LETTER

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Kink confinement in the antiferromagnetic XXZ spin-(1/2) chain in a weak staggered magnetic field

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Abstract – The Heisenberg XXZ spin-(1/2) chain is considered in the massive antiferromagnetic regime in the presence of a staggered longitudinal magnetic field. The Hamiltonian of the model is characterised by the anisotropy parameter $\Delta < -1$ and by the magnetic-field strength h. At zero magnetic field, the model is exactly solvable. In the thermodynamic limit, it has two degenerate vacua and the kinks (which are also called spinons) interpolating between these vacua, as elementary excitations. Application of the staggered magnetic field breaks integrability of the model and induces the long-range attractive potential between two adjacent kinks leading to their confinement into the bound states. The energy spectra of the resulting two-kink bound states are perturbatively calculated in the extreme anisotropic (Ising) limit $\Delta \to -\infty$ to the first order in the inverse anisotropy constant $|\Delta|^{-1}$, and also for any $\Delta < -1$ to the first order in the weak magnetic field h.

Introduction. – The confinement phenomenon occurs when the constituents of a compound particle cannot be separated from each other and, therefore, cannot be observed directly. A prominent and, important, example in high-energy physics is the confinement of quarks in hadrons. It is remarkable, that confinement can also be realized in such condensed-matter systems, as quantum quasi–one-dimensional ferro- and anti-ferromagnets [1–6]. The present theoretical understanding [7,8] of the confinement in such systems originates from the Wu and McCoy scenario [9], in which the two kinks are treated as quantum particles moving in the line and attracting one another with a linear potential proportional to the external magnetic field.

Very recently [5], the magnetic excitations energy spectra in the quasi–one-dimensional spin-(1/2) antiferromagnetic compound $SrCo_2V_2O_8$ in the confinement regime have been studied by means of the inelastic neutron scattering. The experimentally observed energy spectra were interpreted in [5] in terms of the one-dimensional XXZ spin-(1/2) chain Hamiltonian. We write this Hamiltonian directly in the thermodynamic limit in a slightly different form using the more traditional parametrization (see, *e.g.*, eq. (1.1) in [10]),

$$\mathcal{H}(\Delta,h) = -\frac{1}{2}\sum_{j=-\infty}^{\infty}\left[\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \Delta\left(\sigma_j^z\sigma_{j+1}^z + 1\right)\right] - h\sum_{j=-\infty}^{\infty}(-1)^j\sigma_j^z. \tag{1}$$

Here σ_j^a are the Pauli matrices, $\alpha = x, y, z$, Δ is the anisotropy parameter, h is the strength of the staggered magnetic field, which mimics [5] in the 1D Hamiltonian (1) the weak interchain interaction in the 3D array of parallel spin chains in the 3D ordered phase of the compound $SrCo_2V_2O_8$. The massive antiferromagnetic phase is realised at $\Delta < -1$. The dynamical structure factors and the spectrum of magnetic excitations in the model (1) were numerically studied in [5] in three different cases: i) in the extreme anisotropic (Ising) limit $|\Delta| \gg 1$, ii) close to the isotropic point $\Delta \approx -1$, and iii) for generic $\Delta \in (-\infty, -1)$. The resulting energy spectra of the magnetic excitations were presented graphically in figs. 8–15, and in phenomenological formulas like (26), which contain fitting parameters.

The aim of the present paper is to find analytic representations for the energy spectra of the two-kink bound states in the whole Brillouin zone in model (1) expressed solely in terms of the Hamiltonian parameters Δ and h. The problem is solved perturbatively in two asymptotical regimes: in the extreme anisotropic limit $\Delta \to -\infty$, and for any $\Delta < -1$ at small h.

The Hamiltonian symmetries. – The Hamiltonian (1) commutes with the z-projection of the total spin

$$S^z = \frac{1}{2}\sum_{j=-\infty}^{\infty} \sigma_j^z,$$

and with the modified translation operator $\widetilde{T}_1 = T_1 U$, where T_1 stands for the unit translation, and $U = \otimes_{j\in\mathbb{Z}} \sigma_j^x$ is the global rotation by π around the x-axis. For short, the operator S^z will be called the "total spin" in the following.

Ising limit. – In the extreme anisotropic limit $\Delta \to -\infty$, it is convenient to rescale the Hamiltonian (1) to the form

$$\mathcal{H}_I(\epsilon, h) = |\Delta|^{-1}\mathcal{H}(\Delta, h)\big|_{\Delta=-1/\epsilon} = -\epsilon h \sum_{j=-\infty}^{\infty} (-1)^j \sigma_j^z + \sum_{j=-\infty}^{\infty} \left[\frac{1}{2}(\sigma_j^z\sigma_{j+1}^z + 1) - \epsilon\,(\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+)\right], \quad (2)$$

where $\sigma_j^{\pm} = \frac{1}{2}(\sigma_j^x \pm i\sigma_j^y)$. The ground states and the low-energy excitations of the Hamiltonian (2) can be effectively studied [5,10] by means of the Rayleigh-Schrödinger perturbation theory in the small parameter ϵ. We shall describe these straightforward calculations to the first order in ϵ in order to gain insight into the nature of the two-kink bound states of the Hamiltonian (1) in the case of a generic $\Delta < -1$.

