18/VI 84

объединенный
институт
ядерных
исследований
дубна

E17-84-223

V.K.Fedyanin, V.Lisý

CONTRIBUTION OF BREATHERS TO THE EQUILIBRIUM AND DYNAMICAL CHARACTERISTICS OF QUASI-ONE-DIMENSIONAL SYSTEMS

Submitted to "Физика низких температур"

1984

1. For the description of a large number of physical phenomena in quasi-one-dimensional models of condensed matter physics the following Hamiltonian has been widely used over the past years :

$$H = A a_0 \sum_n \left[\frac{1}{2} \dot{\varphi}_n^2 + \frac{c_0^2}{2a_0^2} (\varphi_n - \varphi_{n-1})^2 + \omega_0^2 V(\varphi_n) \right] . \quad (1)$$

Here $\varphi_n(t)$ is the scalar field in the site "n", $V(\varphi_n)$ is a local potential, a_0 is the lattice constant, c_0 , ω_0 are characteristic parameters having the dimension of velocity and frequency. A is a constant with the dimension $[\text{energy}\cdot\text{length}^{-1}\cdot\text{time}^2] = [\text{mass}\cdot\text{length}]$ and it determines the energy scale. (We use the notation of the works [1,2]. These works, by the way, contain a list of many physical problems which may be described by the Hamiltonian (1)). If the relation $d = c_0/\omega_0 \gg a_0$ is satisfied the continuum approximation $\varphi_n \to \varphi(x,t)$, $\sum_n \to \int dx/a_0$ is true and eq.(1) yields a differential equation

$$\varphi_{tt} - c_0^2 \varphi_{xx} + \omega_0^2 \frac{dV}{d\varphi} = 0 . \quad (2)$$

A choice of the potential $V(\varphi)$ is determined by the physical specificity of a problem. So, for $V(\varphi) = 1 - \cos\varphi$ (the sine-Gordon potential) we come to the completely integrable system[3]. In the action-angle variables (1) is represented as a sum of three Hamiltonians corresponding to "phonons", solitons (kinks and antikinks) and breathers (bions). The stability of two later solutions with respect to external perturbations allows us to use them for the description of real particle-like objects. There are significant experimental reasons[4] for such a consideration.

However, for the interpretation of the experimental data (mainly the scattering of neutrons on the "classical" ferromagnet $CsNiF_3$) only solitons have been used. Their contribution to the thermodynamics is negligible because of the large activation energy but a number of remarkable features of the central peak (CP) (the dependence of the CP on temperature and magnetic field at low temperatures (4K - 15K)) predicted in/5/ may be explained using a picture of a soliton gas. Beginning from /5,6/ various structure factors responsible to the scattering on solitons have been calculated in the "nonrelativistic" approximation ($v \ll c_0$, v is the velocity of a soliton) in a series of papers. A general formula which is true for all v, $-c_0 < v < c_0$, has been obtained in/7/ +/. Especially much attention was given to the so-called "parallel" formfactor $S_{\parallel}(q,\omega)$. In recent experimental investigations (the works/4/ give the up-to-date situation about the investigations of solitons in one-dimensional magnets) some discrepancies between its behaviour predicted by the soliton-gas theory and the experiment have been found.

We underline that for explaining the experimental data on equilibrium and dynamic properties of quasi-one-dimensional systems breathers have nearly not been exploited. The necessity to use them, especially with the aim to describe $S_{\parallel}$, has been noted for the first time in/8/. The parallel structure factor has been calculated in/9/. It was shown that breathers give a contribution to the CP, however, analytical expressions for $S_{\parallel}$ and its structure were not obtained. The mean density of the breather gas and the formfactor in the first approximation (about it see bellow) have been calculated in/10/ (see also/11/).

+/We note that this is not only of a pure academic interest: for the description of scattering on solitons in DNA/13/, where in the first approximation the SG-equation takes place, it is necessary to calculate $S(q,\omega)$ in the whole range $-c_0 < v < c_0$.

The results of these calculations allow us to draw two conclusions: a) breathers apparently give a considerable contribution to the CP of $S_{\parallel}(q,\omega)$; b) there arise additionally two narrow side peaks ("satellites").

In the present work general analytical expressions for the parallel and perpendicular DSF are obtained for the scattering of neutrons on the ideal breather gas. The basis of the calculations is quite similar to that proposed in/7/. It is shown that the DSF consists of the CP and an infinite series of satellites. The relations obtained are rather cumbersome and we reduce them to approximate analytical "working" formulae for the CP and satellites. The location of the satellites is found and some properties of them are discussed. The intensities of the satellites are shown to decrease sharply as the distance between the satellite and the CP increases. Comparatively with/10,11/ the behaviour of the CP changes essentially. Furthermore, in the framework of the ideal gas model the thermodynamic functions of the breather subsystem are calculated.

