{1}{2} \int_{-\infty}^{\infty} [\phi_x^2 + p^2 + m^2\phi^2] \, dx. \tag{2.16}$$

To be consistent with the results based on the spectral transform, which in the case of linear systems is reduced to an ordinary Fourier transform, we have used the Fourier transformed form of eq. (2.16):

$$H = \frac{1}{2} \int_{-\infty}^{\infty} [(k^2 + m^2)\tilde{\phi}^2 + \tilde{p}^2] \, dk. \tag{2.17}$$

When the system is made discrete and finite the number of available modes is of course limited. We can take this fact into account in eq. (2.15), but in the limit $n \to \infty$ there is no effect from this limitation.

When the system is quantised the only effect on the kinks is a mass renormalisation[24]. The kink density (2.11a) should thus be satisfactory even when quantum effects are important. This seems indeed to be the case[25]. Breathers and "phonons" are, however, greatly modified when the system is quantised. The phase space available for the internal oscillation mode of the breather is compact, and this produces a discrete breather band[24]. Furthermore, the role of quantised phonons is taken over by the lowest-lying breather in the breather band[24], which has the same mass m as the phonons. Considerable changes in the thermal behaviour of the system are thus expected when the temperature approaches the value mk_B^{-1}.

Perhaps the most important conclusion from the classical densities (2.13) is that unless there is strong damping present[10], the breather

density is actually much higher than the kink density at low enough temperatures. This is a feature which should be appreciated in every case where sine-Gordon like elementary excitations can be expected to contribute to the observable properties.

The method applied here to the sine-Gordon field can easily be extended to the whole class of non-linear fields which can be diagonalised via the spectral transform. Essentially the only defect of the method is that a functional integral can only be defined as a limit of a discrete (multi-dimensional) integral; and so far it has not been proved that the diagonal form (2.7) of the sine-Gordon Hamiltonian is valid also in the discretised version of the system. The Toda lattice is the only discrete system which is known to have a spectral transform. A continuum limit of the Toda lattice is the Korteweg - de Vries field which belongs to the class of exactly soluble models, too. This pair of systems can thus be used for testing the effects of discretisation, and this analysis we hope to provide shortly.

3. APPEARANCE OF NON-LINEAR FEATURES IN PHYSICAL SYSTEMS

As was pointed out already in the introduction, there is a wealth of applications of the non-linear methods to physical systems[11]. The range of applications is, however, limited to systems which can be considered as one- or two-dimensional, and even the truly two-dimesional systems have offered severe difficulties. The reason for this lies in the fact that the systematic method for treating genuinely non-linear solutions has so far been limited to one space dimension only[7]. There are computer solutions and some special solutions to non-linear equations in more than one space dimension[11], and these show that similar kinds of mode appear also in higher dimensions. In the absence of systematic method it is, nevertheless, quite difficult to find the line of generalisation. Furthermore, it is apparent that effects of non-linearities are most striking in one-dimensional systems.

A further limitation is the field nature of the soluble models. We have to work in the continuum approximation, thus neglecting the short-wave-length phenomena. For other reasons too, as indicated in chapter 2, it would be desirable to find spectral transforms for the discretised versions of the models. The Hamiltonians used for describing various physical systems must be considered as being of a phenomenological nature, but nevertheless it is possible[12,17] to compare the theoretical results for spin excitations with the experimental observations in great detail and essentially without any adjustable parameters.

3.1. The commensurate-incommensurate transition

Many physical systems undergo transformations to periodic ordered phases which are incommensurate with the underlying lattices, i.e. the wave vectors describing the modulation cannot be formed by simple rational fractions of the reciprocal lattice vectors. The incommesurate structure may be a condensed charge-density wave (CDW), a static distortion or even a separate atomic lattice[25]. The periodic potential of the underlying lattice causes complicated non-linear distortions of the condensed wave and may eventually drive a separate phase transition where the ordered phase becomes commensurate with the lattice. Physically, the "lock in" at the commensurate wave vector is a consequence of the competition between local "Umklapp" terms in the Hamiltonian, which favour the commensurate phase, and the remaining terms which must favour a wave vector slightly different from the commensurate one.

McMillan[26] has devised a Landau-Ginzburg type of phenomenological theory to describe the observed commensurate-incommensurate (C-I) transition in charge-density wave systems. He showed that the change in the electron density of the disordered phase can be taken as the real part of the order parameter. He further assumed that the absolute value of the order parameter is almost constant near the transition and allowed changes only in the phase of the order parameter. Physically this means that a change in the amplitude of the charge-density modulation costs much more energy than a change in its wave vector.

As a result of a numerical minimisation of the free energy the theory predicts that the incommensurate phase near the phase transition

consists of regions which are almost commensurate with the underlying lattice, separated by relatively narrow domain walls or "discommensurations" where the phase of the commensurate ordering changes rapidly.

The theory was subsequently analysed by Bak and Emery[27], who found that the discommensurations in fact appear as the solutions of the sine-Gordon equation, i.e. as solitons. Furthermore, the density of solitons may now serve as the order parameter of the transition, and this goes smoothly to zero in the transition which is thus of second order. Later on Bruce et al.[28] considered the coupling of the phase order parameter to a uniform strain in the case of one-dimensional modulation. They found that such a coupling will necessarily drive the transition first order.

We consider[14] the coupling when the strain is allowed to change in space and find that the strain is actually of a very inhomogeneous nature and the transition remains of second order. Our starting point is McMillan's free-energy density

$$F(x) = \frac{1}{2}(\phi_x - q_0)^2 - V[\cos(p\phi) - 1] - \frac{1}{2} q_0^2 , \qquad (3.1)$$

where q_0 is the incommensurate wave vector, V the strength of the "commensurable potential", p the degree of commensurability, and $\phi = \phi(x)$ is the phase of the order parameter. The strain η is coupled linearly[28] to the phase giving rise to additional terms in the free-energy density

$$F_\eta(x) = w\eta\phi_x + \frac{1}{2} c\eta^2 + \frac{1}{2} d\eta_x^2 , \qquad (3.2)$$

where $\eta = \eta(x)$ and w and c are parameters depending on the elastic constants of the system.

Minimisation of the resulting total free energy

$$F = \frac{1}{L} \int_{-L/2}^{L/2} F(x)dx \ , \tag{3.3a}$$

where

$$F(x) = \frac{1}{2} (\phi' - q_0)^2 + V[\phi] - \frac{1}{2} q_0^2 + w\eta\phi' + \frac{1}{2} c\eta^2 \ ,$$

$$V[\phi] = V[1 - \cos(p\phi)] \ , \tag{3.3b}$$

leads to coupled non-linear differential equations which cannot be solved exactly. We therefore approximate the potential $V[\phi]$ by a periodic parabolic potential

$$V[\phi] = \frac{1}{2} vp^2\phi^2(x) \equiv \frac{1}{2} r\phi^2(x) \ , \quad -\pi/p \leq \phi < \pi/p \ ,$$

$$V[\phi + \frac{2\pi}{p}] = V[\phi] \ , \tag{3.4}$$

which allows an exact solution. This approximation does not change the physical picture because it provides the same answer to the non-coupled problem as the original sine-Gordon potential. Furthermore, the actual form of the periodic potential imposed on the system by the underlying lattice is not known; the cosine potential of eq. (3.3b) can be considered as the first term in the Fourier series of that potential.

With this potential the Euler equations determining the extrema of the free energy functional are

$$\phi''(x) - r\phi(x) + w\eta'(x) = 0$$
$$d\eta''(x) - c\eta(x) - w\phi'(x) = 0. \tag{3.5}$$

When the condition $w < |\sqrt{c} - \sqrt{rd}|$ is satisfied, these equations have the solutions

$$\phi(x) = A \sinh(\kappa x), \quad -L/2 \leq x < L/2 ,$$

$$\phi(x + L) = \phi(x) + 2\pi/p ;$$

$$\eta(x) = B \cosh(\kappa x), \quad -L/2 \leq x < L/2 ,$$

$$\eta(x + L) = \eta(x) , \tag{3.6}$$

where

$$\kappa^2 = \frac{1}{2d} \{c + rd - w^2 - [(c + rd - w^2)^2 - 4rdc]^{1/2} ,$$

$$A = \pi/p \sinh(\kappa L/2) ,$$

$$B = Aw\kappa / (d\kappa^2 - c) . \tag{3.7}$$

The solutions (3.6) describe a soliton lattice formed by the phase $\phi(x)$ and an accompanying strain field $\eta(x)$ which also forms a soliton-like pattern peaked at $x = \pm L/2, \pm 3L/2, \ldots$ where the gradient of $\phi(x)$ is largest. The strain is thus of very inhomogeneous nature and follows the changes in the phase $\phi(x)$. The length L gives the spacing of the soliton lattice and κ^{-1} is the width of each soliton.

