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Spin–spin correlation function for the free-fermion model: crossover from two-dimensional Ising to Pokrovsky–Talapov critical behaviour

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Abstract. We calculate the spin–spin correlation function for a $(1+1)$-dimensional free-fermion model displaying crossover from the two-dimensional Ising to Pokrovsky–Talapov critical behaviour. In the Ising limit our results reduce to the well known exact representations reported by Wu *et al*. Correspondence between the obtained correlation function and an exactly solvable classical Hamiltonian system is established.

Calculation of correlation functions in exactly solvable models of statistical mechanics is of considerable interest both for physical and mathematical reasons. On the one hand, it helps one to interpret correctly the extensive information provided by scattering experiments in real condensed matter systems undergoing phase transitions [1, 2]. On the other hand, correlation functions possess remarkable mathematical properties having a deep relationship with classical integrable systems and quantum groups [3, 4].

In this paper we report results of the calculation of the Ising spin correlation function in the continuous free-fermion model defined by the Hamiltonian

$$\mathcal{E} = \int_0^L \mathrm{d}x \left\{ \Omega\, \psi^+ \psi + s \frac{\mathrm{d}\psi^+}{\mathrm{d}x} \frac{\mathrm{d}\psi}{\mathrm{d}x} + \frac{\mathrm{i}\Gamma}{2} \left(\frac{\mathrm{d}\psi^+}{\mathrm{d}x} \psi^+ + \frac{\mathrm{d}\psi}{\mathrm{d}x} \psi \right) \right\}. \tag{1}$$

Here L is the system length in the x-direction and operators $\psi(x)$ and $\psi^+(x)$ describe a spinless fermionic field obeying standard anticommutational relations. By rescaling of the energy, space coordinate and fermionic operators one can easily show that model (1) can be characterized completely by the sign of Ω and the single parameter g given by

$$g \equiv \frac{\Gamma}{(4s|\Omega|)^{1/2}}.$$

Being considered as $(1+1)$-dimensional quantum field theory, model (1) describes non-relativistic fermions which move in the x-line and can appear and annihilate in pairs. The main physical motivation for studying such fermionic models lies, however, in two-dimensional statistical mechanics. In particular, the fermionic approach is widely used in the theory of the commensurate–incommensurate phase transition in a system of atoms adsorbed on a crystalline substrate [5–7]. After conventional mapping of the Euclidean $(1+1)$-dimensional field theory defined by (1) onto two-dimensional classical statistical mechanics the time variable τ is interpreted as the second space variable in the plane

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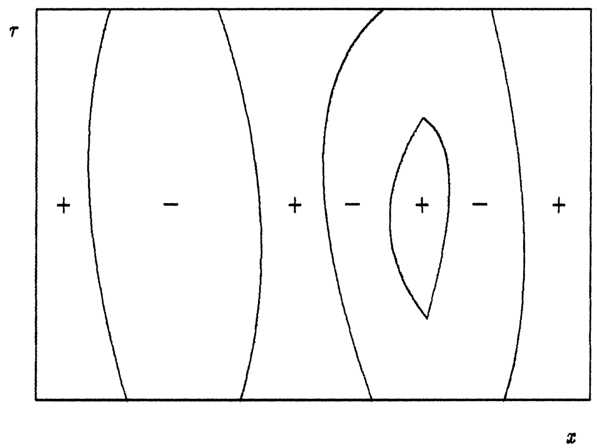

Figure 1. A typical configuration of domain walls and Ising spins described by the Hamiltonian (1).

(x, τ). Fermion trajectories $x(\tau)$ correspond to domain wall lines (solitons) in the (x, τ) plane. Such a wall separates alternating regions, where values $+1$ and -1 are assigned to the discrete order parameter $\sigma(x, \tau)$ (see figure 1). We shall use magnetic terminology and name the variable $\sigma(x, \tau)$ by 'Ising spin'. One can easily express the product of two Ising spin operators $\hat{\sigma}(x_1)$ and $\hat{\sigma}(x_2)$ in terms of fermionic fields

$$\hat{\sigma}(x_2)\hat{\sigma}(x_1) = \exp\left\{\mathrm{i}\pi \int_{x_1}^{x_2} \mathrm{d}x\, \psi^+(x)\psi(x)\right\}. \tag{2}$$

This relation means, simply, that spins at the points x_1 and x_2 are the same or opposite, if the number of domain walls between these two points is even or odd, respectively.

