I-75

e
f

объединенный
институт
ядерных
исследований
дубна

E17-81-575

U.Lindner*

SOLITARY EXCITATION IN Λ-D SYSTEMS WITH FINITE BAND WIDTH

Submitted to "physica status solidi"

* Sektion Physik, Karl-Marx-Universität, Leipzig, DDR.

1981

The experimental results in quasi- 1-d -antiferromagnets, e.g., TMMC, CPC [1], which suggest nonlinear effects, have been interpreted as yet in terms of the antiferromagnetic Heisenberg model.

Here we consider a 1-d model with finite band width, for which we have shown recently [2-4,5] that in continuum approximation solitary solutions exist. We calculate the excitation energy and in the way as Krumhansl and Schrieffer [6] the free energy, the static correlation function of the lattice motion and the width of the central peak of the dynamic structure factor connected with the solitary excitations.

Formerly we have shown [4] that the model in time-dependent mean-field approximation and in continuum limit is given by the following Lagrangian density

$$\mathfrak{L} = i \sum_\sigma (\Phi^*_\sigma \dot{\Phi}_\sigma - \dot{\Phi}^*_\sigma \Phi_\sigma) + Ma^2 \dot{x}^2 - \underset{\sim}{\mathcal{H}} =$$

$$= i \sum_\sigma (\Phi^*_\sigma \dot{\Phi}_\sigma - \dot{\Phi}^*_\sigma \Phi_\sigma) + \frac{M}{2} a^2 \dot{x}^2 - \frac{M}{2} a^2 \omega_0^2 x'^2 -$$

$$- 2[-t + Ja(\lambda - x')] \sum_\sigma \Phi^*_{\mp\sigma} \Phi_\sigma + [-t + Ja] \sum_\sigma \Phi^{*\prime}_{\mp\sigma} \Phi'_\sigma - \tag{1}$$

$$- \frac{U}{2} (\sum_\sigma \Phi^*_\sigma \Phi_{-\sigma})^2 + \mu \sum_\sigma |\Phi_\sigma|^2 ,$$

with the condition that $\frac{\partial}{\partial \xi} \sum_\sigma \Phi^*_\sigma \Phi_{\mp\sigma} = 0$ at the boundary of the system. $\mathcal{H}$ is the Hamiltonian density and for the other notations see ref. [1]. Instead of $t < 0$ in ref. [1] we write here $-t$. In continuum limit we have $R_{j0} \to a\xi$ and $\check{u}_j(t) \to ax(\xi, t)$. The upper signs in (1) concern the antiferromagnetic case; the lower signs, the ferromagnetic one. In the following we restrict ourselves to the antiferromagnetic case. Instead of the complex probability amplitudes $\Phi_\sigma(\xi, t)$ and $\Phi_{-\sigma}(\xi, t)$ to find an electron with spin σ or $-\sigma$ at the time t at the place $a\xi$ in the chain we use the fields $C_\pm(\xi, t) = \frac{1}{\sqrt{2}}(\Phi_\sigma \pm \Phi_{-\sigma})$.

For the equations of motion $\frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial \dot\phi} + \frac{\partial}{\partial \xi}\frac{\partial \mathcal{L}}{\partial \phi'} - \frac{\partial \mathcal{L}}{\partial \phi} = 0$, where $\phi \hat{=} \{r, C_+, C_-\}$ we obtain

$$M\ddot{x} = M\omega_0^2 x'' - \frac{2J}{a}\frac{\partial}{\partial \xi}(|C_+|^2 - |C_-|^2),$$

$$i\dot{C}_+ - T_0 C_+'' - (2T_0 - \mu)C_+ + 2Jax'C_+ - U(|C_+|^2 - |C_-|^2)C_+ = 0, \tag{2}$$

$$i\dot{C}_- + T_0 C_-'' - (-2T_0 - \mu)C_- - 2Jax'C_- + U(|C_+|^2 - |C_-|^2)C_- = 0,$$

with $T_0 = -t + Ja$.