When the condition for w is not satisfied, i.e. the coupling to the strain is strong, there is no solution of the form (3.6), and this we interpret to mean that the phase soliton picture breaks down.

When the solutions (3.6) are substituted back in eq. (3.3) we find the free energy as a function of the average soliton density $\bar{q} = 2\pi/pL$:

$$F = (\pi u/2p\kappa)\bar{q}\,[1 + 2\exp(-2\pi\kappa/p\bar{q})] - q_0\bar{q}\ , \qquad (3.8)$$

where $u = r + d\,(\kappa B/A)^2$. Soliton density can be taken as the order parameter and its value is found by minimising the free energy (3.8). As a result we find

$$\bar{q} = \begin{cases} 0, & q_0 \leq Q \\ b\left[\ln\left(\dfrac{2Q}{q_0 - Q}\right)\right]^{-1}, & q_0 > Q\ , \end{cases} \qquad (3.9)$$

where $Q = \pi u/2p\kappa$ and $b = 2\pi\kappa/p$. There follows a transition from a commensurate ($\bar{q} = 0$) to an incommesurate ($\bar{q} \neq 0$) phase. The transition pressure (temperature) is given by $q_0 = Q$ where q_0 is the experimentally varied quantity. In the transition $\bar{q}$ goes smoothly to zero and the transition, therefore, remains of second order. The only effect of the coupling is to change the transition pressure (temperature) and the soliton width κ^{-1}.

$\bar{q}$ describes the average wave vector of the incommesurate phase, which is observed, for example, in a neutron scattering experiment. Since thermal fluctuations will modify the behaviour, the prediction given by eq. (3.9) is not expected to be exact. The main result, however, i.e. the behaviour of the system is not changed due to not too strong a coupling to the strain, is not affected by the inclusion of fluctuations. One reservation we have to make; a transverse strain component is not allowed to change in the modulation direction and coupling to this will cause a first order transition as predicted by Bruce and Cowley[28]. If we include transverse strain components, however, we should make a proper two-dimensional analysis, and this is

still to be done.

As a further result we can calculate the macroscopic measurable strain $\bar{\eta}$:

$$\bar{\eta} = \frac{1}{L} \int_{-L/2}^{L/2} \eta(x)dx \simeq (B/\kappa A)\bar{q}. \tag{3.10}$$

The macroscopic strain is thus proportional to the soliton density, and in principle this result makes it possible to measure soliton density by a measuring stick.

In ref. 15 the non-coupled problem is extended to the case where the other dimension of the overlayer is also included and thermal fluctuations around the ground state are allowed. The free energy is given now by

$$F[\phi] = \frac{1}{2} \int d^{2}\vec{r}\, [\mu\,(\phi_x - q_0)^2 + \mu\phi_y^{\,2} - 2V\cos\phi\,], \tag{3.11a}$$

describing one-dimensionally modulated displacements of the adatoms; μ is an elastic constant.

It is well known[29] that the thermodynamic free energy

$$\bar{F} = -\beta^{-1} \ln\left\{ \int \mathcal{D}\phi\, e^{-\beta F_c[\phi]} \right\}, \tag{3.11b}$$

where $F_c[\phi]$ is given by eq. (3.11) with $q_0 = 0$, is equal to the ground state energy of the quantum sine-Gordon Hamiltonian, provided that the coupling constant of the latter problem is chosen to be an appropriate function of the temperature appearing in eq. (3.12). Furthermore, the correlation functions of the two problems are also equivalent with the

identification $t \leftrightarrow iy$. The time evolution in the quantum problem thus produces the other dimension in the classical problem, and the one-dimensional quantum fluctuations correspond to the two-dimensional phase fluctuations.

Now we have the extra factor q_0, but it is easily seen to multiply a quantity which gives the soliton density in the system, and thus plays the role of chemical potential. This property is carried over to the quantum version of the problem which is described by the Hamiltonian

$$H = \frac{1}{2} \int dx \left[(\bar{\phi}_x - q_0)^2 + \Pi^2 - 2V \cos(g\bar{\phi}) \right] , \qquad (3.12)$$

in which $\bar{\phi}$ and Π are canonical variables, and $g = (k_B T/\mu)^{1/2}$.

The quantum sine-Gordon problem can again be mapped[30] onto the massive Luttinger model which is a one-dimensional fermion problem. The transformation formulas are given by eq. (A.9) in the appendix. The fermion problem can be solved exactly only with a single value $g^2 = 4\pi$ of the coupling constant[30], corresponding to a fixed temperature in the original problem. At that special temperature the fermions are not interacting and the eigenvalue spectrum is easily found; it consists of two bands separated by a gap V (see appendix). In the ground state the "valence" band is completely filled and the "conduction" band is empty. It is easy to show that the chemical potential of the quantum sine-Gordon Hamiltonian (3.12) is mapped onto the chemical potential of the fermion problem within a constant multiplying factor.

This formulation of the problem allows a pictorial description of the C-I transition. The average soliton density can again be taken as the order parameter, i.e. the average fermion density above the filled valence band. The quantity q_0 is the one which is varied in the experiments by changing the pressure of the gas providing the adatoms of the overlayer, and this corresponds to changing the chemical potential in the fermion problem. When the pressure is increased nothing happens, i.e. the system remains in the commensurate phase, until the chemical potential reaches the edge of the conduction band. At this value fermions begin to appear in the conduction band and the system goes into the commensurate phase. Furthermore, the density of states has a square-root singularity at the band edge in the one-dimensional fermion problem, and this integrates to a square-root behaviour of the fermion density. This is the experimentally observed quantity, so we expect the kind of behaviour

$$\bar{q} \text{ (observed)} \begin{cases} = 0, & q_0 \leq V \\ \propto (\bar{q}_0^2 - V^2)^{\frac{1}{2}}, & \bar{q}_0 > V \end{cases} \qquad (3.13)$$

where $\bar{q}_0 = (\pi/2)^{1/2} q_0$. This kind of behaviour is actually observed, and the observed power law[31] is not too far from 0,5.

Above the special temperature $T_c = 4\pi\mu k_B^{-1}$ at which the problem was solved, the fermion problem cannot be solved exactly, but we can argue that the behaviour is qualitatively similar because the excitation spectrum of the sine-Gordon version of the problem is known to be the same. The value of the gap is naturally changed, and it has been shown[30] to be proportional to $V^{1/(2-g^2/4\pi)}$. This argument holds until we reach the temperature $T_A = 2T_c$ ($g^2 = 8\pi$), which is a singular point of the sine-Gordon theory[30,32]. Above this temperature only the

commensurate phase is possible.

We have also shown that if we consider the two-dimensionally modulated overlayer in the case of a rectangular lattice, the two displacement fields decouple in the approximation used, i.e. we take into account only the first component from the Fourier series of the periodic potential imposed on the overlayer by the underlying lattice (cosine potential). The same analysis can now be made of the two fields separately.

The method described above can be used for calculating other quantities of interest, too. We have calculated in the appendix the phase-phase correlation function

$$G(x,y) = \langle [\phi(x,y) - \phi(0,0)]^2 \rangle . \tag{3.14}$$

In the commensurate phase ($q_0 \leq V$) this is shown to approach a constant at large distances, which means[33] that a crystalline order is established. In the incommensurate phase near the transition, the correlation function behaves in the direction of the modulation as

$$G(x,0) - G_c(x,0) \sim \begin{cases} \bar{q}^2 x^2, & x << \bar{q}^{-1} \\ \ln(2\bar{q}x), & x >> \bar{q}^{-1} \end{cases} \tag{3.15}$$

where $\bar{q}$ is given by eq. (3.13) and G_c is the corresponding expression in the commensurate phase. This result tells us that, first of all, at very small distances comparable to V^{-1}, the incommesurate correlation cannot be distinguished from the commensurate one. At distances $x \lesssim \bar{q}$ there is a distinguishable ingredient which can be recognised as representing a regular soliton lattice, which is the ground state given by mean field theories. Near the C-I transition, $\bar{q} << 1$, the range of

regularity is quite large. The logarithmic behaviour at large enough distances shows[33] that there is no true long-range order, however.