2. The breather solution of eq.(2) has the following form:

$$\phi = 4 \,\mathrm{arctg}\, \varkappa, \qquad \varkappa = \frac{\sqrt{1-\Omega^2}}{\Omega} \sin\theta \cosh^{-1}\xi,$$

$$\theta = \omega_0 \Omega (t - vx/c_0^2)\gamma + \theta_0, \qquad \xi = \frac{\omega_0}{c_0}\sqrt{1-\Omega^2}\,\gamma\,(x - vt - x_0), \tag{3}$$

$$\gamma = (1 - v^2/c_0^2)^{-1/2}, \quad -\infty < x; x_0; t < \infty, \quad -c_0 < v < c_0, \quad 0 \le \theta_0 \le 2\pi, \quad 0 < \Omega < 1.$$

Here Ω is the intrinsic frequency of a breather, v is the velocity, x, t are the space and time variables, and x_0, θ_0 are free parameters (the initial location and the phase). Below we need the energy of the breather

$$\bar{E} = E^{(0)}\gamma = [E^{(0)2} + p^2 c_0^2]^{1/2}, \tag{4}$$

where the energy of the static breather, $E^{(0)}$, is

$$E^{(0)} = 16 A \omega_0 c_0 \sqrt{1-\Omega^2},$$

and the momentum

$$p = 16 A \omega_0 \frac{v}{c_0} \gamma \sqrt{1-\Omega^2} . \tag{5}$$

The form of the solution (3) predetermines difficulties with the calculation of the equilibrium and dynamical characteristics of breathers as compared to solitons of the SG-equation/7/: the automodel dependence on $(x - vt - x_0)/\Delta(v)$ vanishes, the averaging over θ_0 becomes nontrivial and the additional intrinsic variable Ω appears, the averaging over which will be carried out using some "reasonable" assumptions (they have been formulated in /10/, see also below).

Let us consider the thermodynamics of breathers. We note that the model of a lattice soliton gas, which was developed in/7,11/ for the description of thermodynamic properties of solitons, is not applicable to breathers. We cannot operate freely with the "size" of breathers. Therefore, we shall develop the thermodynamics of breathers in the model of the ideal one-dimensional gas in the "volume" $0 \div L$ ($L \to \infty$).

The thermodynamics may be constructed proceeding from the partition function of a separate breather

$$j(T) = \frac{1}{h} \int_0^L dx_0 \, \frac{2}{\pi} \int_0^1 \frac{d\Omega}{\sqrt{1-\Omega^2}} \int dp \, e^{-\beta E(p)} , \tag{6}$$

where h is the Planck constant, T is the temperature, and $\beta = (kT)^{-1}$. The partition function thus determined gives, as we shall see later, the expression for the breather density which agrees with the assumption of the papers/10,11/. After the integration we obtain

$$j(T) = 16 \pi L A \omega_0 h^{-1} \left[K_1(\tfrac{\alpha}{2}) I_0(\tfrac{\alpha}{2}) - I_1(\tfrac{\alpha}{2}) K_0(\tfrac{\alpha}{2}) \right], \tag{7}$$

where the dimensionless parameter

$$\alpha = 16 A \omega_0 c_0 \beta , \tag{8}$$

and K , I are the modified Bessel functions. At "low" temperatures ($\alpha \gg 1$, in some systems, e.g., in/13/ "low" may mean the room temperatures)

$$j(T) \simeq \frac{L}{8 h A \omega_0 c_0^2} (kT)^2 . \tag{7a}$$

The grand partition function of the breather gas is defined by

$$\Xi = \sum_{N=0}^{\infty} e^{\beta \mu N} [j(T)]^N / N! = \exp[j(T) \exp(\beta\mu)], \tag{9}$$

with the chemical potential μ . Since there are no external limitations on the number of breathers and it is determined only by the temperature, after calculations with Ξ one must put $\mu = 0$ in the resulting formulae. Using the thermodynamical potential $\Omega = -kT \ln \Xi$ we find the breather density

$$n = - \frac{1}{L} \frac{\partial \Omega}{\partial \mu} \bigg|_{\mu=0} = \frac{j(T)}{L} , \tag{10}$$

so, the mean number of breathers in the system is $j(T)$. This expression need to be used by us below in the calculation of the structure factors.

By analogy with the breather density all other thermodynamic characteristics are calculated. Here we give the results in the case $\alpha \gg 1$

$$n \simeq \frac{(kT)^2}{8 h A \omega_0 c_0^2} \qquad \text{(density)} ,$$

$$F = -kTn \qquad \text{(free-energy density)},$$

$$u \simeq (kT)^3 / 4 h A \omega_0 c_0^2 \qquad \text{(internal-energy density)},$$

$$C_L \simeq 3k (kT)^2 / 4 h A \omega_0 c_0^2 \qquad \text{(heat capacity)}.$$

In the "high" temperature case ($\alpha \ll 1$, $j(T) \simeq 2LkT/hc_0$) $n \simeq 2kT/hc_0$, $F \simeq -2(kT)^2/hc_0$, $u \simeq 2(kT)^2/hc_0$, $C_L \simeq 4k^2T/hc_0$. Putting in eqs.(7) and (10) $A = \omega_0 = c_0 = 1$ and changing $h \to h/4$, we obtain the breather density found in /10/.

(The last substitution is due to the fact that in[10] the phase volume of the kink was taken 2π-times smaller than the one of the breather, and the averaging over Ω was carried out without the normalizing factor $2/\pi$).

The given formulae allow us to conclude that unlike the soliton gas, due to the absence of the cut-off factor $\sim exp(-\beta E_K^0)$, breathers may essentially influence the thermodynamic characteristics of the SG-systems.

3. Now we shall calculate the DSF of the scattering of neutrons (or light) on breathers. We proceed in the framework of the calculation scheme given in[7]. As was mentioned above the additional averaging over θ_0 and Ω arises. The parallel DSF is determined by averaging the product $\cos\varphi(x,t)\cos\varphi(0,0)$, where according to (3)

$$1-\cos\varphi = 8\,\varkappa^2(1+\varkappa^2)^{-2}. \tag{11}$$

A general analytic formula for $\langle 1-\cos\varphi(x,t), 1-\cos\varphi(0,0)\rangle$ obtained below describes the essential contribution of the breather mode to the parallel DSF; naturally, in the complete correlator $\langle\cos\varphi(x,t)\cos\varphi(0,0)\rangle$ there are terms which give a contribution to the Bragg scattering and are added to the corresponding soliton contribution[5,7]. However, we shall be interested in a modified picture of the quasielastic scattering from breathers.