This system possesses in the case of constant electron density $n(\xi, t) = |C_+|^2 + |C_-|^2 = \text{const.}$ solitary solutions of the type

$$x(\xi, t) = x_0 \tanh\{\kappa(\xi - \xi_0 - \omega t)\}, \tag{3a}$$

$$C_+(\xi, t) = C_+^0 \,\mathrm{sech}\{\gamma(\xi - \xi_0 - \check{u}t)\}\exp\{i\beta(\xi - \xi_0) - i\nu_+ t\},$$

$$C_-(\xi, t) = C_-^0 \tanh\{\gamma(\xi - \xi_0 - \check{u}t)\}\exp\{i\delta(\xi - \xi_0) - i\nu_- t\}. \tag{3b}$$

(If the quantity $\gamma^2 > 0$ then $C_+(\xi, t)$ is of the type "tahn" and $C_-(\xi, t)$ is of the type "sech"). The frequency $\omega = \check{u}$ and the centre position ξ_0 are arbitrary. For the other parameters in (3) we obtain [3]

$$\kappa = \gamma = \sqrt{\frac{(U - \hat{J})n}{T_0}}, \quad C_+^0 = C_-^0 = \sqrt{n}, \quad x_0 = \frac{\hat{J}n}{Ja\kappa},$$

$$\beta = -\delta = -\frac{\check{u}}{2T_0}, \quad \nu_+ = 2T_0 - \hat{J}n - \mu - \frac{\check{u}^2}{4T_0}, \quad \nu_- = -2T_0 + Un - \mu + \frac{\check{u}^2}{4T_0} \tag{4}$$

with $\hat{J} = (2J)^2 / M(\omega_0^2 - \check{u}^2)$. We can interpret the solution (3) as solitary spin distortion (domain wall) of the antiferromagnetic ground state order (3b) which is accompanied by a solitary lattice distortion (3a)[4]. The non-linearity responsible for the solitary solutions is caused by the electron correlation as well as by the electron-phonon interaction. For the case of constant electron density one can give the N-soliton solution, too [7].

Solitary solutions of the type (3) with $\check{u} = \omega$, $\kappa = \gamma$ and $\beta = -\delta = -\frac{\check{u}}{2T_0}$ are also possible; if the amplitudes C_+^0 and C_-^0 are different, then the domain wall is accompanied by a solitary electron density wave

$$n(\xi, t) = C_+^{02} \operatorname{sech}^2\{\gamma(\xi-\xi_0-\check{u}t)\} + C_-^{02}\tanh^2\{\gamma(\xi-\xi_0-\check{u}t)\}, \quad (5)$$

where

$$\overline{n(\xi, t)}^{\,t} = n = C_-^{02} + \frac{2}{\gamma}(C_-^{02} - C_+^{02}) .$$

Makhankov et al.[8,9] described a further type of solitary spin distortions of the system (2) but it is not stable against small perturbations of the differential system in contrast to domain walls. Therefore we restrict ourselves to solution of the type (3).

The solitary lattice distortion (3a) is connected with the well-known Peierls instability of Λ-d systems and lowers the total zero-point energy of the system. A lattice particle at the point $a\cdot\xi$ of the chain has in the ground state two possibilities $a\xi \pm ax_0$ and owing to the solitary distortion it flips in. The one-site double-well potential $\phi_D(x) = \frac{A}{2}a^2x^2 + \frac{B}{4}a^4x^4$ with $A < 0$, and $B>0$, which is caused by the electronic system follows from $-\frac{2J}{a}\frac{\partial}{\partial\xi}(|C_+|^2 - |C_-|^2| \hat{=} -Ax - Ba^2x^2$. One obtains $|A| = Ba^2x_0^2 = 2\frac{(2J)^2}{\hat{J}}\kappa^2$, and $\phi_D(\pm x_0) = -\hat{J}(C_+^{02} + C_-^{02})$. In the case of $n(\xi, t) = \text{const}$ we get for the lowest energy of a lattice particle $\phi_D(\pm x_0) = -2\hat{J}n^2$. We remark that the investigation has been extended also to systems [4], where the Hamiltonian includes an additional one-site double-well potential ϕ such that the lattice is described by the standard model Hamiltonian for quasi- Λ-d-systems [6] which may undergo a structural phase transition. For vanishing electron correlation energy U these systems (modified Peierls chains) show also solitary solution of the type (3) with $\kappa = \gamma$, $\check{u} = \omega$ and $\beta = -\delta = -\frac{\check{u}}{2T_0}$, which are accompanied by solitary electron density waves. The amplitude x_0 of the solitary lattice distrotion is given by the width of the additional double-well potential. The depth of the additional potential increases in consequence of the solitary spin distortion by the term $-\hat{J}(C_+^{02} + C_-^{02})$.

Now we calculate the excitation energy $\int \mathcal{H}\, d\xi = E_{DK} + E_{DP}$ of the domain walls (3). The Hamilton density $\mathcal{H}$ we obtain from (1). The kinetic energy

$$E_{DK} = \int \frac{M}{2}a^2\dot{x}^2 d\xi = \frac{4}{3\kappa}\,\frac{M}{2}a^2x_0^2\check{u}^2\kappa^2 \quad (6)$$

can be written for slow moving walls $\check{u}^2 \ll \omega_0^2$ in the form $E_{DK}^0 = \frac{m_D}{2}\nu_D^2$, where $m_D = \frac{4}{3}\frac{M}{2}x_0^2\kappa$ for $\check{u}^2 \ll \omega_0^2$ is the kinetic effective mass and $\nu_D = a\check{u}$ is the velocity of the soliton (wall).

