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Exactly Solvable *XY* Model of the Spin Peierls Transition

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The exact solution of the problem of the ground state of the *XY*-spin system on a deformed chain is found. At finite magnetization m it is characterized by the double periodic structure and has a finite-band spectrum of spin excitations. At $m \neq 0$ the phase transition from the incommensurate into the dimerized state is accompanied by the soliton lattice formation.

KEY WORDS: Commensurability; finite-band potentials; solitons.

1. INTRODUCTION

A common property of quasi-one-dimensional systems is formation of various periodic and quasiperiodic superstructures. A possible formation of the so-called charge or spin density waves and lattice superstructures depends on the character of interactions in the system. Their formation is accompanied by various physical effects: appearance of gaps in the initial electron spectra, appearance of new soliton-type excitations and collective modes. Most sophisticated phenomena are due to commensurability effects resulting from the interaction of a superstructure with the original periodic structure (see, e.g., the review in Ref. 1).

There are two limit cases in the phenomena of lattice superstructure formation due to the interaction of lattice deformations with an electron subsystem. If the direct electron–electron interaction is weak, there is the so-called Peierls effect,[2] giving rise to formation of the $2k_F$ superstructure (k_F is the Fermi momentum for free electrons) and to the appearance of gaps in the spectra of one-particle states and spin excitations. (Detailed discussion of this problem is in Ref. 3.) In the strong interaction limit when the electron–electron repulsion energy per a site v exceeds the value of the transfer

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integral between the sites t ($v \gg t$), charge and spin degrees of freedom are split. Charge excitations are described by the equivalent system of spinless fermions[4] and they correspond to the Peierls effect with the doubled wave vector. This effect generates the both theoretically and experimentally known problem of the $4k_F$ anomaly.[5] Spin excitations are described by the Hamiltonian of the Heisenberg antiferromagnet with the exchange integral $\mathfrak{I} \sim t^2/v$.

It is known that a quasi-one-dimensional antiferromagnet on a lattice, subject to deformations, is unstable with respect to displacements of its sites, modulating the exchange integrals. This instability, called the spin Peierls transition,[6] has been the subject of numerous theoretical and experimental studies (see the review in Ref. 7). It has been established that in the absence of magnetic field, dimerization of the chain, accompanied by the transition of the system into the singlet state, takes place, i.e., is accompanied by the appearance of a gap in the magnon spectrum.

There is probably a certain critical value of the magnetic field H_c above which a finite magnetic moment m emerges. It is most important that this transition belongs to the commensurate–incommensurate type: at $|H| > H_c$ $m \neq 0$ there is a soliton superstructure with the mean period $\sim m^{-1}$. As a result, the spin lattice becomes nonperiodic and there appear numerous fine phenomena due to the commensurability effect.

The existing researches of the spin Peierls transition have been performed within the continual models where these effects have been neglected. Therefore it is of interest to investigate an exactly solvable discrete model of the spin Peierls transition. The model we consider below in essence coincides with the discrete Peierls model we have studied previously in Refs. 8 and 9. As should be expected, an exactly solvable model is a system of XY spins per $\mathcal{N}$ sites of the lattice x_n. The spin interaction is described by the standard Hamiltonian

$$\mathscr{H} = \sum_n \mathfrak{I}_n (S_n^X S_{n+1}^X + S_n^Y S_{n+1}^Y)$$
$$\mathfrak{I}_n = \mathfrak{I}_0 (x_{n+1} - x_n), \qquad x_n = na + u_n, \qquad n = 1, 2, \ldots, \mathcal{N} \tag{1}$$

Values of the exchange integrals are determined by the spacing between the neighboring sites and, consequently, depend on deformations of the lattice u_n.

Treating the coordinates of the lattice x_n as classical variables, we must define the states of the system from the condition of the minimum of the energy functional of the system

$$\mathcal{N} W_s = W_s\{x_n\} = \mathrm{Sp}\, \mathscr{H} + \sum_n V_n\{x_n\} \tag{2}$$

where $V\{x_n\}$ is the energy of the elastic interaction between lattice sites.