The correlation function $P(x, \tau)$ we are going to study is defined as

$$P(x, \tau) = \langle\Phi|U(-\tau)\hat{\sigma}(x)U(\tau)\hat{\sigma}(0)|\Phi\rangle. \tag{3}$$

Here $|\Phi\rangle$ denotes the Hamiltonian ground state and $U(\tau) = \mathrm{e}^{-\tau\mathcal{E}}$ is the Euclidean evolution operator. The product of two Ising spin operators at $\tau = 0$ is defined by (2); for different time momenta formula (2) is generalized below (see (15), (16)).

The phase diagram of the model defined by Hamiltonian (1) is typical for the free-fermionic models [7, 8]. In the point $\Omega = 0$ the phase transition takes place from the ordered ($\Omega > 0$) to the disordered phase ($\Omega < 0$). It belongs to the two-dimensional Ising universality class for all $\Gamma \neq 0$. If $\Gamma = 0$, the number of domain walls is the same in each section $\tau =$ constant, and finite-size domains are not allowed. This constraint is crucial for the Pokrovsky–Talapov phase transition [9]. We review briefly its main properties. After the Fourier transfer of the fermionic field

$$a_p = L^{-\frac{1}{2}} \int_0^L \mathrm{d}x\, \psi(x) \exp(\mathrm{i}px)$$

Hamiltonian (1) becomes diagonal

$$\mathcal{E} = \sum_p \epsilon(p) a_p^+ a_p \tag{4}$$

where $\epsilon(p) = \Omega + sp^2$ is the fermion spectrum. If $\Omega > 0$, the energy $\epsilon(p)$ is positive for all p, and the ground state is the vacuum vector of the a_p-operators. Thus, there are no domain walls in this ordered (commensurate) phase, and the free energy is zero. If $\Omega < 0$, states with negative $\epsilon(p) < 0$ appear under the Fermi sphere $-p_{\mathrm{F}} < p < p_{\mathrm{F}}$, where $p_{\mathrm{F}} = (|\Omega|/s)^{1/2}$ is the Fermi momentum. All these states are occupied by fermions in the ground state. This means that domain walls appear in the (x, τ)-plane (see figure 1). They are aligned in average in the τ-direction and form a one-dimensional lattice in the x-direction with the density $p_{\mathrm{F}}/\pi \sim |\Omega|^{1/2}$ vanishing in the phase transition point $\Omega = 0$.

So, two asymptotic regions can be separated in the (Ω, Γ)-plane. If $g \gg 1$, the model (1) is equivalent to the critical two-dimensional Ising model, which is isotropic in certain coordinates [10]. In the opposite limit $g \ll 1$, the concentration of finite-size domains vanishes and fluctuations become strongly unisotropic, approaching the Pokrovsky–Talapov picture described above. These two regions can be illustrated in the exact formula for the spontaneous magnetization M in the ordered phase:

$$M = (1 + g^2)^{-1/8}. \tag{5}$$

It is almost equal to unity in the Pokrovsky–Talapov region and goes to zero $\sim\Omega^{1/8}$ in the Ising limit.

It should be noted that the continuous free-fermion model (1) can be mapped by the Jordan–Wigner transformation onto the double scaling limit of the XY-model, which was studied by Jimbo *et al* [11]. The latter model is defined by the quantum spin chain Hamiltonian

$$\mathcal{H}_{XY} = -\frac{1}{4}\sum_{m\in Z}((1+\gamma)\sigma_m^x\sigma_{m+1}^x + (1-\gamma)\sigma_m^y\sigma_{m+1}^y + 2h\sigma_m^z). \tag{6}$$

Correspondence of the Hamiltonian parameters is given by

$$\gamma = \frac{\Gamma}{2\sqrt{s}} \qquad h = 1 + \frac{\Omega}{2}.$$

The double scaling limit of the model (6) is described by relations

$$\delta = (|1 - h^2|)^{1/2} \qquad \gamma = g\delta \qquad g = \text{constant} > 0, \delta \to 0.$$

The Ising spin operator $\hat{\sigma}(x)$ defined by (2) takes the form

$$\hat{\sigma}(x) = \exp\left(\mathrm{i}\pi \sum_{j=-\infty}^{m-1} \sigma_j^+\sigma_j^-\right) \prod_{j=-\infty}^{m-1} (-1)^j \tag{7}$$

where $\sigma_j^{\pm} = \frac{1}{2}(\sigma_j^x \pm \mathrm{i}\sigma_j^y)$ and $x = m\sqrt{s}$.