For the potential energy E_{DP} we obtain

$$\begin{aligned} E_{DP} = {} & \frac{2}{\kappa}\{\frac{1}{3}[(U-\hat{J})(C_+^{02}+C_-^{02})-T_0\kappa^2](C_+^{02}-2C_-^{02}) + \\ & + 2T_0(C_+^{02}+C_-^{02}) - T_0(\beta^2 C_+^{02}+\delta^2 C_-^{02}) - \mu(C_+^{02}-C_-^{02})\} = \\ & = \frac{2}{\kappa}\{\frac{1}{3}[(U-\hat{J})(C_+^{02}+C_-^{02})-T_0\kappa^2](C_+^{02}-2C_-^{02}) + \\ & + 4T_0[1-\frac{1}{4}(\beta^2+\delta^2)]C_+^{02}\}, \end{aligned} \tag{7}$$

because of

$$\mu = \frac{U}{2}C_-^{02} - 2T_0 + T_0\delta^2 .$$

For better understanding we discuss the result (7) for the case of constant electron density according to (4). Then it follows

$$E_{DP}(n=\text{const}) = \frac{2}{\kappa}\{-\frac{1}{3}(U-\hat{J})n^2 + 4T_0(\Lambda - \frac{\check{u}^2}{8T_0^2})n\}.$$

For slow moving walls, this means $\check{u}^2 \ll \omega_0^2$, $8T_0^2$ and $\hat{J} \to (2J)^2/M\omega_0^2$ we get

$$E_{DP}^0(n=\text{const}) = \frac{2}{\kappa}n\{4T_0 - \frac{1}{3}Un\} + \frac{2}{\kappa}\frac{1}{3}\hat{J}n \quad . \tag{8}$$

Considering (3) one sees that $2a/\kappa$ is the thickness of walls, and, because we have chosen ξ dimensionless, $2/\kappa$ is the number of lattice particles in the wall. Then $2n/\kappa$ is the number of electrons in the wall and we can interpret the first term in (8) as mean potential energy of electrons in the wall $\frac{2}{\kappa}n(\epsilon-\mu)$. The mean potential energy of an electron (related to zero) $\epsilon = \mu + 4T_0 - \frac{1}{3}Un = 2T_0 + \frac{1}{6}Un$ is higher than the lower edge of the s-band $2T_0 = -2t + 2Ja$ from which we have to count because of the long-wave approximation (continuum limit). The second term in (8) is the potential energy connected with the motion of lattice particles in the wall (we remember that we used a rigid-ion model). The mean potential energy of a lattice particle $\frac{1}{3}\hat{J}n^2$ is related to zero in (8) according to the selection of the Hamiltonian. (If we would count from the lowest energy of a lattice particle in the wall $\phi_D(\pm x_0) = -2\hat{J}n^2$ we would get $-\frac{5}{3}\hat{J}n^2$). To summarize we can say the excitation energy for slow moving walls lies very closed to the ground state energy of the system.

Because the excitation energy is finite for $\check{u} \to 0$ we can regard the slow moving solitons (walls) for low temperatures as a dilute gas of quasiparticles with the kinetic energy E^0_{DK} and the potential energy $\hat{E}^0_{DP}$ (related to the ground state energy) in a one-dimensional volume $aN = L$.

If we calculate the partition function Z_0, in the simple approximation of Krimhansl and Schrieffer /6/ ,dividing the one-dimensional volume in $n_s = L/\Delta$ segments of the thickness of a wall $\Delta = 2a/\kappa$, we get

$$Z_D = \sum_{n_w} \frac{n_s!}{n_w!\,(n_s - n_w)!} e^{-\beta n_w \hat{E}^0_{DP}} \left(\int \frac{d\nu_D}{B} e^{-\beta \frac{m_D}{2}\nu_D^2}\right)^{n_w}, \tag{9}$$

where n_w is the number of segments occupied by walls and B is an appropriate phase space normalization. In the approximation that Z_D is dominated by the most probable number n_w which if $\exp\{-\beta \hat{E}^0_{DP}\} \ll 1$ is also the mean value $\bar{n}_w = n_s \exp\{-\beta \hat{E}^0_{DP}\}$, from (9) we get using the Stirling formula

$$Z_D \simeq Z_{DK} \cdot Z_{DP} \simeq \left(\frac{2\pi k_B T}{B^2 m_D}\right)^{\bar{n}_w/2} e^{\bar{n}_w} .$$

Thus we obtain for the free energy connected with the walls

$$F_D = -k_B T \ln Z_D = -k_B T N \frac{\kappa}{2}\left[1 + \frac{1}{2}\ln\frac{2\pi k_B T}{B^2 m_D}\right] e^{-\hat{E}^0_{DP}/k_B T} . \tag{10}$$

This means, the free energy and the concentration $\bar{n}_w/n_s$ of the walls drop exponentially with decreasing temperature. The linear excitations of the lattice part (phonons) /6/ as well as of the electronic part of the system /10/ give contributions to the free energy proportional only to the temperature T.