The zero-order Hamiltonian $\mathcal{H}_I(0,h) = \mathcal{H}_I(0,0)$ has two antiferromagnetic ground states,

$$|\Phi_1\rangle = |\ldots\downarrow \overset{0}{\underline{\uparrow}}\overset{1}{\downarrow}\uparrow\downarrow\ldots\rangle, \quad |\Phi_2\rangle = |\ldots\uparrow \overset{0}{\underline{\downarrow}}\overset{1}{\uparrow}\downarrow\uparrow\ldots\rangle, \quad (3)$$

which are degenerate in energy, $\mathcal{H}_I(0,0)|\Phi_{1,2}\rangle = 0$.

The localized one-kink states $|K_{\alpha\beta}(j)\rangle$ interpolate between the vacua $|\Phi_\alpha\rangle$ and $|\Phi_\beta\rangle$ to the left and to the right, respectively, from the bond connecting the sites j, $j+1$. In the state $|K_{\alpha\beta}(j)\rangle$, only two adjacent spins at the sites j and $j+1$ have the same orientations. The one-kink states can be classified also by their spin $s = \pm 1/2$. Namely $S^z|K_{\alpha\beta}(j)\rangle = s\,|K_{\alpha\beta}(j)\rangle$, where $s = 1/2$ if the neighbouring spins $j, j+1$ forming the kink are orientated "up", and $s = -1/2$ if the spins $j, j+1$ have the "down" orientation. For the given localized one-kink state $|K_{\alpha\beta}(j)\rangle$, let us denote by $\rho = 0, 1$ the parity of the kink location j, $\rho = j \bmod 2$. One can easily see that the three discrete parameters ρ, α, s characterising the localized kink are not independent. For example, the kink $|K_{12}(j)\rangle$ has the spin $s = 1/2$ for even j, and $s = -1/2$ otherwise. In the general case, the relation between parameters ρ, α, s can be described by the function $\rho(s,\alpha) = \frac{1}{2}[1 + (-1)^\alpha 2s]$.

In the topologically neutral sector, the lowest-energy excitations are the two-kink states. The basis of localized two-kink states is formed by the vectors $|K_{\alpha\beta}(j_1)K_{\beta\alpha}(j_2)\rangle$ where $j_1, j_2 \in \mathbb{Z}$, $j_1 < j_2$. These states can be classified by the total spin

$$S^z|K_{\alpha\beta}(j_1)K_{\beta\alpha}(j_2)\rangle = s\,|K_{\alpha\beta}(j_1)K_{\beta\alpha}(j_2)\rangle, \quad (4)$$

where $s = 0, \pm 1$, $s = s_1 + s_2$, with $s_{1,2}$ denoting the spins of the individual kinks. One can easily see, that $s = 0$ for even $(j_2 - j_1)$, and $s = \pm 1$ for odd $(j_2 - j_1)$. So, $|s| = \kappa$ where $\kappa = (j_2 - j_1) \bmod 2$.

Denote by P_2 the orthogonal projector onto the two-kink subspace $\mathcal{L}_2$ spanned by the basis $|K_{\alpha\beta}(j_1)K_{\beta\alpha}(j_2)\rangle$, and by $\mathcal{H}_2(\epsilon, h) = P_2\mathcal{H}_I(\epsilon, h)P_2$ the restriction of the Hamiltonian (2) on $\mathcal{L}_2$. At $\epsilon = 0$, all the two-kink states $|\Psi\rangle \in \mathcal{L}_2$ are characterized by the same energy, $\mathcal{H}_I(0,h)|\Psi\rangle = 2|\Psi\rangle$. At $\epsilon > 0$, this degeneracy is removed in the linear order in ϵ. This allows one to restrict the first-order analysis of the low-lying excitation energy spectra of the Hamiltonian (2) to the subspace $\mathcal{L}_2$.

The reduced two-kink Hamiltonian $\mathcal{H}_2(\epsilon, h)$ acts on the basis states of $\mathcal{L}_2$ as follows:

$$\begin{aligned}
&\mathcal{H}_2(\epsilon,h)\,|K_{\alpha\beta}(j_1)K_{\beta\alpha}(j_2)\rangle = \\
&[2 + f_0(j_2 - j_1)]\,|K_{\alpha\beta}(j_1)K_{\beta\alpha}(j_2)\rangle \\
&-\epsilon\big\{|K_{\alpha\beta}(j_1 - 2)K_{\beta\alpha}(j_2)\rangle + |K_{\alpha\beta}(j_1)K_{\beta\alpha}(j_2 + 2)\rangle \\
&+ [|K_{\alpha\beta}(j_1 + 2)K_{\beta\alpha}(j_2)\rangle + |K_{\alpha\beta}(j_1)K_{\beta\alpha}(j_2 - 2)\rangle] \\
&\times (1 - \delta_{j_2-j_1,1})(1 - \delta_{j_2-j_1,2})\big\}. \quad (5)
\end{aligned}$$

Here $f_0 = 2h\epsilon$ is the "string tension", which determines the linear attractive potential acting between the two kinks.