For the ideal breather gas

$$S_{\parallel}(q,\omega) = N_b\, S_1(q,\omega) \,. \tag{12}$$

Here N_b is the mean number of breathers in the system and

$$S_1(q,\omega) = \frac{1}{4\pi^2 h j}\int dx\,dt\,dp\,dx_0\,\frac{d\theta_0}{2\pi}\,\frac{2}{\pi}\,\frac{d\Omega}{\sqrt{1-\Omega^2}}\,e^{i(qx-\omega t)-\beta E(p)}\big(1-\cos\varphi(0,0),1-\cos\varphi(x,t)\big). \tag{13}$$

The integration is taken over the ranges shown in (3); $E(p)$ is given by eq.(4) and $j(T)$ by eqs.(7)-(7a).

Passing in (13) into the breather rest frame with the help of the transformation

$$x = \gamma(\xi' + vt'), \quad t = \gamma(t' + v\xi'/c_0^2), \tag{14}$$

substituting then

$$t' = \frac{\tau-\theta_0}{\omega_0\Omega}, \quad x_0 = \frac{c_0}{\omega_0}\,\frac{z}{\gamma\sqrt{1-\Omega^2}}, \quad \xi' = \frac{c_0 y}{\omega_0\sqrt{1-\Omega^2}} + \gamma x_0, \tag{15}$$

and using (10), we obtain instead of (13)

$$S_{\parallel}(q,\omega) = \frac{2^2 c_0^2}{\pi^4 h\omega_0^3}\int dy\,d\tau\,dp\,dz\,d\theta_0\,\frac{d\Omega}{\Omega(1-\Omega^2)^{3/2}\gamma}\exp\big[-\beta E(p) + i(a\tau - a\theta_0 + by + bz)\big]\iint_0^\infty d\xi\,d\eta\,e^{-\xi}e^{-\eta}(1-\xi)(1-\eta)\cos[\xi X(\tau,y)]\cos[\eta X(\theta_0,z)], \tag{16}$$

where we have introduced

$$a = \gamma\,\frac{qv-\omega}{\omega_0\Omega}, \quad b = \frac{\gamma c_0}{\omega_0}\,\frac{q-\omega v/c_0^2}{\sqrt{1-\Omega^2}}, \tag{17}$$

An identical representation

$$X^2(1+X^2)^{-2} = \frac{1}{2}\int_0^\infty d\xi\,e^{-\xi}(1-\xi)\cos\xi X, \qquad X^2(\tau,y) = \frac{1-\Omega^2}{\Omega^2}\,\frac{\sin^2\tau}{\cosh^2 y},$$

and an analogous representation for the functions of variables θ_0, z have been used. Then, we use the expansion of $\cos\xi X$ which is true for all ξX:

$$\cos\xi X = \sum_{n=0}^{\infty}\sum_{m=0}^{2n}\frac{(-1)^m\,\xi^{2n}}{2^{2n}(2n-m)!\,m!}\left(\frac{1-\Omega^2}{\Omega^2}\right)^n\frac{e^{i\tau(2n-2m)}}{\cosh^{2n}y}.$$

Now the y and z-integration is easily realized[12]:

$$\int\frac{e^{iby}\,dy}{\cosh^{2n}y} = \frac{2^{2n-1}}{(2n-1)!}\left|\Gamma\!\left(n+\frac{ib}{2}\right)\right|^2,$$

and after the integration over τ the Dirac delta-function $\delta(a+2n-2m)$ arises. Possible values of a are thus limited to integer numbers $a = 2m-2n$. This is important for the θ_0-integration. After expanding $\cos[\eta X(\theta_0,z)]$

into the series $\sum_{k,\ell}$ as it was done above, the following integral appears

$$\int_0^{2\pi} d\theta_0 \exp\left[-ia\theta_0 + i\theta_0(2k-2\ell)\right] = 2\pi, \text{ if } \quad 0 \le n-m+k \le 2k$$
$$= 0, \text{ in the opposite case.}$$

The ξ and η -integrations are elementary, too. Finally, we pass from the integration over p, by means of (5), to $v \in (-c_0, c_0)$.

Joining all stages of the calculations given above, we obtain for $S_{\parallel}$ from (16)

$$S_{\parallel}(q,\omega) = \frac{2^{10} A c_0}{\pi^2 h \omega_0^2} \int dv \frac{d\Omega}{\Omega(1-\Omega^2)} \gamma^2 e^{-\beta E(v)} \sum_{\substack{n=0}}^{\infty} \sum_{m=0}^{2n} \sum_{\substack{k=0 \\ 0 \le n-m+k \le 2k}}^{\infty} C_{nkm} \left(\frac{1-\Omega^2}{\Omega^2}\right)^{n+k}$$
$$\times \left|\Gamma\left(n+\frac{ib}{2}\right)\right|^2 \left|\Gamma\left(k+\frac{ib}{2}\right)\right|^2 \delta(a+2n-2m), \tag{18}$$

