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# Dimerization of magnetic lattice influenced by an ensemble of neutral magnetic dipoles

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**Abstract.** – We have studied bound states of a neutral non-relativistic spin-(1/2) particle in a one-dimensional system of magnetic barriers and magnetic delta-functions. If such non-rigid lattice is a host lattice of an ensemble of non-interacting neutral particles, this structure is unstable in dimerizations of the Peierls type.

In recent years there has been considerable interest in the periodical magnetic structures in experiments with polarized particles [1] and a spin resonator for control neutrons [2]. In 1992 Barut and Dowling [3] showed that the solution to the Pauli spinor equation for a magnetic dipole in a periodic magnetic field gives rise to an energy band structure as a consequence of Bloch's theorem. For example, it is possible that with cold neutrons the kinetic energy is about $E \sim 1.27 \cdot 10^{-7}$ eV. For the band structure we find that the lattice period would be $l = 127$ nm and the magnetic-field strength $B \sim 2.15$ T. Hence, a very efficient polarizing filter is proposed. The presence of neutronic band gaps in a periodic magnetic potential has also been demonstrated experimentally [4].

Most magnetic systems enter a long-range order in a model of exchange-coupled spins on a rigid lattice. If allowance is made for the possibility of an elastic distortion of the lattice, a new type of ordering can occur at low temperatures which is magnetoelastic. This ordering is called a spin-Peierls transition [5]. The situation strongly resembles that in a 1D conductor, where Peierls [6] was able to demonstrate that a half-filled conducting band is unstable against a dimerization of the lattice ions which introduces a gap in the Fermi energy. The result is a filled valence band, an empty conduction band, and an overall lowering of the energy of the system. Hence it is a metal-insulator transition. However, spin-Peierls systems are insulating at all temperatures while the structural and magnetic phase transition may coalesce.

In this work, we combine these ideas to study bound states of a neutral non-relativistic particle with spin-(1/2) in a non-rigid one-dimensional system of magnetic barriers.

First we consider a system such as a neutron or a neutral atom interacting with the periodically varying magnetic field in the form of dimerized rectangular barriers (fig. 1). The

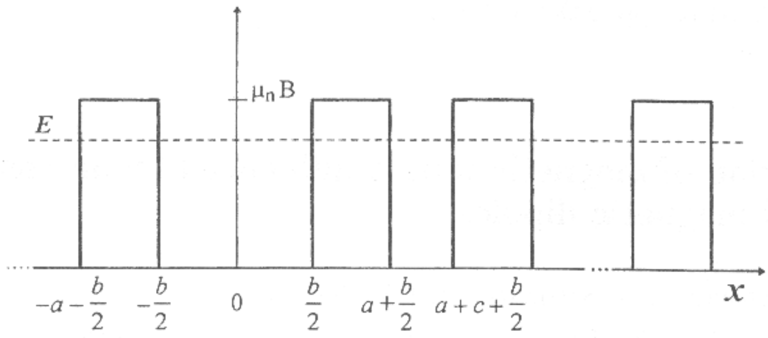


Fig. 1. – Dimerized rectangular potential barriers.

one-dimensional Pauli spinor Hamiltonian $\widehat{H}$ for the dipoles becomes

$$\widehat{H} = -\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2} - \mu_n \widehat{\sigma}_z B \times$$
$$\times \sum_{j=-\infty}^{\infty}\Big[h\Big(x+\frac{b}{2}+jl\Big)-h\Big(x+\frac{b}{2}+a+jl\Big)+h\Big(x+\frac{b}{2}+a+c+jl\Big)-h\Big(x+\frac{b}{2}+2a+c+jl\Big)\Big], \quad (1)$$

where $m$ is the mass of the particle, $\mu_n$ is the magnetic moment, $\widehat{\sigma}_z$ is the Dirac spin matrix, $h(x)$ is the Heaviside function, $B$ is the magnetic field, and $l = 2a+b+c$ is the period of lattice of the barriers.