3.2. Insulator-to-metal transition in doped polyacetylene

Polyacetylene is a simple linear conjugated polymer with a simple chain structure. The thermodynamically stable trans configuration is a dimerized structure consisting of alternating single and double bonds. Because of the possibility of two degenerate structures, which transform to each other by interchanging the single and double bonds, one expects the appearance of domain wall kinds of excitation separating these types of structures. Excitations of this kind were suggested to explain the results of spin resonance experiments[34] in the undoped polymer.

Recent experiments[35] have demonstrated that doping with various acceptor and donor species is possible in a wide range while controlling the electrical properties of the polyacetylene samples at the same time. Measurements in lightly doped samples[36] led to the suggestion that doping may proceed through formation of charged domain walls. Subsequent phenomenological calculations[37,38] showed indeed that it is energetically more favourable for an extra electron or hole to go into the localized state at the centre of the band gap produced by the domain-wall distortion than into the available π-electron band states.

The experiments on polyacetylene films[35] also revealed that when these films are doped, an insulator-to-metal transition occurs at

dopant concentrations $y \approx 1$ %. We have extended[16] the idea of charged-domain-wall formation under doping to take into account an arbitrary number of carriers. We base our model on two assumptions:

(1) Slowly varying spatial and temporal deformations in the amplitude u(x) of the bond alternation are governed by the classical Lagrangian density

$$L(x) = \text{const.} + C\left[\frac{1}{2}u_t^2 - \frac{1}{2}c_0^2 u_x^2 - \frac{1}{8}V_0\left(1 - \frac{u^2}{u_0^2}\right)^2\right], \qquad (3.16)$$

where C and V_0 are known constants depending on the parameters of the system, c_0 is the characteristic velocity, and u_0 is the uniform bond alternation amplitude of regular polyacetylene. The form of the potential is suggested by the presence of the two degenerate structures in the polyacetylene chains.

(2) In order to accommodate carriers the polyacetylene chains develop a periodic distortion in u.

Minimization of the Lagrangian leads to the equation

$$c_0^2 u_{xx} - u_{tt} + \frac{1}{2}u(1 - u^2) = 0 \qquad (3.17)$$

for the amplitude u(x). The required periodic solution to this equation is

$$u(x) = A(k)\,sn([x/\ell(k)] + x_0; k), \qquad (3.18)$$

where

$$u(k) = u_0[2k^2/(1 + k^2)]^{1/2},$$
$$\ell(k) = \ell_0[2(1 + k^2)]^{1/2}, \qquad (3.19)$$

sn(z;k) is the Jacobian elliptic sine function[23], x_0 is an arbitrary initial phase, and $\ell_0 = c_0/\omega_0$ where ω_0 is the optical phonon frequency of the system. The modulus k is fixed by the magnitude of the extra charge carrier concentration y:

$$4K(k)\left[2(1 + k^2)\right]^{1/2} = 2a/y\ell_0 \ , \tag{3.20}$$

where K(k) denotes the complete elliptic integral of the first kind[23], and a is the lattice constant.

In the limit of a vanishing carrier (dopant) concentration $y \to 0$, the single domain wall (soliton) description of refs. 37 and 38 is obtained. As y approaches the critical value $y_* = a/\sqrt{2}\pi\ell_0$, then $k \to 0$, and consequently the amplitude of the bond alternation vanishes. This means that the gap in the electron spectrum vanishes and an insulator-to-metal transition results. The transition may be viewed physically as resulting from an overlapping of localized electron states described by the solution as a "soliton lattice".

It has been estimated[37,38] that $\ell_0/a \approx 10$ for polyacetylene, and this leads to the estimate $y_* \approx 9$ % for the critical carrier concentration. The experimentally studied films of polyacetylene consist of loosely packed fibrils[36] of diameter ≈ 200 Å, and rather large dopant species adhere mainly to the surfaces of the fibrils[39]. This leads to the localization of the charge in the surface layers of the fibrils. If we take this effect into account, our estimate for y_* is in agreement with the experimentally observed value $y_* \approx 1$ % with a localization depth of ≈ 5 Å.

3.3. Non-linear spin excitations in the one-dimensional magnetic systems $CsNiF_3$ and $(CH_3)_4NMnCl_3$ (TMMC)

Some of the quasi-one-dimensional magnetic materials are considered as being among the best candidates for exhibiting soliton-like excitations. Neutron scattering experiments[40] on $CsNiF_3$ have revealed a quasi-elastic central peak which cannot be explained with linear spin waves. Mikeska[41] showed that the excitations are governed by the sine-Gordon equation (2.2) to a good approximation. Following him a number of attempts[40-44] have been made to explain the observations in terms of the kink solution to that equation. This is, however, only one of the non-linear "normal modes" which are present in a sine-Gordon system. In refs. 12 and 17 we report the results of the first throrough analysis of $CsNiF_3$ and a partial analysis of TMMC, including especially the breather excitations.

Studies[45] of $CsNiF_3$ show that it consists of ferromagnetic chains of Ni^{++} ions along the $\vec{c}$-axis of a hexagonal structure with weak antiferromagnetic coupling between the chains. Above the three-dimensional ordering temperature $T_c \approx 2.7$ K the system can be considered one-dimensional, whilst for $T \lesssim 11$ K the spins (which have $S = 1$) are nearly confined to the xy plane by a single-ion anisotropy. Thus for $T \lesssim 3$ K, and in a transverse magnetic field B, the Hamiltonian is believed to be

$$H = -J \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + A \sum_n (S_n^z)^2 - g\mu_B B \sum_n S_n^x \qquad (3.21)$$

with classical values $Jk_B^{-1} = 23.6$ K, $Ak_B^{-1} \simeq 5$ K and $g = 2.4$.

In the long-wave-length and classical limits, when $T \lesssim 11$ K, the Hamiltonian (3.21) can be linearised in $\frac{\pi}{2} - \bar{\theta}(z)$: $\bar{\theta}(na)$ measures

the deviation of the n^{th} spin from the $\vec{c}$-axis; the lattice spacing is a. The spin commutation relations imposed on (3.21) mean in the classical limit that with $\hbar = 1$ and $g\mu_B B << 2A$, the spin angles satisfy

$$\phi_t = 2AS(\frac{\pi}{2} - \bar{\theta}) \ ,$$

$$\bar{\theta}_t = c^2(2AS)^{-1} \left[-\phi_{zz} + m^2 \sin\phi\right] \ , \tag{3.22a}$$

where $c^2 = a^2S^2(2AJ)$, $m^2 = g\mu_B B/JSa^2$, and ϕ is the azimuthal spin angle. This is essentially the sine-Gordon system with momentum $\mathbb{I}$ conjugate to θ, $\mathbb{I} = a^{-1} S(\frac{\pi}{2} - \bar{\Theta})$. In units chosen so that $\hbar = c = a = 1$ we then find

$$H \approx \gamma_0^{-1} \int \left[\frac{1}{2} \phi_z^{\ 2} + \frac{1}{2} \phi_t^{\ 2} + m^2(1 - \cos\phi)\right] dz \ , \tag{3.22b}$$

in which $\gamma_0 = (2A/JS^2)^{1/2} \approx 0.65$ is a dimensionless coupling constant, $\mathbb{I} = (c\gamma_0)^{-1}\phi_t$, $\{\phi_t, \phi\} = c\gamma_0\delta(z - z')$, and the equation of motion is precisely the sine-Gordon equation with this bracket. The mass m is the mass of the linear spin waves. The energy scale is set to $(2AJS^2)^{1/2}$ ≈ 15.4 K. The spin excitations are thus given by the sine-Gordon equation (2.2) which has the kink(+) and antikink(-) solution

$$\phi(z,t) = 4\tan^{-1}\exp\left[\pm m\gamma(z - ut - z_0)\right] \tag{3.23}$$

and the breather solution

$$\phi(z,t) = 4\tan^{-1}\left\{\tan\theta \ \frac{\sin\left[\omega_b\gamma(t - uz - t_0)\right]}{\cosh\left[m\gamma \sin\theta(z - ut - z_0)\right]}\right\}; \tag{3.24}$$

$\gamma \equiv (1 - u^2)^{-1/2}$, $\omega_b = \omega_0 \cos\phi$ is the frequency of the internal oscillation of the breather, and ω_0 is the frequency m ($= mc^2\hbar^{-1}$).