$$C_{nkm} = (-1)^{n+k} n^2 k^2 / \left[m!(2n-2m)!(n-m+k)!(k-n+m)!\right].$$

After some manipulations with the sum in (18), the last formula may be written in a more compact form. It is natural to confront the terms, which are determined by the condition $n = m$, with the contribution to the CP, and the other terms with the contribution to satellites. Then

$$S_{\parallel}(q,\omega) = S_c(q,\omega) + \sum_{N=1}^{\infty} S_{\parallel sat}^{N}(q,\omega), \tag{19}$$

where

$$S_c(q,\omega) = \frac{2^{10} A c_0}{\pi^2 h \omega_0^2} \int dv\, d\Omega \frac{\gamma^2 e^{-\beta E(v)}}{\Omega(1-\Omega^2)} \left[\sum_{n=1}^{\infty} \frac{(-1)^n}{[(n-1)!]^2} \left(\frac{1-\Omega^2}{\Omega^2}\right)^n \left|\Gamma\left(n+\frac{ib}{2}\right)\right|^2\right]^2$$
$$\times \delta(a), \tag{20}$$

$$S_{\parallel sat}^{N}(q,\omega) = \frac{2^{10} A c_0}{\pi^2 h \omega_0^2} \int dv\, d\Omega \frac{\gamma^2 e^{-\beta E(v)}}{\Omega(1-\Omega^2)} \left[\sum_{n=N}^{\infty} \frac{(-1)^n n^2}{(n+N)!(n-N)!} \left(\frac{1-\Omega^2}{\Omega^2}\right)^n\right.$$
$$\left.\times \left|\Gamma\left(n+\frac{ib}{2}\right)\right|^2\right]^2 \left[\delta(a-2N)+\delta(a+2N)\right]. \tag{21}$$

These equations may be rewritten briefly by means of the hypergeometric function $F \equiv {}_2F_1$, e.g., the CP is described by the following expression (after the integration over v)

$$S_c(q,\omega) = \frac{2^8 A c_0^3 |q|}{h \omega_0^3 \gamma(v_0)} \int_0^1 d\Omega \frac{e^{-\beta E(v_0)}}{\sinh^2 \frac{\pi b(v_0)}{2}} \left|F\left(\frac{ib}{2}, 1+\frac{ib}{2}; 1; 1-\Omega^2\right)\right|^2,$$
$$v_0 = \omega/q. \tag{20a}$$

We note that the first satellites (N = 1) have been predicted for the first time in/10/ (see also/11/ and below).

One integration in (20),(21) is easily carried out due to the delta-functions. The last integration may be fulfilled approximately, e.g., as it has been done in/10/. Since one can carry out the calculations in the exact formulae (19)-(21) in various ways, we shall give further calculations in a separate section.

4. Let us first consider in more detail the CP. After the integration (we choose the integration over v) we obtain (20a), or

$$S_c(q,\omega) = \frac{2^{10} A c_0}{\pi^2 h \omega_0 |q|} \int_0^1 d\Omega \frac{1-\Omega^2}{\Omega^4} \gamma(v_0) e^{-\beta E(v_0)} \left[\sum_{n=0}^{\infty} \frac{(-1)^n}{(n!)^2} \left(\frac{1-\Omega^2}{\Omega^2}\right)^n\right.$$
$$\left.\times \left|\Gamma\left(n+1+\frac{ib(v_0)}{2}\right)\right|^2\right]^2. \tag{22}$$

The integrand in (22) converges to 0 at $\Omega \to 0;1$. Indeed, the inequality $|\Gamma(x+iy)| \le |\Gamma(x)|$ yields the following limitations on the integrand $S_c(q,\omega,\Omega)$

$$S_c(q,\omega,\Omega \to 1) \le \frac{2^{10} A c_0}{\pi^2 h \omega_0 |q|} \gamma(v_0)(1-\Omega^2) \to 0,$$

$$S_c(q,\omega,\Omega \to 0) \le \frac{2^{10} A c_0}{\pi^2 h \omega_0 |q|} \gamma(v_0) e^{-\alpha\gamma(v_0)} \approx 0 \quad (\alpha \gg 1).$$

The last estimation, which is written for low temperatures, may be specified remembering that for breathers $1-\cos\phi \to 0$ at $\Omega \to 0$ (see (3) and (11)). $S_{\parallel}$ is expressed as a sum of nonnegative terms, thus all the terms, particularly S_c, approach zero if $\Omega \to 0$.

On the other hand, S_c may be written in the form

$$S_c(q,\omega) = \frac{2^{10} A c_0 \delta^2}{\pi^2 h \omega_0 |q| \gamma(v_0)} \int_0^1 d\Omega\, e^{f(\Omega)} g(\Omega), \tag{22a}$$

where

$$f(\Omega) = -\alpha\,\gamma(v_0)\sqrt{1-\Omega^2} + \delta/\gamma(v_0)\sqrt{1-\Omega^2}\,, \qquad \delta = \pi q c_0/\omega_0\,,$$

$$g(\Omega) = \Omega^{-4}\left(1 - e^{-\delta/\gamma(v_0)\sqrt{1-\Omega^2}}\right)^{-2}\left[1 + \sum_{n=1}^{\infty}\frac{(-1)^n}{(n!)^2}\left(\frac{1-\Omega^2}{\Omega^2}\right)^n\prod_{\ell=1}^{n}\left(\ell^2+\frac{b^2}{4}\right)\right]^2.$$