The solution of the eigenvalue equation $\widehat{H}\Psi = E\Psi$, where $\widehat{H}$ is given by (), has a travelling wave (or exponentially decaying) form. The matching conditions for eigenvectors on the magnetic barriers determine the coefficients of what is called the $M$-matrix [7] which is very useful in studying such Kroning-Penney [8] type problems. In our example, because of the spinor character of the Hamiltonian (), the $M$-matrix for one barrier is $4 \times 4$, *i.e.*

$$M_{E>\mu_n B} = \begin{pmatrix} \widehat{M}^1 & \widehat{O} \\ \widehat{O} & \widehat{M}^2 \end{pmatrix}, \qquad M_{E<\mu_n B} = \begin{pmatrix} \widehat{M}^1 & \widehat{O} \\ \widehat{O} & \widehat{M}^{2'} \end{pmatrix}, \quad (2)$$

where $\widehat{M'}^1$, $\widehat{M}^2$, $\widehat{M}^{2'}$ and $\widehat{O}$ are $2\times 2$ matrices with the matrix elements

$$M^j_{11} = e^{i\mu_j}\cosh\lambda_j, \quad M^j_{12} = i\sinh\lambda_j, \quad M^j_{21} = -M^j_{12},\ M^j_{22} = e^{-i\mu_j}\cosh\lambda_j, \quad (3)$$

and the following notation has been introduced:

$$\mu_j = k_0 a - \arctan\big(\frac{\eta_j}{2}\tan k_j a\big), \qquad \lambda_j = -\sinh^{-1}\big(\frac{\varepsilon_j}{2}\sin k_j a\big),$$

$$\varepsilon_j = \frac{k_j}{k_0} - \frac{k_0}{k_j}, \qquad \eta_j = \frac{k_j}{k_0} + \frac{k_0}{k_j} \qquad (j = 1, 2, 2'), \quad (4)$$

$$k_0 = \frac{\sqrt{2mE}}{\hbar}, \qquad v_0 = \frac{\sqrt{2m\mu_n B}}{\hbar},$$

$$k_{1,2} = \sqrt{k_0^2 \pm v_0^2}, \qquad k_{2'} = \sqrt{v_0^2 - k_0^2}.$$

The product of the $M$-matrix and the propagation matrix

$$T = \begin{pmatrix} \widehat{T} & \widehat{O} \\ \widehat{O} & \widehat{T} \end{pmatrix}, \qquad \widehat{T} = \begin{pmatrix} e^{-ik_0 l} & \widehat{O} \\ \widehat{O} & e^{ik_0 l} \end{pmatrix} \tag{5}$$

determines what is called the $P$-matrix, $P^{-1} = MT$. The condition that the solutions of the eigenvalue equations of the $P$-matrix are purely imaginary leads to the equations of band structure [9]

$$\cos\gamma = \frac{1}{4}\frac{1}{\bar{k}^2(1+\bar{k}^2)}\sin^2\alpha\sqrt{1+\bar{k}^2}\left(\cos 2\alpha\bar{k}^2\Delta' - \cos 2\alpha\bar{k}d'\right) +$$

$$+\cosh 2\alpha\sqrt{1+\bar{k}^2}\cos 2\alpha\bar{k}d' - \frac{2\bar{k}^2+1}{2\bar{k}\sqrt{1+\bar{k}^2}}\sin 2\alpha\sqrt{1+\bar{k}^2}\sin 2\alpha\bar{k}d', \tag{6a}$$

$$\cos\gamma = \frac{1}{4}\frac{1}{\bar{k}^2(1-\bar{k}^2)}\sinh^2\alpha\sqrt{1-\bar{k}^2}\left(\cos 2\alpha\bar{k}^2\Delta' - \cos 2\alpha\bar{k}d'\right) +$$

$$+\cosh 2\alpha\sqrt{1-\bar{k}^2}\cos 2\alpha\bar{k}d' - \frac{1-2\bar{k}^2}{2\bar{k}\sqrt{1-\bar{k}^2}}\sinh 2\alpha\sqrt{1-\bar{k}^2}\sin 2\alpha\bar{k}d', \tag{6b}$$

where $0 \le \bar{k} \le 1$ and the renormalized variables are given by

$$b' = \frac{b}{a}, \quad c' = \frac{c}{a}, \quad d' = \frac{b'+c'}{2}, \quad \bar{k} = \frac{k}{v_0}, \quad \alpha = av_0 . \tag{7}$$

The order parameter $\Delta'$ (known as the parameter of distortion) has been introduced in the following way: $\Delta' = d' - c'$.