In the neutron scattering experiments the measured quantity is essentially the in-plane dynamical correlation function

$$S(q,\omega) = \int dt\, dz\, e^{i(qz-\omega t)} \langle \Phi(z,t)\Phi(0,0)\rangle \ . \tag{3.25}$$

Parallel to $\vec{B}$ the component $\Phi = 1 - \cos\phi$; transverse to $\vec{B}$, $\Phi = \sin\phi$. In a dilute gas approximation, which takes for Φ the asymptotic form of the multisoliton solutions of the sine-Gordon equation, we find for the kinks and antikinks that

$$S_k^{\parallel,\perp}(q,\omega) = N' \int_{-\infty}^{\infty} dp\, e^{-\beta(p^2 + M^2)^{1/2}} \int_{-\infty}^{\infty} dt \cdot$$

$$\cdot e^{i(qu - \omega)t} \left[G_k^{\parallel,\perp}(q)\right]^2 \ , \tag{3.26}$$

in which N' is a number and $G_k^{\parallel,\perp}(q)$ is the Fourier transformation of $\Phi(z - ut)$ for a single kink (antikink) solution,

$$G_k^{\parallel}(q) = 4\pi q\left[m^2\gamma \sinh(\pi q/2m\gamma)\right]^{-1} \ , \tag{3.27}$$

and in the transverse component sinh is replaced by cosh. If parallel and transverse components are given equal weight we thus find

$$S_k(q,\omega) = N(49mq)^{-1}\ \Gamma \exp(-M\beta\Gamma)(\pi q/2m\Gamma)^2 \cdot$$

$$\cdot\left|\sinh^{-2}(\pi q/2m\Gamma) + \cosh^{-2}(\pi q/2m\Gamma)\right] \ , \tag{3.28}$$

where $\Gamma \equiv (1 - \omega^2/q^2)^{-1/2}$ and N is a number (different from N').

The "non-relativistic" approximation to (3.28) coincides with the result derived by Mikeska[41] when $\gamma_0 = 1$.

For B = 5 kG, the kink energy M ≈ 35 K and there is an energy gap, but $M_b = 2M\sin\theta$ for the breather and these can always be excited for $T \gtrsim T_c$. The internal oscillation of the breathers give more structure to $S(q,\omega)$: there is a central peak contribution overlapping the form (3.19) due to the centre-of-mass motion and additional side bands associated with each value of ω_b. Only the parallel component $S_b^{\parallel}(q,\omega)$ contains a central peak contribution. In addition to the kink and breather contributions, there are spin wave side bands which at q = 0 lie at $\pm \omega_0$.

In a dilute gas approximation we find for the breathers

$$S_b(q,\omega) = N_b \int_0^{\pi/2} d\theta \int_{-\infty}^{\infty} dp\, e^{-\beta(p^2 + 4M^2\sin^2\theta)^{1/2}} \int_{\infty}^{\infty} d\tau \cdot$$

$$\cdot e^{i(qu - \omega)\tau} \int_{-\infty}^{\infty} dz\, e^{iqz} \int_{-\infty}^{\infty} dz' \cdot$$

$$\cdot \langle \Phi_b(z + z',\, t' - t_0)\Phi_b(z',\, t - t_0)\rangle_{t_0} \,, \qquad (3.29)$$

where N_b is a number, $\tau \equiv t - t'$, $\Phi_b(x - ut,t)$ is the parallel or transverse component for the single breather solution (3.24), and $\langle\cdot\rangle_{t_0}$ means an average over the initial phase of the internal oscillation.

The parallel component is given by

$$\Phi_b^{\parallel}(x,t - t_0) = 8\tan^2\theta\, \sin^2[\gamma^{-1}\omega_b(t - t_0)] \cdot$$

$$\cdot \left\{ \frac{\cosh(\gamma m\sin\theta x)}{\tan^2\theta\, \sin^2[\gamma^{-1}\omega_b(t - t_0)] + \cosh^2(\gamma m\sin\theta x)} \right\}^2 . \qquad (3.30)$$

If the quantity inside the curly bracket in eq. (3.30) did not depend on t_0, the only factor entering the average would be $\sin^2[\gamma^{-1}\omega_b(t - t_0)]$. Since

$$\langle \sin^2[\gamma^{-1}\omega_b(t - t_0)]\, \sin^2[\gamma^{-1}\omega_b(t' - t_0)] \rangle_{t_0}$$

$$= \frac{1}{4} + \frac{1}{16}\,(e^{2i\gamma^{-1}\omega_b\tau} + \text{c.c.}) \,, \tag{3.31}$$

the result for the central peak contribution given by the term $\frac{1}{4}$ in eq. (3.31) is equivalent to replacing $\sin^2(\cdot)$ by its average of $\frac{1}{2}$. This actually applies to the whole formula (3.30) because by expanding the denominator in the curly bracket in powers of $\cos[2\gamma^{-1}\omega_b(t - t_0)]$ one will generate only further side bands labelled by $\pm 4\omega_b$, $\pm 6\omega_b$,... In the transverse component only sidebands labelled by $\pm \omega_b, \pm 3\omega_b$,... appear.

For the central peak contribution of the breathers we thus find

$$S_b(q,\omega) = N\Gamma q^{-1} \int_0^{\pi/2} d\theta \tan^4\theta (\sin\theta)^{-1} \exp(-2\beta M\Gamma \sin\theta) \cdot$$

$$\cdot \sinh^{-2}(\pi q/2m\Gamma\sin\theta)\; F^2(q,\omega) \,, \tag{3.32}$$

where

$$F(q,\omega) = 2\pi(\tan\theta)^{-1}(2 + \tan^2\theta)^{-3/2}\sin(\pi qb/m\Gamma\sin\theta) +$$

$$+ \pi q[m\Gamma \sin\theta(2 + \tan^2\theta)]^{-1} \cos(\pi qb/m\Gamma\sin\theta) \,, \tag{3.33}$$

and $b = \ln[\tan\theta + (2 + \tan^2\theta)^{1/2}] - \frac{1}{2}\ln 2$. The constant multiplicative factor N, which is the same as in eq. (3.28), is the only free parameter setting the absolute scale, which is not known anyway. The last integration left in eq. (3.32) we have done numerically. The total contribution to the central peak $S(q,\omega) = S_k(q,\omega) + S^{\parallel}_b(q,\omega)$ is found to be

totally dominated by breathers when $q \lesssim 0.05\ \pi$, and the kink and breather contributions are found to be roughly of equal weight when $0.05\ \pi \lesssim q \lesssim 0.1\ \pi$. The peak flattens quickly as q is increased. This is in agreement with the recent computer simulation results[46].

Before comparing the results with the available neutron scattering data we recall that, in a first comparison based on kinks alone[40,47], a good qualitative fit was found in all respects[40] except that the integrated intensity $I(q;T) = \int S(q,\omega)d\omega$ dropped much too rapidly[47] as a function of q (at fixed temperature and magnetic field). This is controlled by the parameter m^{-1} ($= m^{-1}c^{-1}\hbar$), the measure of the width of the kink, and the experimental curve was fitted[47] by using twice the theoretical value in the field B = 5 kG. However, the theoretical value of m is in good agreement with the spin wave data[48], and the conclusion is that the widths of the kinks are much smaller than is predicted by theory.

We have taken the theoretical value for m and fitted the results from a numerical integration of eq. (3.32) added to eq. (3.28) to all the available data[40,47]. We find the agreement actually worse than that obtained from kinks alone. An example is curve (a) of fig. 1 which shows the temperature dependence of I(q;T) for $q = 0.1\ \pi$ and B = 5 kG; the number N appearing in the formulas is scaled to the topmost experimental point. On the other hand if we retain the same theoretical value for m but fix $\sin\theta = (1 - \omega_b^2\ \omega_b^{-2})^{1/2}$ in the sech envelope of the breather (3.24) close to unity, we obtain curve (c) of fig. 1, which is in excellent agreement with the observations.