By means of the Jordan–Wigner transformation, the system of XY spins is reduced to a system of spinless fermions, characterized by amplitudes of the wave functions ψ_n on the sites x_n. As a result, (2) becomes equivalent to the functional

$$\mathcal{N}W = W\{x_n\} = \sum_{E \leqslant \mu} E + V\{x_n\} \tag{3}$$

where $E = E\{x_n\}$ are eigenvalues of the difference Schrödinger equation

$$c_n \psi_{n+1} + c_{n-1}\psi_{n-1} = E\psi_n, \qquad c_n = \tfrac{1}{2}\mathfrak{I}_n \tag{4}$$

with the periodicity conditions

$$\psi_{n+\mathcal{N}} = \psi_n, \qquad c_{n+\mathcal{N}} = c_n \tag{4a}$$

The functional (3), (4) should be considered at a given mean value of magnetization

$$m = \frac{1}{\mathcal{N}} \sum_n \langle S_n^z \rangle, \qquad \langle S_n^z \rangle = \frac{1}{2} - \sum_{E \leqslant \mu} \psi_n^*(E)\, \psi_n(E) \tag{5}$$

The respective magnetic field is determined by the relation

$$H = \partial W_0 / \partial m$$

where

$$W_0 = \min_{\{x_n\}} W\{x_n\}$$

It is clear that $\mu = -H$ serves as the chemical potential.

In Refs. 8 and 9 it has been shown that the extremum problem for functionals of the (3), (4) types admits an exact solution if we confine ourselves to a special functional relation between the potential energy $V\{x_n\}$ and the set

$$c_n = c(x_{n+1} - x_n) = \exp(x_n - x_{n+1}) \tag{6}$$

Namely, the functional $V\{x_n\}$ should be represented as a sum of a finite or infinite number of even Toda integrals $I_{2\alpha}$:

$$V\{x_n\} = \sum_{\alpha=0}^{l} \kappa_\alpha I_{2\alpha}\{c_n\} \tag{7}$$

$$I_0 = \frac{1}{\mathcal{N}} \sum_n \ln c_n, \qquad I_2 = \frac{1}{\mathcal{N}} \sum_n c_n^2$$

$$I_4 = \frac{1}{\mathcal{N}} \sum_n (c_n^2 c_{n-1}^2 + \tfrac{1}{4} c_n^4), \ldots \tag{8}$$

In the problem under study the functionals I_n occur as coefficients of the asymptotic expansion of the quasimomentum $p(E)$ for solutions of the spectral problem (4), (4a)

$$ip(E) = \pm(\ln E - I_0 - I_2 E^{-2} - \cdots) \tag{9}$$

Confining ourselves to the interaction of spins with their nearest neighbors, we must retain in the sum over α in (7) only the first two terms. In the thermodynamic limit we obtain the energy functional in the form

$$W = \frac{1}{\pi}\int_{E<\mu} E\,dp - PI_0 + \kappa I_2, \qquad P = -\kappa_0, \qquad \kappa = \kappa_2 \tag{10}$$

where the integration is performed over all occupied allowed bands. The functional (9) varies at given pressures P and an average number of fermions per an atom ρ

$$\rho = \frac{1}{2} - m = \frac{1}{2\pi}\int_{E<\mu} dp \tag{11}$$

In (10) where P is regarded as pressure, it has been used that according to (6) and (8) the quantity

$$-\mathcal{N}I_0 = x_n - x_0 = \mathcal{N}a \tag{12}$$

is the total length of the chain.

The method of solving the extremum problem for the functionals (10) or in a more general form for the functionals (3), (7), is grounded on the study of their variations in the functional space I_n. Previously it has been shown[9,10] that all the extrema of W belong to the class of the so-called finite-band potentials of the Schrödinger operators (4), the number of allowed bands $q+1$ not exceeding $4l-1$, where $2l$ is a number of terms in the sum of formula (7). It has also been proved that the chemical potential is always in one of the forbidden bands.