At $h = 0$, the reduced Hamiltonian (5) is diagonalised by the the two-kink states $|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{s_1 s_2} \in \mathcal{L}_2$ characterised by the momenta $p_1, p_2 \in \mathbb{R}/\pi\mathbb{Z}$, and the spins $s_1, s_2 = \pm 1/2$ of the individual kinks,

$$\begin{aligned}
&\mathcal{H}_2(\epsilon,0)\,|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{s_1 s_2} = \quad (6)\\
&[\omega_0(p_1) + \omega_0(p_2)]\,|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{s_1 s_2}, \\
&|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{s_1 s_2} = \\
&\sum_{m_1=-\infty}^{\infty} \sum_{m_2 > m_1 + (\rho_2 - \rho_1)/2}^{\infty} \Big\{\Big[e^{i(p_1 j_1 + p_2 j_2)} \\
&+ S_s(p_1,p_2)e^{i(p_2 j_1 + p_1 j_2)}\Big]|K_{\alpha\beta}(j_1)K_{\beta\alpha}(j_2)\rangle\Big\}_{\substack{j_1 = 2m_1 - \rho_1 \\ j_2 = 2m_2 - \rho_2}}, \quad (7)
\end{aligned}$$

where $\rho_1 = \rho(s_1, \alpha), \rho_2 = \rho(s_2, \beta)$, $s = s_1 + s_2 = 0, \pm 1$, $S_s(p_1, p_2)$ denotes the two-kink scattering amplitude

$$S_s(p_1,p_2) = -e^{i(p_1 - p_2)|s|}, \quad (8)$$

and $\omega_0(p)$ is the kink dispersion law,

$$\omega_0(p) = 1 - 2\epsilon\cos(2p). \tag{9}$$

The two-kink states (7) transform in a simple way under the action of the modified translation operator $\widetilde{T}_1$,

$$\widetilde{T}_1|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{s_1 s_2} = e^{i(p_1+p_2)}|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{-s_1,-s_2}, \tag{10}$$

and satisfy the Faddeev-Zamolodchikov commutation relations,

$$|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{s_1 s_2} = S_{s_1+s_2}(p_1,p_2)|K_{\alpha\beta}(p_2)K_{\beta\alpha}(p_1)\rangle_{s_1 s_2}. \tag{11}$$

At $h > 0$, the eigenvalue problem for the Hamiltonian $\mathcal{H}_2(\epsilon, h)$ can be solved following the procedure described in [8,11]. To this end, let us represent the eigenstate of the Hamiltonian $\mathcal{H}_2(\epsilon, h)$ in the form

$$|\Psi(P,\kappa,\rho_1)\rangle = \sum_{m=-\infty}^{\infty}\sum_{r=1}^{\infty}\Big[e^{iP(j_1+r)}\psi(r|P,\kappa,\rho_1) \times |K_{12}(j_1)K_{21}(j_1+j)\rangle\Big]_{j_1=2m-\rho_1,\, j=2r-\kappa}, \tag{12}$$

where $P \in \mathbb{R}/(\pi\mathbb{Z})$ is the total quasi-momentum of two kinks, and the discrete parameters κ and ρ_1 take the values $0, 1$. As was explained earlier, the parameter κ equals the absolute value of the total spin of the two-kink state, $\kappa = |s|$. The eigenstate problem $\mathcal{H}_2(\epsilon, h)|\Psi(P,\kappa,\rho_1)\rangle = E(P,\kappa)|\Psi(P,\kappa,\rho_1)\rangle$ reduces due to (5) to the discrete Sturm-Liouville problem with the linear potential in the half-line for the wave function $\psi(r)$,

$$[2 + f_0\,(2r-\kappa) - E(P,\kappa)]\psi(r) - 2\epsilon\cos P\ \ [\psi(r+1) + \psi(r-1)] = 0, \tag{13}$$

where $r = 1, 2, \ldots$, and the Dirichlet boundary condition $\psi(0) = 0$ is imposed. Note that the distance between the two kinks is $(2r - \kappa)$.

Exploiting the equality

$$J_{\nu+1}(Z) + J_{\nu-1}(Z) = \frac{2\nu}{Z}\,J_\nu(Z),$$

one can immediately write down [12] the explicit solution of the discrete Sturm-Liouville problem (13) in terms of the Bessel function $J_\nu(Z)$. The resulting energy spectrum reads

$$E_n(P,\kappa) = 2 - 2\epsilon\,h\,[\kappa + 2\nu_n(P)], \tag{14}$$

where $\nu_n(P)$ are the solutions of the equation

$$J_{\nu_n(P)}(h^{-1}\cos P) = 0,$$

with $n = 1, 2, \ldots$.