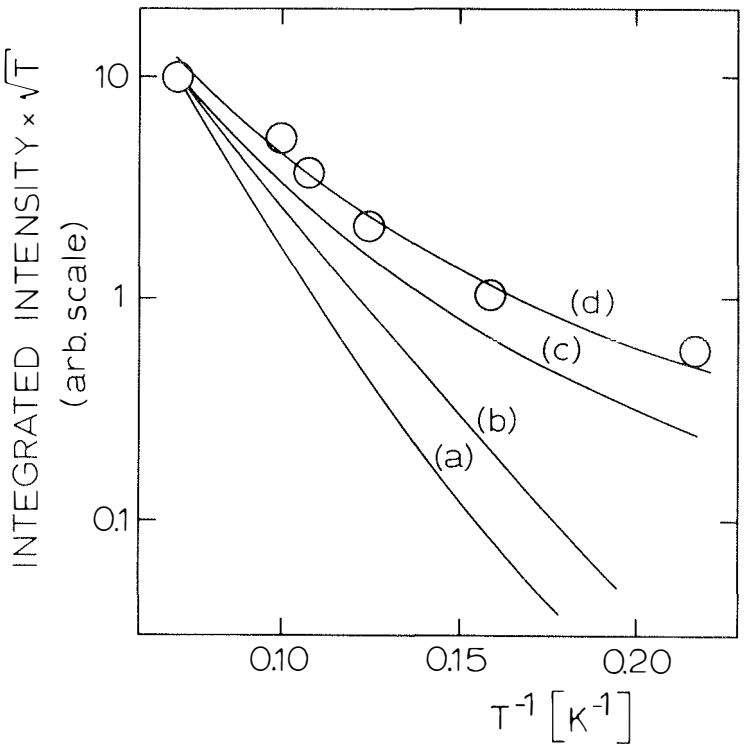

Fig. 1. Plots of $I(q;T)\sqrt{k_B T/M}$ vs. T^{-1} for $q = 0.1\,\pi$ and $B = 5$ kG. The circles are observed data due to Kjems and Steiner[40], curve (a) is the exact numerical result, curve (b) gives the kinks alone plot, curve (c) results from the approximation on widths of breathers, all scaled to the topmost experimental point, and curve (d) is the best fit given by eq. (3.34).

The approximation has the consequence of excluding the very large breathers; an equivalent natural analytical approximation enables us to derive a closed formula for $I(q;T)$ which at $q = 0.1\,\pi$ takes the form

$$I(0.1\,\pi;T) = C\left[n_k + n_{\bar{k}} + (1.2\,\gamma_0/4\sqrt{2\pi})n_b\right] , \qquad (3.34)$$

where $n_k = n_{\bar{k}}$ and n_b are the thermal densities of the kink, antikink and breather excitations given by eq. (2.11), and C is a constant. The curve (3.34) retraces curve (c) of fig. 1 when C is fitted to the topmost point, and the best fit gives curve (d) which is in exceptional agreement with the observations.

We have not made a detailed perturbation analysis of $CsNiF_3$ to find a physical mechanism for reduction of breather widths, but there is one we can think of producing this kind of effect. If we add an extra periodic potential $-\lambda\left[1 - \cos(\phi/2)\right]$ to the Hamiltonian (3.22), the oscillatory solution[49] of the resulting double sine-Gordon equation, viewed as a perturbed breather of the sine-Gordon equation, persists over a range of initial data until a maximum size is reached. Beyond this maximum initial size an unbinding into kink-antikink pairs happens. It is evident from the phase planes of the corresponding field equations that this property is not restricted to the case of double sine-Gordon, but will equally well appear for any potential $\cos(\phi/n)$, $n = 2,3,\ldots$. Interaction between adjacent chains in the hexagonal structure of $CsNiF_3$ may thus produce a reduction of maximum breather widths.

The other observational data reported[40] for the central peak are all well fitted by the approximated correlation function. But although the approximation greatly improves the fit for $I(q;T)$ against q, the predicted fall with q in the range $0.05\,\pi \leq q \leq 0.1\,\pi$ is still twice as

rapid as is observed[47]. Although a fit is possible by adjusting m we believe there must be another explanation for this anomalous behaviour. One point is the method adopted to remove the background scattering due to Cs ions[40]. This is estimated by determining the scattering for B = 30 kG and T = 3.1 K. The kink contribution is now irrelevant, but this does not remove the contribution of the Ni^{++} because breathers can still be excited. If, furthermore, the system is quantised, and we suggest below that it is, the lowest-lying breather level is greater than zero and lies at m ≈ 6.9 K. This level can be sufficiently excited at T = 3.1 K. The precise contribution of quantised breathers is still to be evaluated, but if a steeply q-dependent part is subtracted with the background a great deal of the anomaly can be removed.

In conclusion from the above analysis we can say that $CsNiF_3$ is not a pure classical sine-Gordon system. However, quantum corrections may be important to the measured function. In the following we develop an argument leading to the right quantum value of the coupling constant γ_0, and this enables us to estimate the size of quantum corrections.

It is well known[50] that the one-dimensional Heisenberg chain with single-ion anisotropy and with arbitrary spin does not have a gap in its excitation spectrum but that a gap appears when a transverse magnetic field is applied. In the $S = \frac{1}{2}$ case it has been shown[30] how the Heisenberg Hamiltonian can be mapped to a quantised free scalar field problem when the plane perpendicular to the chain direction, the xy plane, is a plane of rotational symmetry, and how an asymmetry in that plane leads to a quantised sine-Gordon type mass term. Luther and Scalapino[51] have shown that the continuum limit of the S = 1 xy Hamiltonian with single-ion anisotropy has the quantised free field as

the equation of motion. They show that in the continuum limit a set of equal time commutation relations can be assigned so that $S^x = C \cos(\sqrt{\gamma_0}\phi)$ and $S^y = C \sin(\sqrt{\gamma_0}\phi)$, where γ_0 plays the role of the coupling constant in the theory. They further show that inclusion of an interaction term which leads to the appearance of a sine-Gordon type mass term does not affect the commutation relations.

We can therefore conjecture that the S = 1 Heisenberg chain with single-ion anisotropy can be mapped to a quantum sine-Gordon problem. Notice that there is only one gap in the argument; we have not proved that adding $-J \sum_n S_n^z S_{n+1}^z$ to the xy Hamiltonian does not change the equation of motion in the continuum limit from the quantised free field equation of motion. That this is so is suggested strongly by the gapless spectrum in the Heisenberg case (the value of γ_0 will change).

The spectrum under consideration can thus be quantised by quantising the sine-Gordon Hamiltonian we got as a classical approximation. From Coleman[32] we know that for the quantised sine-Gordon system at T = 0 the correlation function is

$$\langle S^x(z,t) S^x(0,0) \rangle \propto \langle \cos\left[\sqrt{\gamma_0}\phi(z,t)\right] \cos\left[\sqrt{\gamma_0}\phi(0,0)\right] \rangle$$

$$\propto |z^2 - t^2|^{-\alpha/2} , \qquad (3.35)$$

where $\alpha = \gamma_0^2/2\pi$. Since γ_0 does not depend on the mass $m \propto B^2$, it follows that the same result must apply in the limit $B \to 0$. On the other hand, Mikeska and Patzak[52] have calculated the T = 0 quantal correlation for the Hamiltonian (3.21) with B = 0 in the form (3.35), and find the exponent

$$\alpha = \frac{\sqrt{\Delta}}{\pi\bar{S}} \left\{ 1 + \frac{1}{4\pi\bar{S}} \left[\sqrt{\Delta} + (1+\Delta)\left(\frac{\pi}{2} - \arctan\sqrt{\Delta}\right) \right] \right\}, \tag{3.36}$$

where $\Delta = A/4J$ and $\bar{S} = \left[S(S+1)\right]^{1/2}$. We can now equate this result[53] with $\gamma_0^2/2\pi$ given by the sine-Gordon theory, and we find $\gamma_0 \approx 0.48$. This has still to be renormalized[24] to get the true quantal value

$$\gamma_0' = \gamma_0(1 - \gamma_0/8\pi)^{-1} \approx 0.49 \ . \tag{3.37}$$

This is to be compared with the classical value $\gamma_0 \approx 0.65$. We note that the quantal value of the coupling constant can be achieved with the naive "quantum substitution" $S \to \left[S(S+1)\right]^{1/2}$, which gives $\gamma_0' \approx 0.47$. In this way we get the quantum corrected masses $m \approx 3.4$ K and $M \approx 57.5$ K at $B = 5$ kG, to be compared with $m \approx 2.8$ K and $M \approx 35$ K given by the classical calculation.