The wave functions ψ_n and the potentials c_n are completely determined by the values of the lower $E_1, E_3, \ldots, E_{2q+1}$ and upper $E_2, E_4, \ldots, E_{2q+2}$ boundaries of the allowed bands as well as by the points γ_i in each of the forbidden bands $E_{2i}^2 \leqslant \gamma_i \leqslant E_{2i+1}^2$ of the spectrum. It is important that values of the functional W depend only on E_i but not on γ_i. An arbitrary choice of the values of γ_i at fixed E_i leads to the existence of zero gapless modes.

The boundaries of the bands determine the so-called hyperelliptical Riemannian surface Γ

$$y^2 = R(E^2), \qquad R(\varepsilon) = \prod_{k=1}^{q+1}(\varepsilon - E_k^2) \tag{13}$$

The latter in its turn determines the Riemann θ function in terms of q complex variables by which it is possible to express the wave functions ψ_n and potentials c_n. The method of constructing the θ functions for the surface Γ in application to the discrete equation (4) is in detail described in Ref. 11. All the necessary data are in brief given in Ref. 10. The quasimomentum $p(E)$, the asymptotic expansion of which has been given above in (9), is introduced on the surface Γ by means of the relation

$$i\,dp = \frac{E^q + r_1 E^{q-2} + \cdots}{[R(E^2)]^{1/2}}\,dE \tag{14}$$

The coefficients r_1,... are determined from the physically evident conditions that the integrals of the quasimomentum over the forbidden bands are zero.

Calculation of quasimomentum variations (see Ref. 9) yields the mutual independence of the first q integrals $I_{2\alpha}$. As a result, the extremum problem for the functionals is reduced to an algebraic system of equations.

Apart from the above-mentioned general assertions, we have a possibility of calculating all the necessary physical quantities. Below we shall give the results of these calculations.

2. PHYSICAL QUANTITIES

In the ground state of the model under study at $m \neq 0$ the lattice possesses an incommensurate double periodic structure. It is possible to regard it as a superposition of two lattices for odd and even sites, periodic with the period $T = 1/|m|$. Displacements of the sites are

$$u_n = u(n - n_0) = \frac{1}{2} \ln \frac{\theta_4((n - n_0 - 1)\,|m| + (-1)^n/4)}{\theta_4((n - n_0 + 1)\,|m| + (-1)^n/4)} \tag{15}$$
$$\theta_4(\xi) = \theta_4(\xi, \tau), \qquad \tau = iK'(k)/K(k)$$

Here and henceforth we follow Ref. 13 in designations for the elliptical functions and θ functions. The parameters τ or k are defined below. The deformation (15) is accompanied by the spin density modulation

$$S_n^z = m - \frac{1}{8\,|m|} \frac{K'(k)}{K(k)} \frac{\partial}{\partial n_0} u(n - n_0) \tag{16}$$

Note that in formulas (15) and (16) n_0 is an arbitrary, generally speaking, noninteger, so that the ground state is continuously degenerate with respect to the superstructure translation despite the absence of the translational invariance symmetry in the energy functional. This translational degeneracy

corresponds to the above-mentioned arbitrary choice of the parameters γ_i. This circumstance is closely associated with the exact integrability of the model.

The parameters $\tau = \tau(m)$ and $k = k(m)$ in (15), (16) are determined by one of the two self-consistency conditions:

(a) At a given mean intersite spacing a

$$\frac{K(r)}{\mathrm{cn}(u,k)} \frac{\theta_4^2(0)}{\theta_4^2(m)} = 2\pi\kappa\bar{c} = \lambda_0^{-1}, \qquad \bar{c} = e^{-a} \tag{17}$$

where

$$u = 2|m|K(k), \qquad r = \mathrm{dn}(u,k)$$

(b) At a given pressure P

$$P = \frac{K(r)}{2\pi^2\kappa}\left[1 + \frac{\mathrm{sn}^2(u,k)\,\mathrm{dn}^2(u,k)}{\mathrm{cn}^2(u,k)} - 2\frac{E(r)}{K(r)}\right] \tag{18}$$