Equation (14) determines, for arbitrary $h > 0$, the exact small-ϵ asymptotics for the energy spectrum of the two-kink bound states for the Hamiltonian (2) to the first order in ϵ. A very similar energy spectrum was found in [8] (see eqs. (54), (59), (60) therein), where the kink confinement in the quantum Ising spin-chain was studied.

In the case of small $h \to +0$, two asymptotical expansions can be obtained [8] from (14), using the well-known properties of the Bessel function. For not very large $n = 1, 2, 3, \ldots$, the *low-energy expansion* in the fractional powers of h holds,

$$E_n(P,\kappa) = 2 - 4\epsilon\cos P + 4\epsilon\left(\frac{\cos P}{2}\right)^{1/3} h^{2/3}\mathrm{z}_n - 2\epsilon\kappa h + O(h^{4/3}), \tag{15}$$

where $-\mathrm{z}_n$ are the zeroes of the Airy function. In the case of large $n \gg 1$, one can use instead the *semi-classical expansion*

$$E_n(P,\kappa) = 2 - 2\epsilon h\kappa - 4\epsilon\cos P\,\cos(2p_a(P)). \tag{16}$$

Here $p_a(P)$ is the solution of two equations

$$2p_a\lambda_a + \sin(2p_a) = \frac{\pi h}{\cos P}\left(n - \frac{1}{4}\right) + O(h^2), \tag{17}$$

$$\cos(2p_a) = -\lambda_a, \tag{18}$$

which determine also the parameter λ_a. Derivation of the asymptotic formulas (15), (16) from the exact energy spectrum (14) almost literally reproduces the derivation of the similar small-h asymptotics for the exact energy spectrum in the Toy model 1, which was described in much detail in sect. 6.1 of [8].

It turns out, that the small-h asymptotic representations (15), (16) for the two-kink bound-state energy spectra can be also derived by means of a different, semi-heuristic approach, which was initially developed for the Ising field theory [7,13], and then applied to the quantum Ising spin-chain model [8], and to the Potts Field Theory (PFT) [14]. The high accuracy of the analytical predictions obtained by this technique was confirmed later [15,16] by direct numerical calculations of the kink bound-state energy spectra in the confinement regime for all three models mentioned above. In the cases of the Ising field theory and the Ising spin chain model, the semi-heuristic technique reproduces the initial terms of the asymptotical expansions for the bound-state energy spectra obtained by the more powerful technique based on the Bethe-Salpeter equation. For the PFT, the meson mass spectra calculation by means of the latter method is still lacking. In what follows, we shall describe the semi-heuristic technique for the case of the extreme anisotropic limit $\Delta \to -\infty$ of the antiferromagnetic XXZ model, and then apply it to the general case $\Delta < -1$.

Let us treat the two kinks as classical particles having the z-projections of the spin $s_i = \pm 1/2$, $i = 1, 2$, moving along the line, and attracting one another with a linear potential. Their Hamiltonian will be taken in the form

$$H(x_1, x_2, p_1, p_2, s_1, s_2) = \omega_0(p_1) + \omega_0(p_2) + f_0[|x_2 - x_1| - \kappa(s_1, s_2)]. \tag{19}$$

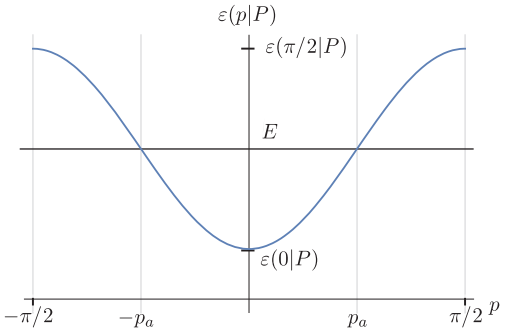

Fig. 1: (Colour online) Kinetic energy (22) of two kinks as a function of p. For the energy E, the classically allowed region is $[-p_a, p_a]$.

Here $x_1, x_2 \in \mathbb{R}$ are the kink spacial coordinates, $\kappa(s_1, s_2) = \delta_{s_1,s_2}$, and $\omega_0(p)$ is the kink dispersion law (9).

After the canonical transformation

$$X = \frac{x_1 + x_2}{2}, \qquad x = x_2 - x_1, \tag{20a}$$

$$P = p_1 + p_2, \qquad p = \frac{p_2 - p_1}{2}, \tag{20b}$$

the Hamiltonian (19) takes the form

$$H(p, x|P) = \varepsilon(p|P) + f_0|x|, \tag{21}$$

where

$$\varepsilon(p|P) = \omega_0(p + P/2) + \omega_0(p - P/2) - f_0\kappa. \tag{22}$$

In order to simplify notations, we have dropped here the spin arguments s_1, s_2, as well as the argument κ in the function $\varepsilon(p|P, \kappa)$ defined by (22).