So long as $\alpha \gg 1$ the function $f(\Omega)$ has a sharp maximum at $\Omega = \bar{\Omega} \sim 1$ (an importance of the contributions to $S(q,\omega)$ with $\Omega \sim 1$ has been postulated in[10]). Therefore, for the estimation of (22a) one may use[9,10] the saddle-point method. This gives $1 - \bar{\Omega}^2 = \delta/\alpha\gamma^2(v_0)$,

$$\int_0^1 d\Omega\, e^{f(\Omega)} g(\Omega) \approx \frac{\sqrt{\pi}\, g(\bar{\Omega})\, e^{f(\bar{\Omega})}}{2\sqrt{|f''(\bar{\Omega})|/2}}\left[\operatorname{erf}\left(\bar{\Omega}\sqrt{|f''(\bar{\Omega})|/2}\right) + \operatorname{erf}\left((1-\bar{\Omega})\sqrt{|f''(\bar{\Omega})|/2}\right)\right],$$

or, taking into account once more that $\alpha \gg 1$,

$$\int_0^1 d\Omega\, e^{f(\Omega)} g(\Omega) \approx \sqrt{\pi}\, g(\bar{\Omega})\, e^{f(\bar{\Omega})}\left(|f''(\bar{\Omega})|/2\right)^{-1/2}.$$

After substitution of this estimation in (22a), we finally obtain

$$S_c(q,\omega) \approx \frac{2^{10} A c_0 \delta^{11/4}}{\pi^{3/2} h\omega_0 |q|}\,\alpha^{-\frac{5}{4}}\gamma^{-3}(v_0)\, e^{-2\sqrt{\alpha\delta}}\left[1 + \sum_{n=1}^{\infty}\frac{(-1)^n}{\gamma^{2n}}\prod_{\ell=1}^{n}\left(\frac{\delta}{\alpha} + \frac{\delta^2}{4\pi^2\ell^2}\right)\right]^2. \quad (23)$$

The leading term of the approximation (the factor before the square brackets) was found before[10,11] (in [10,11] $A = \omega_0 = c_0 = 1$). However, our result is essentially modified by the factor

$$\left[1 - \nu^2 + \nu^4/4 - \nu^6/36 + \cdots\right]^2, \qquad \nu = \frac{\delta}{2\pi\gamma}\,, \quad \frac{\delta}{\alpha} \ll 1.$$

For the interpretation of S_c in recent experiments (this will be the subject of our separate investigation) it is not sufficient to use only the first term of the sum. The parameters of the CP (intensity, width) are determined, of course, by concrete values of A, ω_0, c_0.

Now we will estimate $S^N_{\parallel sat}$ (eq.(21)). We use the well-known relation for the delta-function

$$\delta(\varphi(x)) = \sum_s \delta(x - x_s)\,|\varphi'(x_s)|^{-1},$$

where x_s are the roots of the equation $\varphi(x) = 0$. We specify $q, \omega \geq 0$ and solve the equations $a \pm 2N = 0$ relative to v. This leads to the quadratic equations

$$qv - \omega \pm 2N\omega_0\Omega\gamma^{-1} = 0\,.$$

Using the solutions of these equations we obtain after the integration

$$S^N_{\parallel sat}(q,\omega) = \frac{2^{14} A c_0^2}{h\omega_0^2}\int_0^1 d\Omega\, G(\Omega)\left(e^{F_1(\Omega)} + e^{F_2(\Omega)}\right), \quad (24)$$

where

$$F_1(\Omega) = -\frac{B_N(\Omega)}{\sqrt{1-\Omega^2}} - \alpha\sqrt{1-\Omega^2}\,\frac{q^2c_0^2 + (2N\omega_0\Omega)^2}{qc_0\omega_0 B_N(\Omega)/\pi + 2N\omega_0\omega\Omega}\,,$$

$$F_2(\Omega) = -\frac{B_N(\Omega)}{\sqrt{1-\Omega^2}} - \alpha\sqrt{1-\Omega^2}\,\frac{q^2c_0^2 + (2N\omega_0\Omega)^2}{|qc_0\omega_0 B_N(\Omega)/\pi - 2N\omega_0\omega\Omega|}\,,$$

$$G(\Omega) = \pi^3 B_N^{-3}\left(1 - e^{-B_N/\sqrt{1-\Omega^2}}\right)^{-2}\left[\sum_{n \geq N-1}\frac{(-1)^n (n+1)^2}{(n+1-N)!\,(n+1+N)!}\right.$$

$$\left.\times\left(\frac{1-\Omega^2}{\Omega^2}\right)^{n+1}\prod_{\ell=0}^{n}\left(\ell^2 + \frac{B_N^2}{4\pi^2}\right)\right]^2, \qquad B_N(\Omega) = \frac{\pi}{\omega_0}\left(q^2c_0^2 + (2N\omega_0\Omega)^2 - \omega^2\right)^{1/2}. \quad (25)$$