Jimbo *et al* [11] calculated the n-point in-line correlation function

$$\langle\Phi|\sigma_{m_1}^x\sigma_{m_2}^x, \ldots, \sigma_{m_n}^x|\Phi\rangle$$

for the model (6) in the double scaling limit in the phase $|h| < 1$, and expressed it in terms of the ordinary Painlevé V differential equation. Recently, Eßler *et al* [12] established a relation between the Painlevé V differential equation and correlation functions in an exactly solvable model of interacting fermions. We are interested in another, though closely related, set of problems. The differences are as follows.

- We consider the two-point correlation function of the spin operators (7), which naturally appear if model (1) is used to describe the commensurate–incommensurate phase transition. These spin operators are related to σ_m^x by the duality transformation (see [13]). Jimbo *et al* calculated correlation functions of the initial σ_m^x operators.
- We study both $|h| > 1$ and $|h| < 1$ phases, while Jimbo *et al* consider only the phase $|h| < 1$, which is ordered for the σ_m^x operators.

• We calculate the off-line correlation function $P(x, \tau)$ which depends on space and time coordinates, while Jimbo *et al* restrict their consideration to the in-line correlation function depending on x only.

• Correspondingly, we express the result in terms of a not ordinary (Painlevé V), but partial differential equation (see (29)).

Passing to calculations, let us introduce new fermionic operators b_p

$$b_p = a_p \cos\varphi(p) + a^+_{-p} \sin\varphi(p) \tag{8}$$

which are related to the a_p-operators by the Bogoliubov–Valatin transformation characterized by the angle $\varphi(p)$. Then the following representation is valid for the Ising spin operator $\hat{\sigma}(x)$:

$$\hat{\sigma}(x) = M(\varphi) : \exp\left\{\frac{1}{2L}\sum_{pk}[D_{pk}(b_p b_k - b^+_{-k} b^+_{-p}) \exp[-\mathrm{i}(p+k)x] \right. \\ \left. +2b^+_p b_k G_{pk} \exp[\mathrm{i}(p-k)x]]\right\} : \tag{9}$$

where

$$D_{pk} = \frac{1}{p+k}\left[\frac{A(k)}{A(p)} - \frac{A(p)}{A(k)}\right] \qquad G_{pk} = \frac{\mathrm{i}}{k-p-\mathrm{i}0}\left[\frac{A(k)}{A(p)} + \frac{A(p)}{A(k)}\right] \tag{10}$$

$$A(p) = \exp\left[\frac{1}{\pi}\int_{-\infty}^{p} \mathrm{d}k \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{q-k}\frac{\mathrm{d}\varphi(q)}{\mathrm{d}q}\right] \tag{11}$$

$$M(\varphi) = \exp\left\{\frac{1}{2\pi^2}\int_{-\infty}^{\infty} \mathrm{d}p\varphi(p) \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{q-p}\frac{\mathrm{d}\varphi(q)}{\mathrm{d}q}\right\}. \tag{12}$$

Notation : $\exp\{\ldots\}$: has been used for normal ordering with respect to the b^+, b-operators. Integration in q is understood in the sense of the Cauchy principal value. In the above representation the angle of the Bogoliubov–Valatin transformation $\varphi(p)$ is an arbitrary continuous odd function obeying the following conditions:

(i) $-\pi/2 < \varphi(p) \leqslant 0$ for $p \geqslant 0$;

(ii) $\varphi(p)$ has a single minimum in the half-line $p > 0$;

(iii) $\varphi(p)$ goes to zero at $|p| \to \infty$ fast enough so that integrals in (13) defining $M(\varphi)$ converge.