The topology of the phase trajectories in the (x, p)-plane depends on the total energy E of the two kinks, as is clear from fig. 1. The phase trajectories are closed for $\varepsilon(0|P) < E < \varepsilon(\pi/2|P)$. In this case, the solution of the canonical equations describes the oscillatory motion of two kinks in the center-of-mass frame that drifts with a constant average velocity.

There are two different ways to quantize the model (19). For small oscillations, the kinetic-energy term (22) can be expanded to the second order in the momentum p, with the subsequent replacement of the latter by the operator $-i\partial_x$. The resulting Schrödinger equation can be reduced to the Airy equation in the half-line $0 < x < \infty$, which, together with the Dirichlet boundary condition at $x = 0$, gives rise to the energy spectrum (15). For the high-amplitude oscillations with energies in the interval $\varepsilon(0|P) < E < \varepsilon(\pi/2|P)$, the energy levels can be found [8] by means of the Bohr-Sommerfeld quantization rule. The resulting spectrum reads

$$2E_n(P, \kappa)p_a - \int_{-p_a}^{p_a} \mathrm{d}p\, \varepsilon(p|P) = 2\pi f_0\,(n - 1/4), \tag{23}$$

with $E_n(P, \kappa) = \varepsilon(p_a|P)$ and $n \gg 1$, which is equivalent to (16)–(18). Note that the left-hand side of (23) is the Legendre transform of the integral $\int_{-p_a}^{p_a} \varepsilon(p|P)\,\mathrm{d}p$ considered as a function of the variable p_a.

General case $\Delta < -1$. – Let us turn to the general case of the XXZ spin-chain model (1) in the antiferromagnetic phase $\Delta < -1$. We shall use the standard parametrisation for the anisotropy constant $\Delta = -\cosh\gamma$, and $q = \exp\gamma > 1$.

At zero field $h = 0$, the model considered on a finite chain is solvable by the Bethe Ansatz method [17], see also [18,19] for further references. In the thermodynamic limit, it has two degenerate ground states $|\Phi_\alpha\rangle$, $\alpha = 1, 2$, showing a Néel-type order,

$$\langle\Phi_1|\sigma_j^z|\Phi_1\rangle = -\langle\Phi_2|\sigma_j^z|\Phi_2\rangle = (-1)^j\bar{\sigma},$$

with the spontaneous magnetization [20–22]

$$\bar{\sigma} = \prod_{n=1}^{\infty}\left(\frac{1 - q^{-2n}}{1 + q^{-2n}}\right)^2. \tag{24}$$

The lowest-energy excitations are topologically charged, being represented [10,23] by the kinks $|K_{\alpha\beta}(p)\rangle_s$ interpolating between the vacua α and β, and characterised by the quasi-momentum $p \in \mathbb{R}/(\pi\mathbb{Z})$, and by the z-projection of the spin $s = \pm 1/2$. The dispersion relation of these excitations reads [24],

$$\omega(p) = \frac{2K}{\pi}\,\sinh\gamma\,\sqrt{1 - k^2\cos^2 p}. \tag{25}$$

Here K and K' are the complete elliptic integrals of modulus k and $k' = \sqrt{1 - k^2}$, respectively, such that $K'/K = \gamma/\pi$. The dispersion relation (25) can be parametrized in terms of the Jacobi elliptic functions

$$p(\lambda) = \frac{\pi}{2} - \mathrm{am}(2K\lambda/\pi, k), \tag{26}$$

$$\omega(\lambda) = \frac{2K}{\pi}\,\sinh\gamma\,\mathrm{dn}(2K\lambda/\pi, k), \tag{27}$$

with the rapidity variable $\lambda \in [-\pi/2, \pi/2]$.

The number of kinks must be even in the topologically neutral sector. The two-kink basis states $|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{s_1 s_2}$, characterized by the quasi-momenta $p_{1,2}$ and the spins $s_{1,2}$ of the individual kinks, diagonalize the Hamiltonian $\mathcal{H}(\Delta, 0)$ and the total spin S^z with the eigenvalues $\omega(p_1) + \omega(p_2)$ and $s_1 + s_2$, respectively. The translation properties of these states are determined by eq. (10). In the extreme anisotropic limit $\gamma \to \infty$, the two-kink states $|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{s_1 s_2}$ reduce to (7).

Let us define the following basis in the two-kink subspace with $S^z = 0$:

$$|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_\pm \equiv \frac{1}{\sqrt{2}}\Big(|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{1/2,-1/2} \pm |K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{-1/2,1/2}\Big). \tag{28}$$

The modified translation operator becomes diagonal in this basis:

$$\widetilde{T}_1|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_\pm = \pm e^{i(p_1+p_2)}|K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_\pm. \quad (29)$$

The two-kink scattering at $h = 0$ can be described by the Faddeev-Zamolodchikov commutation relations:

$$\begin{aligned} |K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{ss} &= w_0(p_1,p_2)|K_{\alpha\beta}(p_2)K_{\beta\alpha}(p_1)\rangle_{ss}, \\ |K_{\alpha\beta}(p_1)K_{\beta\alpha}(p_2)\rangle_{\pm} &= w_\pm(p_1,p_2)|K_{\alpha\beta}(p_2)K_{\beta\alpha}(p_1)\rangle_{\pm}. \end{aligned} \quad (30)$$