Since the functions F_1, F_2 have sharp maxima at $\Omega \sim 1$, the estimations of the integrals in (24) may be accomplished following[10] with the use of the saddle-point method. For the paper briefness we designate

$$C_N(\Omega) = \alpha\,\frac{q^2c_0^2 + (2N\omega_0\Omega)^2}{qc_0\omega_0 B_N/\pi + 2N\omega_0\omega\Omega}\,, \quad E_N(\Omega) = \alpha\,\frac{q^2c_0^2 + (2N\omega_0\Omega)^2}{|qc_0\omega_0 B_N/\pi - 2N\omega_0\omega\Omega|}\,, \quad (26)$$

and express $S^N_{\parallel sat}$ in the form

$$S^N_{\parallel sat} = S^N_{\parallel sat1} + S^N_{\parallel sat2}\,, \quad (27)$$

where

$$S^N_{\parallel sat1} \approx \frac{2^{14} A c_0^2 \pi^{7/2}}{h\omega_0^2}\left(\frac{B_N(1)}{C_N(1)}\right)^{3/2}\frac{\left(1 - e^{\sqrt{B_N(1)C_N(1)}}\right)^{-2}}{\left(B_N(1)\,C_N(1)\right)^{7/4}}$$

$$\times\left[\sum_{n \geq N-1}\frac{(-1)^n (n+1)^2}{(n+1-N)!\,(n+1+N)!}\left(\frac{B_N(1)}{C_N(1)}\right)^n\prod_{\ell=0}^{n}\left(\ell^2 + \frac{B_N(1)C_N(1)}{4\pi^2}\right)\right]^2, \quad (28)$$

and $S^N_{\parallel sat\,2}$ is obtained from (28) after the substitution $C_N \to E_N$. Because of the cut-off exponential factor in(28), $S^N_{\parallel sat}$ will be appreciably different from zero only in the vicinity of ω determined from the condition

$$B_N(1) \sim \sqrt{q^2 c_0^2 + (2N\omega_0)^2 - \omega^2} \approx 0 ,$$

that is, if ω is near to

$$\omega_N = \sqrt{q^2 c_0^2 + (2N\omega_0)^2} . \tag{29}$$

Thus the satellites are the peaks located near the frequencies $\omega \approx \omega_N$. At low temperatures their positions are almost independent of the temperature. However, taking into account our approximations in obtaining (27)-(29), we see that if T increases, the value of ω_N decreases and the satellites come nearer to the CP.

The quantity B_N is small near ω_N. This allows us to make one more approximation. Instead of (26) we will have

$$E_N \approx C_N \approx \frac{\alpha\omega}{2N\omega_0} , \qquad B_N \approx \frac{\pi}{\omega_0}\sqrt{\omega_N^2 - \omega^2} , \tag{26a}$$

and

$$S^N_{\parallel sat} \approx 2 S^N_{\parallel sat\,1} , \tag{30}$$

if we substitute (26a) in (27)-(30).

As was mentioned above, the first satellite (N=1) has been found in[10,11]. Our expressions determine the series of following satellites, the corrections to the solution[10,11] for $S^1_{\parallel sat}$ and correct the expression for $S^1_{\parallel sat}$ obtained in the cited works (in eq.(28) of the paper[10] one must replace $\mathrm{sgn}(q^2-\omega^2)$ by $\mathrm{sgn}|q^2-\omega^2|$; this alters the following calculations).

We write the expressions for the first two satellites:

$$S^1_{\parallel sat} \approx \frac{2^9 A c_0^2}{\sqrt{\pi}\, h\omega_0^2}\left(\frac{B_1}{C_1}\right)^{3/2}(B_1C_1)^{1/4}\left(1-e^{\sqrt{B_1C_1}}\right)^{-2}[1-\dots]^2, \tag{31}$$

$$S^2_{\parallel sat} \approx \frac{2^9 A c_0^2}{9\sqrt{\pi}\, h\omega_0^2}\left(\frac{B_2}{C_2}\right)^{7/2}(B_2C_2)^{1/4}\left(1+\frac{B_2C_2}{4\pi^2}\right)^2\left(1-e^{\sqrt{B_2C_2}}\right)^{-2}[1-\dots]^2. \tag{31a}$$

The corrections to 1 in the square brackets in these formulae are not important in this case. For $S^1_{\parallel sat}$ we have

$$[1-\dots] = 1 - \frac{4}{3}\left(\frac{B_1}{C_1} + \frac{B_1^2}{4\pi^2}\right) + \dots ,$$

and for $S^2_{\parallel sat}$

$$[1-\dots] = 1 - \frac{9}{5}\frac{B_2}{C_2}\left(1 + \frac{B_2C_2}{16\pi^2}\right) + \dots .$$

Near the maxima (in ω) of the functions $S^1_{\parallel sat}$ and $S^2_{\parallel sat}$ the values C_1 and C_2 remain of the same order but B_1, B_2 are small. Therefore, one may conclude that the heights of the peaks of $S^1_{\parallel sat}$ and $S^2_{\parallel sat}$ much differ in their magnitudes, $S^2_{\parallel sat}$ being much smaller than $S^1_{\parallel sat}$. The same conclusion takes place for other N, too. Thus, the general picture is as follows: the parallel DSF, which is responsible for the scattering from breathers, consists of the CP and the peaks of intensity (the satellites) located near the frequencies ω_N $(N=1,2,\dots)$ with gradually decreasing heights.

5. Usually, in scattering experiments besides the "parallel" DSF (investigated above) the corresponding "perpendicular" DSF, $S_\perp$, is determined. The calculation of the later is connected with the averaging of the product $\sin\Phi(x,t)\,\sin\Phi(0,0)$. $S_\perp$ has been investigated for the first time in[10,11]. There was found in these works that $S_\perp$ gives a very small contribution to the CP (which can be neglected) and represents a satellite located near the frequency $\omega \approx \sqrt{q^2c_0^2+\omega_0^2}$.