If $\varphi(p) \equiv 0$, representation (6) reduces to the relation

$$\hat{\sigma}(x) =: \exp\left(-2\int_x^{\infty} \mathrm{d}y\, \psi^+(y)\psi(y)\right) :$$

which can be easily verified in the $2n$-particle sectors. For arbitrary $\varphi(p)$ we derive (9) from (2) in several steps. First, we consider the matrix entrance $\langle\beta^*|\hat{\sigma}(x_2)\hat{\sigma}(x_1)|\beta\rangle$ between fermionic coherent states

$$\langle\beta^*| \equiv \langle 0_\mathrm{b}| \exp\left(\sum_p b_p \beta^*_p\right) \qquad |\beta\rangle \equiv \exp\left(\sum_p \beta_p b^+_p\right)|0_\mathrm{b}\rangle \tag{13}$$

where $|0_\mathrm{b}\rangle$ is the vacuum vector of operators b_p (i.e. $b_p|0_\mathrm{b}\rangle = 0$ for $\forall p$) and β_p, β^*_p denote the Grassmann variables. We represent this matrix entrance in terms of the Fredholm determinant of some integral operator. Then we express it in the limit $(x_2 - x_1) \to \infty$ as a product of two factors depending on x_2 and x_1, respectively. Identifying these factors with matrix entrances $\langle\beta^*|\hat{\sigma}(x_2)|\beta\rangle$ and $\langle\beta^*|\hat{\sigma}(x_1)|\beta\rangle$, we derive (9)–(12) after some algebra based on the solution of a Riemann–Hilbert problem. The evaluation procedure outlined above is alternative to the Clifford algebra approach to the same problem introduced by Jimbo *et al* [11].

Representation (9) turns out to be a very convenient starting point for the calculation of the vacuum average of products of spin operators. Let us denote by $\sigma(x;\beta_p^*,\beta_p)$ the normal symbol of the operator $\hat\sigma(x)$, which is obtained from (9) by replacing the fermionic operators b_p^+, b_p by their Grassmann counterparts β_p^*, β_p. Denote, further, by $U_0(\tau)$ the free-field evolution operator

$$U_0(\tau)=\exp\left[-\tau\sum_p \omega(p)b_p^+b_p\right]$$

characterized by some frequencies $\omega(p)$. Then the vacuum average $P_0(x,\tau)$ defined by

$$P_0(x,\tau)=\langle 0_b|U_0(-\tau)\hat\sigma(x)U_0(\tau)\hat\sigma(0)|0_b\rangle \tag{14}$$

can be written as a Gaussian continual integral over Grassmann variables:

$$P_0(x,\tau)=\int\left(\prod_p \mathrm{d}\beta_p^*\,\mathrm{d}\beta_p\right)\sigma(x;0,\beta_p\,\mathrm{e}^{-\tau\omega(p)})\sigma(0;\beta_p^*,0)\exp\left(-\sum_p\beta_p^*\beta_p\right). \tag{15}$$

Straightforward integration yields

$$P_0(x,\tau)=M^2(\varphi)\det[1+\hat D(x,\tau)] \tag{16}$$

where $M(\varphi)$ is given by (10), and $\hat D(x,\tau)$ is the integral operator acting on a function $f(p)$ in the following way:

$$\hat D(x,\tau)f(p)=\int_{-\infty}^{\infty}\frac{\mathrm{d}k}{2\pi}D_{pk}f(k)\exp\left\{-\frac12\mathrm{i}x(p+k)-\frac12\tau[\omega(p)+\omega(k)]\right\}. \tag{17}$$

Throughout the above analysis we did not concretize the angle of the Bogoliubov–Valatin transformation $\varphi(p)$. But now let us put

$$\varphi(p)=\tfrac12\arg(\Omega+sp^2-\mathrm{i}\Gamma p) \tag{18}$$

choosing the branch of the argument by the constraint $\varphi(\pm\infty)=0$. Corresponding b-operators diagonalize Hamiltonian (1) in both ordered ($\Omega>0$) and disordered ($\Omega<0$) phases:

$$\mathcal{E}=\sum_p\omega(p)b_p^+b_p+\text{constant}\qquad\text{where } \omega(p)=[(\Omega+sp^2)^2+(\Gamma p)^2]^{1/2}. \tag{19}$$

If $\Omega>0$, function (19) satisfies conditions (i)–(iii). So, one can apply general formula (14) to calculate $P_0(x,\tau)$. This coincides with the desired correlation function $P(x,\tau)$, since $|\Phi\rangle=|0_\mathrm{b}\rangle$ and $U(\tau)=U_0(\tau)$ in this case. Substituting (18) into (9)–(11) one obtains in the ordered phase

$$P(x,\tau)=M^2\det[1+\hat D(x,\tau)]. \tag{20}$$

Here the spontaneous magnetization M is given by (5). Operator $\hat D(x,\tau)$ is defined by relations (10) and (17), where the function $A(p)$ reduces to

$$A(p)=\left(\frac{p^2-p_1^2}{p^2-p_2^2}\right)^{1/4}.$$

We use the notation p_1 and p_2 for two complex solutions of the equation $\omega(p)=0$, which are ordered as follows: $0<\operatorname{Im}p_1\leqslant\operatorname{Im}p_2<\infty$.