The three scattering amplitudes $w_\eta(p_1,p_2)$, with $\eta = 0, \pm$, can be parametrized by the rapidity variable,

$$w_\eta(p_1,p_2) = \exp[-i\pi + i\theta_\eta(p_1,p_2)], \quad (31)$$

$$\theta_\eta(p_1,p_2) = \Theta_\eta(\lambda_1 - \lambda_2), \quad (32)$$

$$\Theta_0(\lambda) = -\lambda - \sum_{n=1}^{\infty} \frac{e^{-n\gamma}\sin(2\lambda n)}{n\cosh(n\gamma)}, \quad (33)$$

$$\Theta_\pm(\lambda) = \Theta_0(\lambda) + \chi_\pm(\lambda), \quad (34)$$

$$\chi_+(\lambda) = -i\ln\left[-\frac{\sin(\lambda - i\gamma)/2)}{\sin(\lambda + i\gamma)/2)}\right], \quad (35)$$

$$\chi_-(\lambda) = -i\ln\left[\frac{\cos(\lambda - i\gamma)/2)}{\cos(\lambda + i\gamma)/2)}\right], \quad (36)$$

where $p_j = p(\lambda_j)$, $j = 1, 2$, and $\Theta_\eta(\lambda)$ are the scattering phases. The scattering amplitude $w_0(p_1,p_2)$ was found by Zabrodin [25], and the whole two-kink scattering matrix was determined by Davies *et al.* [26]. In the extreme anisotropic limit $\gamma \to \infty$, the commutation relations (30) reduce to (11).

The application of a staggered magnetic field $h > 0$ breaks the integrability of the XXZ model and leads at $\Delta < -1$ to the confinement of the kinks into the bound states. The natural way to study their energy spectrum is to apply some perturbative technique in small h around the exact solution at $h = 0$. The most systematic but technically rather hard realization of this idea should exploit the Bethe-Salpeter equation [7,27], together with the appropriate form factor perturbative expansion [28,29]. Here we shall apply instead the more simple semi-heuristic approach, which was outlined above. Since the vacuum $|\Phi_2\rangle$ becomes metastable at $h > 0$, we shall concentrate in the following on the topological neutral sector spanned by the basis states $|K_{12}(p_1)K_{21}(p_2)\rangle_{s_1 s_2}$.

So, let us consider two interacting particles moving in the line, whose classical evolution is determined by the Hamiltonian

$$H(x_1,x_2,p_1,p_2) = \omega(p_1) + \omega(p_2) + f\,|x_2 - x_1|. \quad (37)$$

Now the particle kinetic energy $\omega(p)$ is taken in the form (25), and for the string tension we use its value $f = 2h\bar{\sigma}$ at $h \to +0$, where the spontaneous magnetisation $\bar{\sigma}$ is given by (24). Quantization of the periodical motion of two particles in the center-of-mass frame should allow one to determine the energy spectrum of the two-kink bound states of model (1) at $h \to +0$.

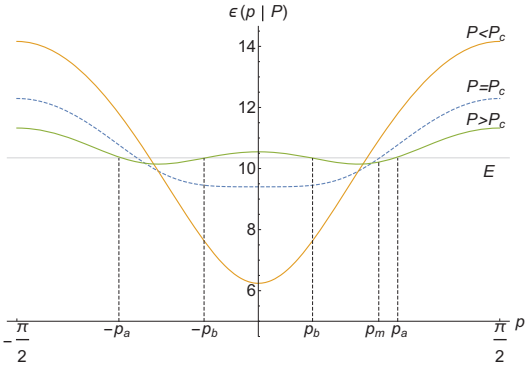

Fig. 2: (Colour online) Kinetic energy (38) of two kinks at $\Delta = -5$ as the function of p for three values of their total momentum P: $P < P_c$, $P = P_c$, and $P > P_c$. For the energy E in the latter case, the classically allowed regions are $[p_b, p_a]$ and $[-p_a, -p_b]$.

Two new features, which modify the analysis, must be taken into account. First, due to the different kink dispersion law (25), the profile of the effective kinetic energy $\varepsilon(p|P)$ in the center-of-mass frame

$$\varepsilon(p|P) = \omega(p + P/2) + \omega(p - P/2), \quad (38)$$

now transforms with increasing total momentum P, as is shown in fig. 2. At small total momenta P, the kinetic energy $\epsilon(p|P)$ takes its minimal value at the origin $p = 0$, and monotonically increases with p at $0 < p < \pi/2$. At large enough P, the kinetic energy becomes non-monotonic. It has a local maximum at $p = 0$, and two minima located at $p = \pm p_m(P)$. The transition between these two regimes takes place at the critical value $P_c(k') = \arccos(\frac{1-k'}{1+k'})$ of the total momentum. As a result, the classical phase portrait of the two-particle relative motion changes at $P > P_c(k')$, which also affects the quantization of their dynamics.