Unfortunately the classically found integrated intensity is quite insensitive to the actual energies[54] and it is difficult to identify observable quantum features that way. The large corrections indicate, however, that $I(T,q)$ may be considerably affected by quantum corrections. And perhaps after further analysis experiments can still be devised which probe the kink energy directly.

In conclusion we can say that a fully quantum mechanical evaluation of the dynamic correlation function is now very much needed. The quantal results may turn out to be compatible with the observations with far fewer modifications than the classical ones.

The classical analysis described above is easily extended to the TMMC compound. Its structure[45] resembles that of $CsNiF_3$, but the coupling between the chain ions (Mn^{++}) is antiferromagnetic. Thus the

Hamiltonian appropriate for TMMC is given by eq. (3.21) with a negative J. In the classical and continuum limits a partial summation over odd (even) spins reduces the Hamiltonian to the sine-Gordon form (3.22). The angle ϕ is now related to the original azimuthal spin angle ϕ' by $\phi = 2\phi' - \pi$. The coupling constant is $\gamma_0 = 4(A/J\bar{S}^2)^{1/2} \approx 1.34$ and $m = 2\mu_B B/44.5$ K; the kink mass $M = 8\gamma_0^{-1} m = 5.97$ m. The contribution to the central peak of $S(q,\omega) = S_k(q,\omega) + S_b(q,\omega)$ is

$$S_k(q,\omega) = N\Gamma(96q)^{-1} \exp(-\beta M\Gamma) \left[\cosh^{-2}(\pi q/2m\Gamma + \right.$$

$$\left. + 0.4\, m^2 q^{-2} f_1^2\right] , \qquad (3.38a)$$

$$S_b(q,\omega) = N\Gamma q^{-1} \int_0^{\pi/2} d\theta\, \tan^4\theta \left[\sin\theta\,(1 + \tan^2\theta + \frac{1}{2}\tan^4\theta)\right]^{-1} \cdot$$

$$\cdot \exp(-2\beta M\Gamma \sin\theta) \cdot f_2^2 , \qquad (3.38b)$$

where

$$f_1 = 1 - \pi q(2m\Gamma)^{-1} \left[\sinh(\pi q/2m\Gamma)\right]^{-1} , \qquad (3.39a)$$

$$f_2 = \sin(qb/m\Gamma\sin\theta) \left[\sinh(\pi q/2m\Gamma\sin\theta)\right]^{-1} , \qquad (3.39b)$$

which are to be compared with eqs. (3.28) and (3.32) where the same symbols appear. The phase shift $\pi/2$ means that the parallel and transverse components exchange their roles. A numerical analysis of eq. (3.38) shows that the width of the central peak is almost a linear function of T and q; $I(q;T)$ behaves much as for $CsNiF_3$ as a function

of T, and falls rapidly with increasing q.

Neutron scattering experiments on TMMC have been started[55] and will subsequently allow a detailed check on these various results.

4. SUMMARY AND DISCUSSION

In this thesis we have demonstrated that many physical systems display soliton-like excitations in accordance with the new[9] concept of non-linear normal modes. As the best example we can consider the quasi-one-dimensional ferromagnet $CsNiF_3$, whose neutron scattering data[40,47] we interpret as the first observation of a breather soliton. This conclusion is based on the first thorough non-linear analysis of the compound, which we have presented in refs. 13 and 17. Especially, we have made the first calculation of the breather contribution to the observable properties of the sine-Gordon systems. We have extended[17] our results to the TMMC compound, which is also a sine-Gordon system, and a more detailed account of the results will be reported later.

We briefly mention a couple of aspects of the theory which deserve further study. At higher temperatures the single-ion anisotropy is not important and, consequently, there should be a crossover to an isotropic Heisenberg chain behaviour. We can apply our method to that system, too, because a spectral transform for the classical continuous isotropic Heisenberg chain has also been found[56-60]. Secondly, we have the whole area of quantum behaviour to be explored. Unfortunately, the dynamical correlation functions of interest can be calculated exactly only with a single value of the coupling constant (see sect. 3.1 and the appendix), which allows the transformation to a non-interacting fermion problem or, equivalently, the exact summation of the perturbation expansion[61] in V. Faddeev and coworkers[62,63] have recently developed a quantum version of the inverse scattering method, and this may provide new possibilities.

In sect. 3.1 we have considered the commensurate-incommensurate (C-I) transition which occurs in overlayers of adsorbed atoms and also in charge-density wave systems. First we considered the coupling of the order parameter to the strain and showed that, if the coupling is not very strong, the transition remains of second order; only the transition temperature is changed. We also found that the strain is of a very inhomogeneous nature. A related problem was subsequently analysed by Gordon and Villain[64]. They concluded that only the longitudinal strain plays a significant role in the case of overlayers, and thus our conclusions are appropriate for these systems. The situation is different in three-dimensional charge-density wave systems, where the coupling[28] to a constant transverse strain will drive the transition in first order.

In the same section 3.1 we further considered the effect of thermal fluctuations on the C-I transition. The problem can be solved exactly at a special temperature T_c, where it is equivalent to a one-dimensional quantum problem of non-interacting fermions. We found that the transition is of second order, and the observed "misfit parameter" has a square-root behaviour near the transition. We conjectured that these results are valid in the temperature range $T_c \leq T < 2T_c$. From the behaviour of the phase-phase correlation function we further concluded that a crystalline order is established in the commensurate phase, but there is no true long-range order in the incommensurate phase; large areas of "soliton-lattice" kinds of structures can occur near the transition, though. The results were extended to the case of two-dimensional modulations on a rectangular lattice; the two displacement fields decouple in this case. Pokrovsky and Talapov[65] have considered a similar problem, but they include the possibility of different orien-

tations of the overlayer and the substrate (orientational epitaxy). They showed that an orientational order can be present also in the incommensurate phase.

The insulator-to-metal transition in the doped trans-polyacetylene was analysed in sect. 3.2. The extra charge carriers (electrons or holes) are assumed to go into localized states at the centre of the band gap. Each localized state is related to a distortion in the dimerized ground state of the chain of carbon atoms, and the dimerization amplitude is chosen to be the order parameter for the system. We showed that, if the distortions feel a "ϕ-four" potential, there follows a transition from an insulating to a metallic state at a critical dopant concentration $y_* \approx 9$ %. If we take into account the inhomogeneous charge distribution in the polyacetylene fibrils, the experimentally observed value $y_* \approx 1$ % is consistent with a charge localisation depth of 5 Å.

In chapter 2 we have considered the classical thermodynamics of the sine-Gordon field. We have used the exact diagonalisation of the sine-Gordon Hamiltonian achieved via the spectral transform of the inverse scattering method, and the partition function was calculated exactly as a functional integral. All the thermal properties can now be calculated, and we have shown the results for the thermal densities of the soliton excitations. The same method can be used to calculate the thermal properties of every member of the class of totally integrable Hamiltonian systems. It also provides a natural definition for any suitable ensemble. In contrast to this, the transfer integral technique[20] cannot specify the contributions of different modes. Furthermore, the existing transfer integral calculations use periodic boundary conditions, which are not appropriate for the spectral transform.

There is another approach[66] to the thermodynamics of non-linear fields which resembles our method, except that a part of the phonon contribution is used to "dress" the kink (breather) mass. This method makes use of periodic boundary conditions for phonons, but as we noted above, these are not appropriate for the spectral transform. If we work consistently[67] in periodic boundary conditions, the excitations are different from those used in chapter 2. The method provides agreement with the transfer integral results if the kink excitations are included, but this agreement is lost if the breather excitations are also included.