According to (3) $\sin\Phi$ is defined by the expression

$$\sin\Phi = 4\varkappa(1-\varkappa^2)(1+\varkappa^2)^{-2}. \tag{32}$$

Substituting (32) instead of $(1-\cos\Phi)$ in (12) and (13) and using the transformations (14) and (18) we obtain

$$S_\perp(q,\omega) = \frac{2^6 A c_0^2}{(2\pi)^4 h\omega_0^3}\sum_{n=0}^{\infty}\sum_{k=0}^{\infty}\int dy\,d\tau\,dz\,dp\,d\theta_0 \frac{d\Omega}{(1-\Omega^2)^{3/2}\Omega\gamma}\exp\Big[-\beta E(p)$$
$$+i\left(-bz+by-a\theta_0-a\tau\right)\Big](-1)^{n+k}(2n+1)(2k+1)\left(\frac{\sin\tau}{\cosh y}\right)^{2n+1}\left(\frac{\sin\theta_0}{\cosh z}\right)^{2k+1}\left(\frac{1-\Omega^2}{\Omega^2}\right)^{n+k+1}. \tag{33}$$

Here the formal expansion has been used

$$\sin\phi = 4\sum_{n=0}^{\infty}(-1)^n(2n+1)\,\varkappa^{2n+1}.$$

Such a way (despite of its formality) gives the same results as the more rigorous method we have used in the calculations of $S_{\parallel}$ and is slightly more fast and straightforward. The values a and b are given in (17). The integrals over y and z, as in Section 3, are expressed in terms of gamma-functions, and the integral over τ gives birth to the sum of delta- functions

$$\sim \sum_{\ell=0}^{2n+1}\binom{2n+1}{\ell}(-1)^{\ell}\,\delta(2n+1-2\ell+a)\,.$$

Possible values of a are now limited to integer numbers, so the integration over θ_0 gives

$$\int_0^{2\pi} d\theta_0\, e^{-ia\theta_0}\sin^{2k+1}\theta_0 = \frac{\pi}{2^{2k}i}\binom{2k+1}{n+k-\ell+1}(-1)^{n-m+2},$$

if $0\le n+k-\ell+1\le 2k+1$, and 0 in the opposite case. Finally, after the substitution $dp = p'(v)\,dv$, (33) is replaced by

$$S_{\perp}(q,\omega) = \frac{2^6 A c_0}{\pi^2 h\omega_0^2}\int dv\, d\Omega\cdot\Omega^{-3}\gamma^2 e^{-\beta E(v)}\sum_{n\geq 0}\sum_{\substack{k\geq 0\\ 0\le n+k-\ell+1\le 2k+1}}\sum_{\ell=0}^{2n+1} C'_{nk\ell}\left(\frac{1-\Omega^2}{\Omega^2}\right)^{n+k}$$

$$\times\,\delta(2n+1-2\ell+a)\,\left|\Gamma\!\left(n+\tfrac{1}{2}+\tfrac{ib}{2}\right)\Gamma\!\left(k+\tfrac{1}{2}+\tfrac{ib}{2}\right)\right|^2,$$

$$C'_{nk\ell} = (-1)^{n+k}(2n+1)^2(2k+1)^2\left[\ell!\,(k-n+\ell)!\,(k+n-\ell+1)!\,(2n+1-\ell)!\right]^{-1}. \qquad (34)$$

Making the substitution $2n+1-2\ell = -2N-1$ and regroupping the terms in the sum, we have

$$S_{\perp}(q,\omega) = \frac{2^6 A c_0}{\pi^2 h\omega_0^2}\int dv\, d\Omega\cdot\Omega^{-3}\gamma^2 e^{-\beta E(v)}\sum_{N=0}^{\infty}\left[\delta(a+2N+1)+\delta(a-2N-1)\right]$$

$$\times\left[\sum_{n\geq N}(-1)^n\frac{(2n+1)^2}{(n+1+N)!\,(n-N)!}\left(\frac{1-\Omega^2}{\Omega^2}\right)^n\left|\Gamma\!\left(n+\tfrac{1}{2}+\tfrac{ib}{2}\right)\right|^2\right]^2. \qquad (34a)$$

The terms which correspond to N = 0, 1, ..., may be called the satellites (there is no separate contribution to the CP

as it was in the case of $S_{\parallel}$). If n = 0 one may obtain from (34a) an expression for the first "odd" satellite (N=0) found in /10,11/ (with corrected numerical factor). Finally, after the integration over v (which is easily realized due to the delta-functions) we obtain from (34a) for the Nth satellite

$$S^N_{\perp sat}(q,\omega) = \frac{2^6 A c_0^2}{\pi h\omega_0^2}\int_0^1 \frac{d\Omega}{\Omega^2 B'_N(\Omega)}\left(e^{-\beta E(v_1)} + e^{-\beta E(v_2)}\right)$$

$$\times\left[\sum_{n\geq N}\frac{(-1)^n(2n+1)^2}{(n+1+N)!\,(n-N)!}\left(\frac{1-\Omega^2}{\Omega^2}\right)^n\left|\Gamma\!\left(n+\tfrac{1}{2}+i\frac{B'_N(\Omega)}{2\pi\sqrt{1-\Omega^2}}\right)\right|^2\right]^2, \qquad (35)$$

where

$$B'_N(\Omega) = \frac{\pi}{\omega_0}\sqrt{q^2c_0^2-\omega^2+(2N+1)^2\omega_0^2\Omega^2}\,,$$

$$\beta E(v_{1,2}) = \alpha\sqrt{1-\Omega^2}\,\frac{(2N+1)^2\omega_0^2\Omega^2+q^2c_0^2}{(2N+1)\omega_0\omega\Omega \mp q c_0\omega_0 B'_N/\pi}\,. \qquad (36)$$

The expression (35) is exact in the model of the ideal breather gas. The integration in (35) may be carried out numarically or using various methods of estimations. We note, however, that the saddle-point method, which was used in /10,11/ and above, must be used with some care. In such an approximation the first satellite /10,11/ diverges at $\omega\to\sqrt{q^2c_0^2+\omega_0^2}$ while it is easy to shaw that $S^N_{\perp sat}\to 0$ as $\omega\to\sqrt{q^2c_0^2+(2N+1)^2\omega_0^2}$.