Fortunately, the kink dispersion law (25) in the antiferromagnetic XXZ-model coincides up to a reparametrization with the kink dispersion law in the Ising spin-(1/2) chain in a transverse magnetic field. This fact allows one to apply the results of the paper [8], in which the same semi-heuristic approach has been used to calculate the two-kink energy spectrum in the latter model, together with the more systematic method based on the Bethe-Salpeter equation.

Then, in contrast to the Ising model, the kinks in the XXZ-model are not free particles, but strongly interact at small distances already at $h = 0$. This short-range interaction leads to the nontrivial two-kink scattering, which must be properly taken into account. The problem of kink confinement in the presence of a nontrivial kink-kink scattering has been already studied in the case of the PFT [14]. The dynamics of two kinks confined into a bound state in the semiclassical regime at $h \ll 1$ was described in [14] in two different ways. At large separations $|x_2 - x_1|$, the two

kinks were treated as classical particles moving according to the canonical equations of motion. When the two kinks approach one another at some point $x_2 = x_1$ having the momenta p_1 and p_2, they undergo quantum scattering, which is described by the Faddeev-Zamolodchikov commutation relations analogous to (30). As a result, the semi-classical energy spectrum of the two-kink bound states becomes explicitly dependent on the kink-kink scattering phases. Applying the same strategy, we calculated the energy spectrum of the two-kink bound states in the XXZ-model for any $\Delta < -1$ to the first order in $h \to +0$. Here we shall present the results only. The details of the calculations, which are to much extent similar to those described in papers [8,14], will be published elsewhere.

There are three spectral modes, which will be distinguished by the parameter η taking the "values" 0 and $\pm$. The twofold degenerate mode with $\eta = 0$ corresponds to the kink bound states with $S^z = \pm 1$. Two other modes $\eta = \pm$ correspond to the kink bound states with $S^z = 0$. The wave functions of such states can be expanded in the bases (28), which diagonalize the scattering matrix at $h = 0$. These two $S^z = 0$ modes, which are degenerate in the Ising limit $\Delta \to -\infty$, split at finite $\Delta < -1$ due to the difference in their two-kink scattering phases. The lowest energy of all three spectral modes has the mode with $\eta = 0$.

At $|P| < P_c(k')$, the initial terms of the low-energy expansion take the form

$$E_n(P,\eta) = 2\,\omega(P/2) + f^{2/3}[\omega''(P/2)]^{1/3}\mathrm{z}_n + f\frac{\sinh\gamma}{\omega(P/2)}\partial_\lambda\Theta_\eta(\lambda)\big|_{\lambda=0} + O(f^{4/3}), \quad (39)$$

where $n = 1, 2, \ldots$, and $-\mathrm{z}_n$ are the zeroes of the Airy function. So, the shifts between the energy spectra of the three modes with different η are proportional to the magnetic field.

The leading term of the semi-classical expansion for the energy spectra of all three modes at $|P| < P_c(k')$ reads

$$2E_n(P,\eta)\,p_a - \int_{-p_a}^{p_a}\varepsilon(p|P)\,\mathrm{d}p = f\left[2\pi\left(n-\frac{1}{4}\right) + \theta_\eta\left(\frac{P}{2}-p_a, \frac{P}{2}+p_a\right)\right] + O(f^2), \quad (40)$$

where $n \gg 1$, $\theta_\eta(p_1, p_2)$ are the scattering phases defined by (32), and $p_a \in (0, \pi/2)$ is the solution of the equation $E_n(P,\eta) = \varepsilon(p_a|P)$.

At $P_c(k') < |P| < \pi/2$, the low-energy expansion takes the form

$$E_n^{(1,2)}(P,\eta) = \varepsilon(p_m|P) + f^{2/3}\left[\frac{\partial_p^2\varepsilon(p|P)\big|_{p=p_m}}{2}\right]^{1/3} x_n^{(1,2)} + \frac{f}{2}\,\partial_p\,\theta_\eta(P/2-p, P/2+p)\big|_{p=p_m} + O(f^{4/3}), \quad (41)$$

where $p_m = \frac{1}{2}\arccos(\cos P/\cos P_c)$ is the location of the minimum of the kinetic energy $\varepsilon(p|P)$, and $-x_n^{(1)} = -\mathrm{z}_n$ and $-x_n^{(2)} = -\mathrm{z}'_n$ are the zeroes of the the Airy function and of its derivative, respectively, $Ai(-\mathrm{z}_n) = 0$, $Ai'(-\mathrm{z}'_n) = 0$, $n = 1, 2, \ldots$. The semi-classical asymptotics at $E_n(P,\eta) \in (\varepsilon(p_m|P), \varepsilon(0|P))$ modifies to the form

$$E_n(P,\eta)\,(p_a - p_b) - \int_{p_b}^{p_a}\varepsilon(p|P)\,\mathrm{d}p = f\pi\left(n-\frac{1}{2}\right) + \frac{f}{2}\left[\theta_\eta\left(\frac{P}{2}+p_b, \frac{P}{2}-p_b\right) + \theta_\eta\left(\frac{P}{2}-p_a, \frac{P}{2}+p_a\right)\right] + O(f^2), \quad (42)$$

where $p_{a,b} \in (0, \pi/2)$ are the positive solutions of the equation

$$E_n(P,\eta) = \varepsilon(p_a|P) = \varepsilon(p_b|P), \qquad p_b < p_a. \quad (43)$$