APPENDIX

Calculation of the phase-phase correlation function

$$G(x,y) = \langle [\phi(x,y) - \phi(0,0)]^2 \rangle$$

As was described in sect. 3.1, the statistical mechanics properties of the classical two-dimensional sine-Gordon problem are given by a one-dimensional fermion problem. We do not go step by step through the transformations involved, because they can be found in the literature[29,30]. We start with the fermion Hamiltonian

$$H = \sum_k \{(a^+_{1k}a_{1k} - a^+_{2k}a_{2k}) + V(a^+_{1k}a_{2k} + a^+_{2k}a_{1k})\} + \\ + q_0 \sum_k (a^+_{1k}a_{1k} + a^+_{2k}a_{2k}) , \qquad (A.1)$$

valid in the special case when the coupling constant is $g^2 = 4\pi$. Different indices are used for right (1) and left (2) going particles. With the transformation

$$a_{1k} = \cos\theta_n \, \bar{a}_{1k} - \sin\theta_k \, \bar{a}_{2k} , \\ a_{2k} = \cos\theta_n \, \bar{a}_{2k} + \sin\theta_k \, \bar{a}_{1k} , \qquad (A.2)$$

the Hamiltonian (A.1) can be diagonalized, and we find

$$\bar{H} = \sum_k E_k (\bar{a}^+_{1k}\bar{a}_{1k} - \bar{a}^+_{2k}\bar{a}_{2k}) + q_0 \sum_k (\bar{a}^+_{1k}\bar{a}_{1k} + \bar{a}^+_{2k}\bar{a}_{2k}) , \qquad (A.3)$$

where

$$E_k = k\left[1 + \left(\frac{V}{k}\right)^2\right]^{1/2} , \tag{A.4}$$

$$\tan 2\theta_k = \frac{V}{k} . \tag{A.5}$$

The equations of motion of the Hamiltonian (A.3) are easily solved:

$$\begin{aligned} \bar{a}_{1k}(t) &= \bar{a}_{1k}(0)\, e^{-i(E_k + q_0)t} , \\ \bar{a}_{2k}(t) &= \bar{a}_{2k}(0)\, e^{-i(-E_k + q_0)t} \end{aligned} \tag{A.6}$$

and corresponding results for the creation operators.

The correlation function needed is given by the corresponding correlation function of the quantum sine-Gordon system

$$G(x,t) = \langle\left[\phi(x,t) - \phi(0,0)\right]^2\rangle , \tag{A.7}$$

and the essential quantity to be calculated is

$$\Gamma(x,t) = \langle\phi(x,t)\phi(0,0)\rangle . \tag{A.8}$$

The transformation from the quantum sine-Gordon field to the fermion problem is given by

$$\begin{aligned} \phi(x,t) &= -i\,\frac{\sqrt{\pi}}{L}\sum_k \frac{1}{k}\, e^{-ikx}\left[\rho_1(k) + \rho_2(k)\right] , \\ \Pi(x,t) &= \frac{\sqrt{\pi}}{L}\sum_k e^{-ikx}\left[\rho_1(k) - \rho_2(k)\right] , \\ \rho_j(k) &= \frac{1}{\sqrt{2}}\sum_p a^{+}_{jk+p} a_{jp} , \end{aligned} \tag{A.9}$$

where L is the length of the system; we have left out the cutoff which is necessary for the convergence of the Fourier transformation. Under this transformation the correlation function $\Gamma(x,t)$ is transformed to

$$\Gamma(x,t) = \frac{\pi}{2L^2} \sum_k \frac{1}{k^2} e^{-ikx} \chi(k,t) \quad , \tag{A.10}$$

where

$$\chi(k,t) = \langle [\rho_1(k,t) + \rho_2(k,t)] [\rho_1(-k,0) + \rho_2(-k,0)] \rangle$$

$$= \sum_{p=\bar{q}}^{\bar{q}-k} d_1(k,p)\, e^{i(E_{k+p} - E_p)t} + \sum_{p=-\bar{q}-k}^{-\bar{q}} d_1(k,p)\, e^{-i(E_{k+p}-E_p)t}$$

$$+ \sum_{p=-\infty}^{Q_1} d_2(k,p)\, e^{i(E_{k+p}+E_p)t} + \sum_{p=Q_2}^{\infty} d_2(k,p)\, e^{-i(E_{k+p}+E_p)t} \quad , \tag{A.11}$$

in which

$$d_1(k,p) = \frac{1}{2}\left\{1 + \mathrm{sgn}[p(k+p)]\ \frac{p(k+p) + V^2}{(p^2+V^2)^{\frac{1}{2}}[(p+k)^2+V^2]^{\frac{1}{2}}}\right\} ,$$

$$d_2(k,p) = \frac{1}{2}\left\{1 - \mathrm{sgn}[p(k+p)]\ \frac{p(k+p) + V^2}{(p^2+V^2)^{\frac{1}{2}}[(p+k)^2+V^2]^{\frac{1}{2}}}\right\} ,$$

$$Q_1 = -\bar{q} + (2\bar{q} - k)\theta(k - 2\bar{q}) \quad ,$$

$$Q_2 = \bar{q} - (k + 2\bar{q})\theta(-k - 2\bar{q}) ,$$

$$\bar{q} = \begin{cases} 0 , & q_0 \leq V ; \\ (q_0^2 - V^2)^{\frac{1}{2}}, & q_0 > V , \end{cases} \tag{A.12}$$

and $\theta(x)$ is the step function.

In the following we work in the continuum limit, where

$$\sum_k \rightarrow \frac{L}{2\pi} \int dk .$$

We first calculate the result in the $q_0 = 0$ case, which is also valid when $0 < q_0 \leq V$. We find

$$\chi(k,t) = \frac{L}{2\pi} \int_{-k}^{0} dp \left[d_1(k,p) - d_2(k,p)\right] e^{-i\varepsilon(k,p)t}$$

$$+ \frac{L}{2\pi} \int_{-\infty}^{\infty} dp\, d_2(k,p)\, e^{-i\varepsilon(k,p)t}, \quad k > 0 ,$$

$$\chi(k,t) = \frac{L}{2\pi} \int_{k}^{0} dp \left[d_1(k,p) - d_2(-k,p)\right] e^{-i\varepsilon(-k,p)t} +$$

$$+ \frac{L}{2\pi} \int_{-\infty}^{\infty} dp\, d_2(-k,p)\, e^{-i\varepsilon(-k,p)t}, \quad k < 0 , \tag{A.13}$$

which can be combined to give

$$\chi(k,t) = \frac{L}{2\pi} \int_{-|k|}^{0} dp\left[d_1(|k|,p) - d_2(|k|,p)\right] e^{-i\varepsilon(|k|,p)t} +$$

$$+ \frac{L}{2\pi} \int_{-\infty}^{\infty} dp\, d_2(|k|,p)\, e^{-i\varepsilon(|k|,p)t}, \qquad (A.14)$$

where

$$\varepsilon(k,p) = \left[(k+p)^2 + V^2\right]^{\frac{1}{2}} + (p^2 + V^2)^{\frac{1}{2}}. \qquad (A.15)$$

We further calculate the Fourier transform of $\chi(k,t)$:

$$\chi(k,\omega) = i \int_{0}^{\infty} dt\, e^{-i\omega t}\chi(k,t) + i \int_{-\infty}^{0} dt\, e^{-i\omega t}\chi^*(-k,t)$$

$$= \frac{L}{2\pi} \int_{-|k|}^{0} dp\left[d_1(|k|,p) - d_2(|k|,p)\right] \frac{-2\varepsilon(|k|,p)}{\omega^2-\varepsilon^2(|k|,p) + i\eta} +$$

$$+ \frac{L}{2\pi} \int_{-\infty}^{\infty} dp\, d_2(|k|,p)\, \frac{-2\varepsilon(|k|,p)}{\omega^2-\varepsilon^2(|k|,p) + i\eta} \qquad (A.16)$$

where we have moved the poles into the complex plane in the usual way. This result is exactly the same as that obtained by Minnhagen, Rosengren and Grinstein[29], and gives the correlation function in the commensurate phase.