Equations (17) and (18) can be interpreted as a parametric equation of state $P = P(a, m)$. Note that $P > 0$ always. The energy of the ground state W_0 is determined by the expression

$$W_0 = W_0(P,m) = \frac{K^2(r)}{4\pi^2}\left[1 + \frac{\mathrm{sn}^2(u,k)\,\mathrm{dn}^2(u,k)}{\mathrm{cn}^2(u,k)} - 4\frac{E(r)}{K(r)} - \frac{\mathrm{sn}(u,k)}{K(k)}\frac{\theta_4'(\frac{1}{2}-|m|)}{\theta_4(\frac{1}{2}-|m|)}\right] + Pa \tag{19}$$

The spectrum (4) at $m \neq 0; \pm 1/2$ in accordance with the situation discussed in Sec. 1, consists of three allowed bands $(-E_3, -E_2)$, $(-E_1, E_1)$, and (E_2, E_3) (see Fig. 1a). The magnitude of the magnetic field H is in one of the forbidden bands $(-E_2, -E_1)$ or (E_1, E_2) at $m > 0$ or $m < 0$, respectively. The edges of the bands are determined by the relations

$$E_3 = 2\bar{c}\frac{\theta_4(m)\,\theta_4(\frac{1}{2}-|m|)}{\theta_4(0)\,\theta_4(1/2)}$$
$$\frac{E_2}{E_3} = \mathrm{sn}(u,k), \qquad \frac{E_1}{E_2} = \frac{k'}{\mathrm{dn}(u,k)} \tag{20}$$

Of greatest interest is the behavior of the physical quantities in the vicinity of the commensurate–incommensurate transition, i.e., at $m \to 0$. In the case of weak coupling this region is

$$|m| \ll \exp(-1/\lambda_0), \qquad \lambda_0 = 1/2\pi\kappa\bar{c} \ll 1 \tag{21}$$

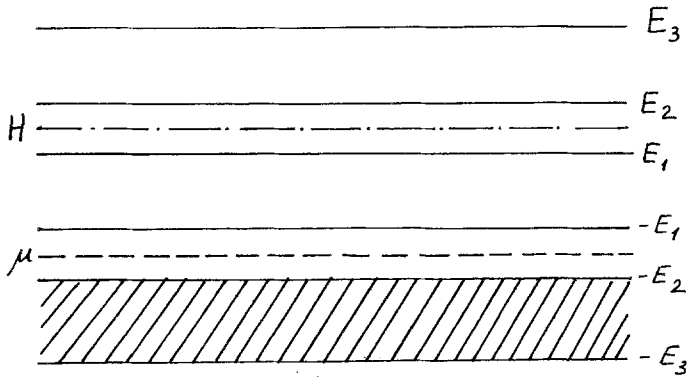

Fig. 1. The spectrum of Fermion's eigenvalues.

In the limit $m \to 0$ formulas (15), (16) yield a dilute lattice of solitons each of which shifts the dimerization structure by a half-period. In the region of a soliton only each second site participates in the deformation of the lattice and spin density, e.g.,

$$u_{2n} = \frac{1}{2} \ln \frac{\mathrm{ch}[\mathscr{S}^{-1}(n - n_0 - 1/2)]}{\mathrm{ch}[\mathscr{S}^{-1}(n - n_0 + 1/2)]} \tag{22}$$

$$u_{2n+1} = \mathrm{const}$$

Then

$$S^z_{2n} - m = \tfrac{1}{4}\{\mathrm{th}[\mathscr{S}^{-1}(n - n_0 + \tfrac{1}{2})] - \mathrm{th}[\mathscr{S}^{-1}(n - n_0 - \tfrac{1}{2})]\} \tag{23}$$

$$\sum_n (S^z_{2n} - m) = 1/2, \qquad S^z_{2n+1} = m$$

Formula (23) shows that each soliton has only one 1/2 spin, distributed over either even or odd sites.

