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ON THE MAGNETIC-RESONANCE LINESHAPE IN INCOMMENSURATE SYSTEMS IN THE MULTI-SOLITON LIMIT

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The appearance of the incommensurate (IC) superstructure is a result of the structural phase transition in some crystal substances. Numerous studies (ref.[1] and references therein) have proved the efficiency and usefulness of the magnetic-resonance technique for the investigation of structurally IC systems. The usefulness is based on the fact that the NMR frequency distribution $I(\omega)$ reflects a spatial variation of the IC modulation and its temperature evolutions. However to compare the measured NMR data with the theoretical predictions one has had to use the approximate expression for $I(\omega)$ so far [1,2]. In the cases where more detailed information on the magnetic-resonance lineshape is required for the comparison one has had to accomplish a lengthy numerical calculation. To avoid this in future the present letter is devoted to a simple derivation of the analytical expression for the frequency distribution $I(\omega)$. The obtained result can be applied practically for the whole temperature interval where the IC phase exists. Further we will not take into account the finite width of individual lines. For this reason the function $I(\omega)$ may be considered as a resonance lineshape.

Our consideration of structurally IC systems is based upon simple concepts developed by McMillan [3] and Bak and Emery [4]. According to these concepts the spatial IC modulation is described in the constant amplitude approximation ($A(x) = A_0$) by using the soliton solutions of the sine-Gordon equation for the phase angle $\phi(x)$:

$$\frac{d^2\phi(x)}{dx^2} = pv \sin p\phi(x), \tag{1}$$

where p is a small integer number $p \geq 2$, and $v \sim A_0^{p-2}$. The one-soliton solution of equation (1) $\phi_s(x - x_0)$ corresponds to the centered at $x = x_0$ single domain wall which separates two commensurate (C) regions: one with $\phi_- = \frac{2\pi}{p} \cdot (n-1)$ and the other with $\phi_+ = \frac{2\pi}{p} \cdot n$ ($n = 1, 2 \ldots,$). A more general type of solutions for the sine-Gordon equation can be expressed by elliptic functions. But now we emphasize only one property of these solutions to be used in further consideration.

Namely, in the "multi-soliton" limit of well separated domain walls the phase $\phi(x)$ is approximately described by

$$\phi(x) = \sum_{n=1}^{N_s} \phi_s(x - x_0 - n\ell_s). \tag{2}$$

Here ℓ_s is the intersoliton spacing which is determined as

$$\ell_s = \frac{2K(1/\sqrt{1+\Delta^2})}{pv^{1/2}\sqrt{1+\Delta^2}}, \quad (3)$$

where K(k) is the complete elliptic integral of the first kind with the parameter $k = 1/\sqrt{1+\Delta^2}$, and Δ is the constant of integration (see, for example, ref.[5]). If the temperature-dependent spacing ℓ_s becomes comparable with the soliton width the representation of $\phi(x)$ by means of (2) is already incorrect. However the following property holds good: the increase of the variable x by the value ℓ_s causes the increase of $\phi(x)$ by $2\pi/p$, i.e.,

$$\phi(x+\ell_s) = \phi(x) + \frac{2\pi}{p}. \quad (4)$$

In the evaluation of the lineshape we confine ourselves to the simplest linear dependence of the resonance frequency on the nuclear displacements $u = A_0\cos[\phi(x)+\phi_0]$ represented in the continuum limit

$$\omega(x) = \omega_0 + \omega_1\cos[\phi(x)+\phi_0], \quad (5)$$

where $\phi_0 (0 \le \phi_0 < 2\pi)$ is an initial phase which is determined by a position in the unit cell of the nucleus under investigation. The lineshape $I(\omega)$ is defined as the Fourier transform of the autocorrelation function $G(t) = \langle\exp[-i\omega(x)t]\rangle$ (see ref.[6]):

$$I(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dt e^{i\omega t}\langle\exp[-i\omega(x)t]\rangle, \quad (6)$$

where the brackets represent the spatial averaging over the system with the length L. On changing the sequence of operations in equation (6) and making use of the δ-function property, we get

$$I(\tilde\omega) = \frac{1}{\omega_1 L}\int_0^L dx \sum_\xi \delta(x-x_\xi)\frac{1}{|\sin[\phi(x)+\phi_0]\cdot d\phi(x)/dx|}, \quad (7)$$

where $x_\xi = x_\xi(\tilde\omega)$ are the solutions of the equation

$$\cos[\phi(x)+\phi_0] = \tilde\omega, \quad (8)$$

with $\tilde\omega = (\omega-\omega_0)/\omega_1$. To evaluate (7) we integrate the sine-Gordon equation (1) at first and get

$$\frac{d\phi(x)}{dx} = \pm 2v^{1/2}\sqrt{\Delta^2 + \sin^2\frac{p}{2}\phi(x)}, \quad (9)$$

where Δ is the constant which is related to ℓ_s through equation (3). Now using equation (8) the expression for $I(\tilde\omega)$ may be written as

$$I(\tilde\omega) = \frac{1}{2\omega_1 Lv^{1/2}}\cdot\frac{1}{\sqrt{1-\tilde\omega^2}}\int_0^1 dx \sum_\xi \delta(x-x_\xi)\frac{1}{\sqrt{\Delta^2+\sin^2\frac{p}{2}\phi(x)}}, \quad (10)$$

Let us further rewrite equation (8) in the equivalent form

$$\phi(x_n^\pm) = \pm\arccos\tilde\omega + 2\pi n - \phi_0, \quad (11)$$

with n = 0, ±1, ±2,... . Formally, to evaluate (10) we should find the sets of solutions $\{x_n^+\}$ and $\{x_n^-\}$ from equation (11) and substitute them into equation (10). However it is sufficient only to count all of them.