First we are interested in the nature of the incommensurate phase, given by the correlation function $G(x,t)$ when $q_0 > V$, i.e. $\bar{q} > 0$. In the case of one-dimensional modulation, the quantity of major interest is the correlation in the direction of modulation $G(x,0)$:

$$G(x,0) = \frac{1}{L}\int_0^\infty \frac{dk}{k^2}(1 - \cos x)\chi(k,0) \tag{A.17}$$

The integrals in eq. (A.11) can be done exactly when $t = 0$, and we find

$$\chi_{IC}(k,0) \equiv \chi(k,0) - \chi_{\text{commensurate}}(k,0)$$

$$= \begin{cases} \frac{L}{4\pi}(|k|-2\bar{q}) + \frac{L}{4\pi}\left[f_1(\bar{q}) - f_1(-\bar{q}-|k|)\right], & |k| \le 2\bar{q} \\ \frac{L}{4\pi}\left[f_1(\bar{q}) - f_1(-\bar{q})\right] + \frac{L}{4\pi}\left[f_1(\bar{q}-|k|) - f_1(-\bar{q}-|k|)\right], & |k| \ge 2\bar{q} \end{cases} \tag{A.18}$$

where

$$f_1(x) = A(k)xf_2(x) + \frac{V}{A(k)}F(\phi(x)|\bar{k}) - VA(k)E(\phi(x)|\bar{k}) ,$$

$$A(k) = \frac{k}{2V} + \left(\frac{k^2}{4V^2} + 1\right)^{1/2} ,$$

$$f_2(x) = \left\{1 - \frac{k}{VA(k)}\frac{\left(\frac{x}{V} - \frac{1}{A(k)}\right)^2}{\left(\frac{x}{V}\right)^2 + 1}\right\}^{1/2} ,$$

$$\bar{k} = 1 - |A(k)|^{-4} ,$$

$$\phi(x) = \arctan\left[\frac{\frac{x}{V}A(k)-1}{\frac{x}{V} + A(k)}\right], \tag{A.19}$$

and $F(\phi|\bar{k})$ and $E(\phi|\bar{k})$ are[23] incomplete elliptic integrals of the first and sedond kind, respectively.

We examine the behaviour of the correlation function near the C-I transition in more detail. In this case $\bar{q} << V$ and we can use the

leading terms in (A.18):

$$\chi_{IC}(k,0) \simeq \begin{cases} \frac{L}{2\pi}\left(|k| - \frac{\bar{q}}{2V^2}k^2 - \frac{|k|^3}{4V^2}\right), & |k| \leq 2\bar{q} \\ \frac{L}{2\pi}\left(2\bar{q} - \frac{\bar{q}}{V^2}k^2\right), & 2\bar{q} < |k| \leq V \\ \frac{L}{2\pi}\left(3\bar{q}\frac{V}{|k|}\right), & |k| > V \,. \end{cases} \tag{A.20}$$

By substituting this into eq. (A.17) we get

$$\begin{aligned} G_{IC}(x,0) &\equiv G(x,0) - G_{\text{commensurate}}(x,0) \\ &\simeq C + \ln(2\bar{q}x) - Ci(2\bar{q}x) + (1 - \cos 2\bar{q}x) \\ &+ \frac{3}{2}\bar{q}x\left[\sin Vx - Vx\,Ci(Vx)\right] \\ &- \frac{q}{V}\left[1 - \frac{\sin Vx}{Vx} + \frac{1}{2}(1 - \cos Vx)\right] \\ &+ \left(\frac{\bar{q}}{V}\right)^2\left[\frac{1}{2} - \frac{1 - \cos 2\bar{q}x}{(2\bar{q}x)^2}\right] + \ldots, \end{aligned} \tag{A.21}$$

where[23] $C = 0{,}577\ldots$ is the Euler-Mascheroni constant and $Ci(x)$ is the cosine integral.

To find the asymptotic behaviour of $G_{IC}(x,0)$ in the regions $x << \bar{q}^{-1}$ and $x >> \bar{q}^{-1}$ we use the expansions[23]

$$Ci(x) \sim \begin{cases} C + \ln x - \frac{1}{4}x^2 + \ldots, & x << 1 \\ \frac{\sin x}{x} - \frac{\cos x}{x^2} + \ldots, & x >> 1 \,, \end{cases} \tag{A.22}$$

and the result is

$$G_{IC}(x,0) \simeq \begin{cases} 3\bar{q}^{-2}x^2, & x << \bar{q}^{-1} \\ \\ \ln(2\bar{q}x), & x >> \bar{q}^{-1} \end{cases} . \qquad (A.23)$$

The physical interpretation of these results is given in sect. 3.1.

We can also examine the nature of ordering in the commensurate phase starting from the result (A.16). As shown[30] by Minnhagen et al., this result can be further simplified with the transformation

$$p' = \frac{1}{\sqrt{2}} \cdot \left\{ kp + p^2 - V^2 + (p^2+V^2)^{\frac{1}{2}} \left[(p+k)^2 + V^2 \right]^{\frac{1}{2}} \right\}^{\frac{1}{2}}$$

$$\cdot \mathrm{sgn}(p + \tfrac{1}{2}k) , \qquad (A.24)$$

under which eq. (A.16) transforms to

$$\chi(k,\omega) = \frac{L}{2\pi} \int_{-\infty}^{\infty} dp \, \frac{V^2}{(p^2+V^2)^{\frac{3}{2}}} \, \frac{k^2}{k^2 - \omega^2 + 4p^2 + 4V^2 + i\delta} , \qquad (A.25)$$

where we have dropped the primed notation. The correlation function $G(x,t)$ can now be obtained as a two-dimensional Fourier transformation

$$G(x,t) = \iint \frac{d^2\vec{k}}{(2\pi)^2} \int_{-\infty}^{\infty} dp \, \frac{V^2}{(p^2+V^2)^{\frac{3}{2}}} \left[\frac{1}{4p^2+4V^2} - \frac{e^{i\vec{k}\cdot\vec{r}}}{\vec{k}^2+4p^2+4\Delta^2} \right] , \qquad (A.26)$$

where we have taken the limit $\delta \to 0$ because the singularity is removed,

and $\vec{k}$ and $\vec{r}$ are to be understood as vectors (k,ω) and (x,t) in a two-dimensional Minkowski space, i.e. $\vec{k}^2 = k^2 - \omega^2$ and $r^2 = x^2 - t^2$.

We can now make a "Wick rotation" $\omega \to iq$, $t \to i\eta$, and obtain the ordinary two-dimensional Fourier transformation of $G(x,y)$. In polar coordinates this reads

$$G(x,y) = \int_0^{a^{-1}} \int_0^{2\pi} \frac{k\, dk\, d\theta}{(2\pi)^2} \int_{-\infty}^{\infty} dp\, \frac{V^2}{4(p^2+V^2)^{5/2}} \cdot$$

$$\cdot \left[1 - \frac{4p^2 + 4V^2}{4p^2+4V^2+k^2}\, e^{ikr\cos\theta} \right] , \qquad (A.27)$$

where a^{-1} is the momentum cutoff.

For simplicity we consider the case $V \gg 1$. Now the term multiplying the exponential in eq. (A.27) can be set equal to one, and we obtain

$$G(x,y) \simeq \frac{1}{8\pi} \int_0^{a^{-1}} [1 - J_0(kr)]\, k\, dk \int_{-\infty}^{\infty} \frac{V^2}{(p^2+V^2)^{\frac{5}{2}}}\, dp , \qquad (A.28)$$

where $J_\nu(x)$ is[23] a Bessel function. The second integral can easily be done and the first integral can be calculated as an asymptotic series[23], and we find

$$G(x,y) \simeq \frac{1}{48\pi V^2} \left[\frac{1}{a^2} - \frac{1}{r^2} \sqrt{\frac{r}{a}} \sin\left(\frac{r}{a} - \frac{\pi}{4}\right) + \frac{1}{4r^2} + O(r^{-5/2}) \right] , \qquad (A.29)$$

where $r = (x^2 + y^2)^{1/2}$. At large distances the correlation function thus approaches a constant which is dependent on the cutoff procedure.

The result (A.29) gives the limiting value of G(x,y) at large distances. To get a feeling for the bahaviour of G(x,y) at small distances, we calculate its value at the origin:

$$G(0,0) = \int_0^{a^{-1}} \int_0^{2\pi} \frac{k\,dk\,d\theta}{(2\pi)^2} \int_{-\infty}^{\infty} dp \; \frac{V^2}{4(p^2+V^2)^{\frac{5}{2}}} \cdot \frac{k^2}{4p^2+4V^2}$$

$$= \frac{1}{32\pi} \int_0^{a^{-1}} k^3 dk \int_{-\infty}^{\infty} dp \; \frac{V^2}{(p^2+V^2)^{\frac{7}{2}}}$$

$$= \frac{1}{120\pi} \cdot (aV)^{-4} \,, \qquad \text{(A.30)}$$

which is to be compared with $(aV)^{-2}/48\pi$, the limiting value at large distances.

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