The width parameter of the soliton $\mathscr{S}$ is found from the equation

$$r = 1/\mathrm{ch}(\mathscr{S}^{-1}) \tag{24}$$

The self-consistency conditions (16), (17) in the limit $m \to 0$ can be simplified if we neglect all the terms $\sim \exp(-4/\mathscr{S}|m|)$. As a result, we get the following equations for the quantity r:

$$rK(r)\left(\frac{1 + r'}{r}\right)^{2|m|} = 2\pi\kappa e^{-a} = \frac{1}{\lambda_0} \tag{25}$$

$$r^2 + r'^2 = 1$$

$$K^2(r)(2 - r^2) - 2E(r)\,K(r) = 2\pi^2\kappa P \tag{26}$$

and the expression for the energy

$$W_0(P, m) = \frac{K^2(r)}{4\pi^2\kappa}\left[2 - r^2 - 4\frac{E(r)}{K(r)} + 4r'|m|\right] + Pa \tag{27}$$

It follows from formulas (25)–(27) that with accuracy up to exponentially small terms, the parameters of the system are uniquely (irrespective of m) determined by the pressure. Then the length and energy are linear with respect to $|m|$, i.e., with respect to soliton concentration. The cusp in the energy dependence on m leads to the appearance of the critical field H_c. For the energy at a given magnetic field H we have

$$\begin{aligned} W(H) &= W_0(m) - mH \\ &= W(0) + 2E_s|m| - Hm + O(e^{-4/\mathscr{S}|m|}) \end{aligned} \tag{28}$$

where E_s is the soliton energy. Note that the spin of each soliton equals 1/2.

From (28) we get that at $|H| > H_c = 2E_s$ the quantity m is determined by the dependence

$$m \sim \mathscr{S}^{-1} \ln \frac{1}{H - H_c} \tag{29}$$

This behavior is typical of the commensurate–incommensurate transitions in classical systems.[14] From formulas (25)–(27) we can find the value of the critical magnetic field

$$\left.\frac{\partial W_0}{\partial m}\right|_{m=0} = H_c \approx \frac{r'}{\pi^2\kappa}K^2(r) - 2P \ln \frac{1 + r'}{r} \tag{30}$$

In the weak coupling limit it follows from (30) that

$$H_c \approx \frac{2}{\pi}\Delta_0 = \frac{16}{\pi}\bar{c}\exp(-1/\lambda_0)$$

where $\Delta_0 \approx E_2|_{m=0}$ is a half-width of the gap in the fermion spectrum due to the spin Peierls transition in the absence of the magnetic field.

3. PROPERTIES OF NONINTEGRABLE MODELS

The character of the spin Peierls transition noticeably changes if the exact integrability of the model is somehow violated. It is sufficient, for instance, as has already been done previously,[12] to add to the elastic energy a small term of the form

$$\mathscr{H}_{n,i} = \lambda \sum_n c_n, \qquad \lambda \to 0 \tag{31}$$

Then already in the linear approximation with respect to λ the dependence of the energy on the mean spin (per an ion) m will become a function, discontinuous in all the points. More exactly (cf. Ref. 14), the value of the energy at "rational" moments

$$m = l/n$$

where l and n are integers, will differ by a finite value from the energy in a close irrational point. The value of the jump is dependent on l/n. If the latter is not too small, i.e., the corresponding central band in Fig. 1 is not too narrow, we believe that there is an almost sinusoidal spin density wave. Its pinning energy at $n \to \infty$ (but finite l/n) will be exponentially low[12]

$$\mathscr{H}_{\text{pinn}} \sim \lambda e^{-n} \tag{32}$$

This means that the discontinuous function is differentiable in all irrational m. The respective dependence of the moment on the field $m(H)$ will be given by the curve with a small number of horizontal regions, corresponding to the pinning under small values of $n = 3, 4, 5, \ldots$.

When the value of the mean moment is close to 1/2, the middle band in Fig. 1 vanishes, and the charge density wave becomes a soliton lattice. Then the pinning energy loses its exponential dependence on n, and the curve becomes a typical "devil's staircase" (see, e.g., Ref. 1). Finally, when the width of the central band is substantially smaller than the perturbation energy λ (32), a chaotic behavior will be observed in the system.[12] We shall not dwell upon this regime, referring all those interested to the above-mentioned review by P. Bak.[1]

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