To be convinced of that the following properties of equations (9)-(11) must be noted and used:

(i) As it follows from equation (9) the phase $\phi(x)$ is the monotonic function of x ; therefore for any n and a certain choice of "±" sign the equation (11) has not more than one solution;

(ii) The expression $\sqrt{\Delta^2+\sin^2\frac{p}{2}\phi(x_n^\pm)}$ depends only on the choice the sign "±" but not on n, as can be proved by direct substitution of equation (11) into (9);

(iii) Excluding the singular point $\omega = \omega_0$ one finds that $x_n^+ \neq x_{n'}^-$ for any n and n'.

Taking into account (i)-(iii) we obtain from (11) the intermediate result

$$I(\tilde\omega) = \frac{1}{2\omega_1 Lv^{1/2}}\cdot\frac{1}{\sqrt{1-\tilde\omega^2}}\left\{\frac{1}{\sqrt{\Delta^2+\sin^2[p/2(\arccos\tilde\omega-\phi_0)]}}\times\sum_{\{x_n^+\}}1 + \frac{1}{\sqrt{\Delta^2+\sin^2[\frac{p}{2}(\arccos\tilde\omega+\phi_0)]}}\sum_{\{x_n^-\}}1\right\}. \quad (12)$$

To determine the limits of summations in (12) we note that equation (11) has solutions as far as the following condition is satisfied

$$\phi(0) \le \pm\arccos\tilde\omega + 2\pi n - \phi_0 \le \phi(L), \quad (13)$$

where $\phi(0)$ and $\phi(L)$ are phase values at the left and the right end of the system, respectively. In view of the relation (4) it is easy to see from (13) that summations in (12) should be executed over all n restricted by the limits

$$\left[\frac{\phi(0)}{2\pi}\right] \le n \le \left[\frac{1}{p}\cdot\frac{L}{\ell_s} + \frac{\phi(0)}{2\pi}\right], \quad (14)$$

where [y] means the integer part of y and small contributions compared to $1/p \cdot L/\ell_s (\gg 1)$ are neglected. Finally we obtain

$$I(\tilde{\omega}) = \frac{\ell_s^{-1}}{2\omega_1 v^{1/2} p \sqrt{1-\tilde{\omega}^2}} \sum_{\nu=\pm 1} \frac{1}{\sqrt{\Delta^2 + \sin^2\left[\frac{p}{2}(\arccos\tilde{\omega} + \nu\phi_0)\right]}}, \quad (15)$$

where the intersoliton spacing ℓ_s is given by equation (3).

Now it would be desirable to compare the obtained expression (15) with the approximate formular for $I(\omega)$ used so far [1,2]. Previously, on the basis of the approximate formular one might only predict the most general features of the lineshape. Now equation (15) may give us not only the same features, but also the detailed information on the lineshape without a rather complicated numerical calculation. Furthermore, the expression (15) with equation (3) gives us more correct dependence of the lineshape on the soliton density (or, equally, on Δ). This density is believed to be the order-parameter for the IC-C phase transition.

In conclusion we should like to note that the suggestion on the long-range order for the solitons arrangement in the system is not necessary for the validity of the expression obtained (15). Actually, one may imagine the situation where the long-range order is broken (by a solitons pinnning on defects, for example), but the form of domain walls is not affected in the whole. It is easy to see that a new function $\phi(x)$ preserved the properties used above. Hence the relation (15) in that case remains valid, too. However the quantity ℓ_s is now not given by equation (3), but should be considered as an adjustable parameter corresponding to a mean distance between two neighbouring domain walls.

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Юшанхай В.Ю. E14-85-273

О форме линии магнитного резонанса в несоразмерных системах в многосолитонном пределе

Аналитическое выражение для распределения ЯМР частот $I(\omega)$ выводится для несоразмерных систем на основе общих свойств уравнения синус-Гордон для фазового угла модуляционной волны. Полученная формула обоснована для произвольных значений солитонной плотности ℓ_s^{-1}, начальной фазы ϕ_0 и при произвольном числе p топологически неэквивалентных соразмерных доменов.

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On the Magnetic-Resonance Lineshape in Incommensurate Systems in the Multi-Soliton Limit

An analytical expression for the NMR frequency distribution $I(\omega)$ is derived in structurally incommensurate systems by using general properties of the sine-Gordon equation for the phase angle $\phi(x)$ of the modulation wave. The obtained formula is valid for arbitrary values of the soliton density ℓ_s^{-1}, the initial phase ϕ_0 and some number p of topologically nonequivalent commensurate domains.

The investigation has been performed at the Laboratory of Nuclear Problems, JINR.

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