In the disordered phase $\Omega<0$, relations (18) and (19) still hold. However, we cannot apply formula (16), since the function $\varphi(p)$ defined by (18) has a discontinuity in the origin: $\varphi(\pm 0) = \mp\pi/2$. Formally, this leads to indeterminacy in the right-hand side of (17): $M^2(\varphi) = 0$, while the function D_{pk} becomes singular in the origin $p \to 0$, $k \to 0$. To avoid this problem, let us replace (19) by the regularized function†

$$\varphi(p;\delta) = \tfrac{1}{2}\arg(\Omega + sp^2 - \mathrm{i}\Gamma p) + \arg(p + \mathrm{i}\delta) \tag{21}$$

with small positive δ. This function is appropriate for satisfying conditions (i)–(iii), so we can calculate $P_0(x, \tau; \delta)$ according to (17). Proceeding then to the limit $\delta \to 0$ one can obtain

$$\lim_{\delta\to 0} P_0(x, \tau; \delta) = C \cdot (f, [1 - \hat{D}_+^2(x, \tau)]^{-1} f) \det[1 + \hat{D}_+(x, \tau)] \tag{22}$$

where

$$f(p) = [\omega(p)]^{-1/2} \exp[-\tfrac{1}{2}\mathrm{i}xp - \tfrac{1}{2}\tau\omega(p)]$$

and operator $\hat{D}_+(x, \tau)$ is defined by relations (10) and (17), where $A(p)$ is replaced by $\sqrt{\omega(p)}$. The scalar product of two functions $f(p)$ and $g(p)$ reads as

$$(f, g) \equiv (2\pi)^{-1} \int_{-\infty}^{\infty} \mathrm{d}p\, f(p)g(p).$$

The constant factor C is determined by the evident requirement that $P(0, 0; \delta) = 1$.

Formulae (20) and (22) are our first main result. Representation (20) relating to the ordered phase is exact. It is not evident, however, that the limiting procedure (21) and (22) leads to the exact correlation function $P(x, \tau)$ in the disordered phase. Nevertheless, *both* formulae (20) and (22) reduce in the limit $|\Omega|s \ll \Gamma^2$ to the *exact* spin–spin correlation function of the two-dimensional Ising model in the critical region, which was reported by Wu *et al* [10]. In this limit we have

$$p_1 = \mathrm{i}|\Omega|/\Gamma \qquad p_2/p_1 = \infty \qquad \omega(p) = [\Omega^2 + (\Gamma p)^2]^{1/2}$$
$$\hat{D}(x, \tau) = \hat{D}_+(x, \tau) \qquad D_{pk} = \frac{1}{p + k} \frac{\omega(k) - \omega(p)}{\sqrt{\omega(k)\omega(p)}}.$$

Then putting $\Omega = \Gamma = 1$, one can easily verify that

$$\det[1 + \hat{D}(x, \tau)] = \hat{F}_-(\sqrt{x^2 + \tau^2}) \qquad (f, [1 - \hat{D}^2(x, \tau)]^{-1} f) = G(\sqrt{x^2 + \tau^2})$$

where $\hat{F}_-(x)$ and $G(x)$ are the universal functions introduced by Wu *et al* in relations (2.26) and (2.29) in their paper [10]. This allows us to suggest that the right-hand side of (22) gives the exact correlation function $P(x, \tau)$ in the disordered phase ($\Omega < 0$) for model (1).

The Fourier transform of the correlation function $P(x, \tau)$ is often called the K-dependent susceptibility $\chi(K)$:

$$\chi(K) = 2 \int_{-\infty}^{\infty} \mathrm{d}x \int_0^{\infty} \mathrm{d}\tau\, P(x, \tau) \exp(\mathrm{i}Kx). \tag{23}$$