6. The expressions found above for the thermodynamic functions and DSF of the breather gas are true for any system governed by the SG-equation (2). In any concrete system one must only specify the values of the constants A, ω_0, c_0 and a_0. We will use the obtained results in a following work for the interpretation of the mentioned neutron scattering experiments on one-dimensional Heisenberg magnets /4/. In spite of the agreement that the spin-dynamics in such magnets (as $CsNiF_3$) is governed by the SG-equation, the breather contribution to the DSF of scattering has not been yet considered quantitatively. It is hoped that the revealed features of the structure of the

DSF (the series of satellites) will stimulate further experiments in this field. One more example which demonstrates the wide range of application of the SG-model may be the problem of "open states" in DNA [13]. Probably, torsion vibrations may exist in DNA which may be described by the SG-equation. The additional condition of low temperatures ($\alpha >> 1$) which has been widely used above is well satisfied in experiments [4]; we note that for DNA "low" temperatures may mean the room tempertatures.

We are grateful to V.G. Makhankov for stimulating remarks and discussions on the results.

References

1. Bishop A.R., Krumhansl J.A., Trullinger S.E. Physica, 1980, 1D, p.1.
2. Currie I.F. et al. Phys.Rev., 1980, B32, p.477.
3. Тахтаджян Л.А., Фаддеев Л.Д. ТМФ, I974,2I, с.I60.
4. Steiner M., J.Magn.Mat., 1983, 31-34, p.1277.
   Steiner M., Kakurai K., Kjems J.K. Physica, 1983, 120B,p.250.
5. Mikeska A.I. J.Phys.C, 1978, 11, p. L29.
6. Kawasaki K. Progr.Theor.Phys., 1876, 55, p.2029.
7. Федянин В.К. ОИЯИ, PI7-82-268, Дубна, I982.
8. Stoll E., Schneider T., Bishop A.R., Phys.RevLett., 1979, 42, p.937.
9. Timonen J., Bullough R.K., Phys.Lett., 1981, 82A, p.183.
10. Маханьков В.Г. ОИЯИ,P2-82-248 Дубна, I982.
11. Fedyanin V.K., Makhankov V.G., JINR, E17-83-30, Dubna, 1983; Physica Scripta, 1983, 28, p.221.
12. Прудников А.П. и др., Интегралы и ряды, Наука, М., I98I.
13. Englander S.W. et al., Proc.Nat.Acad.Sci. USA, 1980, 77, p.7222.

Received by Publishing Department
on April 9,1984.

Федянин В.К., Лиси В. E17-84-223

Вклад бионов в равновесные и динамические характеристики квазиодномерных систем

В работе изучены равновесные и динамические характеристики газа бионов /брифферов/ для моделей статистической механики, описываемых уравнением sine-Gordon. Построена термодинамика бионов. Впервые получены точные аналитические формулы для продольного и поперечного динамических структурных факторов $S_{\parallel}(q,\omega)$ и $S_{\perp}(q,\omega)$. Оказалось, что $S_{\parallel}$ состоит из центрального пика и бесконечной последовательности сателлитов, центры которых расположены вблизи частот $\omega^{\parallel}_N = \sqrt{q^2c_0^2 + (2N\omega_0)^2}$, $N = 1,2,\ldots$; вклад от $S_\perp$ в центральный пик отсутствует, а сателлиты центрированы вблизи частот $\omega^{\perp}_N = \sqrt{q^2c_0^2 + (2N+1)^2\omega_0^2}$, $N = 0,1,\ldots$. Полученные формулы могут быть применены для анализа и интерпретации экспериментальных данных по рассеянию нейтронов и света на квазиодномерных магнетиках, молекуле ДНК, волнах зарядовой плотности и т.п.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1984

Fedyanin V.K., Lisý V. E17-84-223

Contribution of Breathers to the Equilibrium and Dynamical Characteristics of Quasi-One-Dimensional Systems

The equilibrium and dynamical characteristics of a gas of breathers are investigated for statistical mechanical models described by the sine-Gordon equation. The thermodynamics of breathers is constructed. For the first time exact analytical expressions are obtained for the parallel and perpendicular dynamical structure factors $S_{\parallel}(q,\omega)$ and $S_{\perp}(q,\omega)$. These expressions are approximately averaged over the intrinsic frequency Ω of a breather. $S_{\parallel}$ is proved to consist of a central peak and an infinite series of satellites with centres near the frequencies $\omega^{\parallel}_N = \sqrt{q^2c_0^2 + (2N\omega_0)^2}$, $N = 1,2,\ldots$. $S_\perp$ has no central peak while the satellites are centered near the ferquencies $\omega^{\perp}_N = \sqrt{q^2c_0^2 + (2N+1)^2\omega_0^2}$, $N = 0,1,\ldots$. The obtained expressions may be used in the analysis of experimental data from the scattering of neutrons and light on quasi-one-dimensional objects, e.g., magnets, DNA-molecule, charge-density-waves, and others.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1984