For application it is interesting to calculate the static and the dynamic correlation function of the lattice motion. If the lattice particles are in the minima of ϕ_D in the ground state and flip from $x = \pm x_0$ to $\mp x$ owing to a solitary distortion we can use the approximation of Krumhansl and Schrieffer /6/, too.

We obtain for the static two-point correlation function $\langle x(0)\, x(\xi) \rangle$ if $\xi \gg 2/\kappa$ at low temperature, and at low density of walls

$$\langle x(0)\, x(\xi)\rangle = x_0^2 \exp\{-\xi \kappa e^{-\beta \hat{E}^0_{DP}}\} = x_0^2 \exp\{-\xi/\lambda_c\} \tag{11}$$

with the correlation length $\lambda_c = \frac{1}{\kappa} e^{\beta \tilde{E}^0_{DP}}$. For $n(\xi, t) = \mathrm{const}$ according to (4) and (7)

$$x_0^2 = \frac{\hat{J}^2 n\, T_0}{a^2 J^2 (U - \hat{J})},\ \kappa = \sqrt{\frac{(U-\hat{J})n}{T_0}} \text{ and } \hat{E}^0_{DP} = \frac{2n}{\kappa}\left(\frac{1}{6} Un + \frac{1}{3}\hat{J}n\right).$$

Because the lattice distortions are strongly connected with the spin distortions, λ_c gives information about the electronic system, too. For $T \to 0$ we have $\lambda_c \to \infty$ like it is expected for Λ-d system. From the dynamic correlation function $S\langle x(0,0)\, x(\xi, t)\rangle$ or the dynamic structure factor

$$S(q, \omega) = \frac{1}{(2\pi)^2} \iint d\xi\, dt\, e^{i(q\xi - \omega t)} \langle x(0,0)\, x(\xi, t)\rangle$$

we get some features of the frequency spectrum of the lattice part of Hamiltonian. The peaks of $S(q,\omega)$ at $\omega \pm \omega_0$ are connected with linear excitations (phonons) and the central peak is connected with the non-linear excitations. If we calculate the width t_D of the central peak in the phenomenological way as Krumhansl and Schrieffer /6/ we find for $\kappa\xi \gg 2$, $\kappa t \gg 2/\check{u}$, where $\check{u}$ is the mean frequency of solitons (slow moving walls), and at low temperatures

$$t_D = \frac{m_D}{k_B T} \frac{2}{\kappa} e^{\beta \hat{E}^0_{DP}} \tag{12}$$

with parameter according to (4), (6) and (7) in the case of $n(\xi, t) = \mathrm{const}$.

A detailed discussion of the static and dynamic correlation function is in preparation.

ACKNOWLEDGEMENTS

I wish to thank Prof. V.K.Fedyanin and Dr. V.L.Aksenov for interesting discussions and I am indebted for hospitality to the Laboratory of Theoretical Physics of the Joint Institute for Nuclear Research at Dubna.

REFERENCES

1. Mikeska H.J. J.Mag.Mag.Mat., 1979, 13, p.35.
2. Lindner U., Fedyanin V.K. phys.stat.sol.(b), 1978, 89, p.123.

3. Lindner U., Fedyanin V.K. phys.stat.sol.(b), 1978, 95, p.K83.
4. Lindner U. 3rd Int. School on Modern Trends in Solid State Theory, Leipzig, 1980 and Preprint KMU-FKT 3.12.79, and Preprint KWU-FKT 22.11.80.
5. Lindner U. phys.stat.sol.(b) (to be published).
6. Krumhansl J.A., Schrieffer J.K. Phys.Rev., 1975, B11, p.3535.
7. Scherf S. Diplomarbeit, Leipzig, 1981.
8. Makhankov V.G. Phys.Lett., 1981, 81A, p.156.
9. Makhankov V.G., Makhaldiani N.N., Pashaev O.K. Phys.Lett., 1981, 81A, p.161.
10. Schumacher W., Lindner U., Jauch R. phys.stat.sol.(b), 1978, 86, p.621.

Received by Publishing Department
on August 28 1981.