It can be shown from (20) and (22) that its singularities in the complex K-plane lie at the points $\pm(m_1 p_1 + m_2 p_2)$, where $m_1, m_2 = 0, 1, 2, \ldots,$ and $2 \leqslant (m_1 + m_2) = 0 \bmod 2$ in the ordered phase $\Omega > 0$, and $(m_1 + m_2) = 1 \bmod 2$ in the disordered phase $\Omega < 0$. In the Ising limit all singularities are purely imaginary, as was shown by Tracy and McCoy [1]. By contrast, in the Pokrovsky–Talapov limit $g \to 0$ and $\Omega < 0$ singularities fill the lines $\mathrm{Re}K = \pm(m_1 + m_2)p_{\mathrm{F}}$. These singularities correspond to the Bragg ($m_1 + m_2 = 1$) and satellite ($m_1 + m_2 = 3, 5, \ldots$) reflections on the periodic multisoliton lattice, which could

† Physically ansatz (21) corresponds in the BCS approximation to the effect of a small magnetic field $h \sim \sqrt{\delta}$ on the ground state of the system (1) (for details see [14]).

be observed in some scattering experiment in a two-dimensional incommensurate crystal. Perhaps, representation (22) could be also useful in interpretation of scattering patterns in three-dimensional incommensurate crystals [15].

The leading term in $g \to 0$ in the correlation function (22) has a simple form for $xp_{\rm F} \gg 1$:

$$P(x,\tau) = 2\sqrt{g}\hat{F}_+(r)\hat{F}_-(r)\cos xp_{\rm F} \tag{24}$$

where

$$r = g[(xp_F)^2 + 4(\Omega\tau)^2]^{1/2}$$

and $\hat{F}_+(r)$ and $\hat{F}_-(r)$ are the universal correlation functions of the two-dimensional Ising model in the critical region in the paramagnetic and ferromagnetic phases, respectively [10].

It is well known that correlation functions of integrable models of statistical mechanics are closely related with some classical Hamiltonian models, which in turn can be solved exactly by the inverse scattering method (see [4, 10–12]). We establish such a relationship for the correlation function of model (1) in the ordered phase $\Omega > 0$. It is convenient to introduce new independent variables y and t by the relations

$$x(y) = ys[\Gamma^2 + 4s\Omega]^{-1/2} \qquad \tau(t) = -\mathrm{i}ts[\Gamma^2 + 4s\Omega]^{-1}$$

and to modify our definition of the correlation function (3):

$$\tilde{P}(y,t) \equiv P(x(y),\tau(t)). \tag{25}$$

Let us consider a classical Hamiltonian system defined by the Hamiltonian

$$\mathcal{H} = \int \mathrm{d}y H(y) \tag{26}$$

with Hamiltonian density

$$H(y) = \frac{1}{2}\left\{\pi^2(y)[u'^2(y) + (1/4)R(u)] + \frac{[u''(y) + (1/8)\,\mathrm{d}R(u)/\mathrm{d}u]^2}{[u'^2(y) + (1/4)R(u)]} - k^2u^2(y)\right\}. \tag{27}$$

Here $u(y)$ and $\pi(y)$ are the canonical coordinate and momentum functions, $k^2 = \Gamma^2/[\Gamma^2 + 4s\Omega]$, and $R(u) = (1-u^2)(1-k^2u^2)$. The standard Poisson brackets on the coordinate and momentum functions are assumed:

$$\{\pi(y_1), u(y_2)\} = \delta(y_1 - y_2).$$

Then the following equality is valid

$$\frac{\partial^2 \ln \tilde{P}(y,t)}{\partial y^2} = -\frac{1}{2}H(y,t). \tag{28}$$

Here $H(y,t)$ is the time evolution of the Hamiltonian density (27) according to the Hamiltonian dynamics of canonical variables $u(y,t)$ and $\pi(y,t)$, which corresponds to certain initial conditions $u(y,0) = u_0(y)$ and $\pi(y,0) = 0$. Representation (28) is our second main result.

It turns out that the classical Hamiltonian model defined by (26) and (27) is exactly solvable by the quantum inverse scattering method. More precisely, we have obtained for the Hamiltonian equations of this model the zero curvature representation [16], which is known to be equivalent to the Lax representation. In the limit $k \to 1$ the model (26) and (27) reduces to the sine–Gordon model. The evaluation procedure leading to (26)–(28) follows by principal moments to the Faddeev school version of the inverse scattering method [16] passed in the 'backward' direction, however. Starting from the eigenvalue problem for the operator $\hat{D}(x(y),\tau(t))$ defined by (17), through analysis of the associated

Riemann–Hilbert problem, we come to the overdetermined set of zero-curvature equations [16]. Their solvability conditions coincide with the Hamiltonian equations of the model (26) and (27). Details will be published elsewhere.

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