For the energies in the interval $E_n(P,\eta) \in (\varepsilon(0|P), \varepsilon(\pi/2|P))$, the semi-classical spectrum is described by eq. (40).

At $|P| = P_c(k')$, the Taylor expansion of the kinetic energy $\epsilon(p|P_c) = \epsilon(0|P_c) + \frac{p^4}{4!}\partial_p^4\varepsilon(p|P_c)\big|_{p=0} + \ldots$ does not contain the quadratic term. As a result, the low-energy expansion changes to the form

$$E_n(P_c,\eta) = 2\omega(P_c/2) + f^{4/5}\left[\frac{\partial_p^4\varepsilon(p|P_c)\big|_{p=0}}{6}\right]^{1/5} c_n + f\frac{\sinh\gamma}{\omega(P_c/2)}\partial_\lambda\Theta_\eta(\lambda)\big|_{\lambda=0} + O(f^{8/5}), \quad (44)$$

where c_n are the consecutive solutions of eq. (93) in [8]. The numerical values of the first three ones are $c_1 = 1.787$, $c_2 = 3.544$, $c_3 = 5.086$. The low-energy expansion (44) holds for the energies slightly above the lower bound of the spectrum, $E \approx \varepsilon(0|P_c)$. For higher energies in the interva $\varepsilon(0|P_c) < E < \varepsilon(\pi/2|P_c)$, the semi-classical asymptotics (40) can be used.

Conclusions. – The energy spectrum of the two-kink bound states in the XXZ spin-(1/2) chain model (1) in the massive antiferromagnetic phase in the presence of a staggered magnetic field is calculated perturbatively in two asymptotic regimes: i) in the extreme anisotropic limit $\Delta \to -\infty$ to the first order in $\epsilon = 1/|\Delta|$, and ii) for generic $\Delta < -1$ at a weak magnetic field, to the first order in h. Preliminary analysis shows a good agreement[1] of the obtained analytical representations for the energy spectra with the results of numerical calculations performed by Bera *et al.* and presented in figs. 10–15 of [5]. To illustrate this, we have displayed in fig. 3 by solid curves the magnetic-field dependence for the lowest mode energy calculated by eq. (39) at two values of the anisotropy parameter $\Delta = -2$, and $\Delta = -5$. The points in fig. 3

[1]Note that due to (29), only the $\eta = +$ mode with $S^z = 0$ contributes to the longitudinal structure factor $S^{zz}(\omega, Q = \pi)$, which is displayed by red curves in figs. 12–15 of [5], while the other $S^z = 0$ mode with $\eta = -$ contributes to the structure factor $S^{zz}(\omega, Q = 0)$.

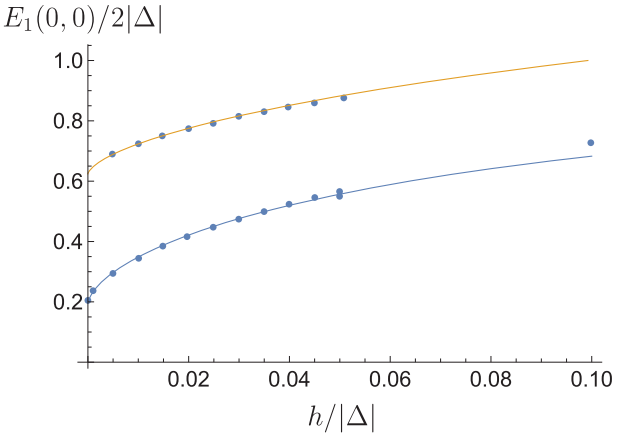

Fig. 3: (Colour online) The energy of the first bound state for the mode $\eta = 0$ at $P = 0$ *vs.* the magnetic field calculated from (39) at $\Delta = -5$ (upper curve), and at $\Delta = -2$ (lower curve). The points display the results of numerical calculations on the finite chains at the same values of the parameters performed by Bera *et al.* and presented in fig. 11 of [5].

represent the numerical results for the same energy spectra extracted from fig. 11 of ref. [5]. Taking into account, that no fitting parameters have been used, the agreement is seen to be excellent.

Of course, the detailed comparison of the obtained analytical results with already existing [5] numerical and experimental data is required. On the other hand, it is desirable to validate the obtained results (39)–(44) by reproducing them in a more powerful and systematic approach based on the Bethe-Salpeter equation.

* * *

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