The first equation (6$a$) corresponds to the up-projection of spin. The second equation (6$b$) corresponds to the down-projection of spin. In the case of higher momentum $\bar{k} \ge 1$, eq. (6$b$) transforms into

$$\cos\gamma = \frac{1}{4}\frac{1}{\bar{k}^2(\bar{k}^2-1)}\sin^2\alpha\sqrt{\bar{k}^2-1}\left(\cos 2\alpha\bar{k}^2\Delta' - \cos 2\alpha\bar{k}d'\right) +$$

$$+\cosh 2\alpha\sqrt{\bar{k}^2-1}\cos 2\alpha\bar{k}d' - \frac{2\bar{k}^2-1}{2\bar{k}\sqrt{\bar{k}^2-1}}\sin 2\alpha\sqrt{\bar{k}^2-1}\sin 2\alpha\bar{k}d', \tag{8}$$

while (6$a$) remains the same. The condition $\cos\gamma > 1$ denotes all energy values which are forbidden. From (6) and (7) the allowed values of the energy ($E \sim \bar{k}^2$) can be calculated in terms of the parameter $\gamma$, and also the parameter of distortion $\Delta'$. This is done numerically with a precision of $10^{-6}$ (fig. 2).

Let us assume that the based magnetic chain is not fixed, then oscillates around the equilibrium positions. In the simplest approximation that there is a macroscopic occupation of one phonon of the type $q_0 = \pi/l$ [5], [10], the free energy of the phonon subsystem has the form $F_{\mathrm{ph}} = N\omega_0'\Delta'^2$, where $N$ is the number of magnetic atoms and $\omega_0' = \omega(q_0)\hbar$.

Let us consider the system of $N$ non-interacting neutral particles with spin-(1/2) embedded in the periodical magnetic potential in fig. 1. Each particle is interacting with the magnetic chain according to the laws of quantum mechanics (6), (8). The free energy of this subsystem can be found by the usual relation $F_{\mathrm{p}} = \mu\langle N\rangle + \Omega$, where $\mu$ and $\Omega$ are the chemical potential

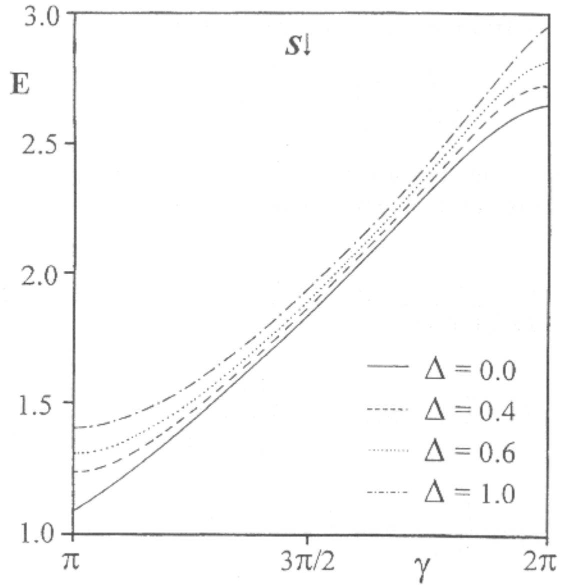


Fig. 2. – The dispersion spectrum of the particle in the second Brillouin zone for different values of the parameter of distortion and down ($s\downarrow$) spin polarization.

and grand canonical potential, respectively. The form of the functions $\langle N\rangle$ and $\Omega$ depends on the model of the density of states. If we propose that the density of states is proportional to $(E-E_{\rm c})^{-1/2}$ [11], where $E_{\rm c}$ is the bottom of the "conducting" band, then $\langle N\rangle$ and $\Omega$ become

$$\langle N\rangle = \frac{4L}{h}(2m)^{1/2}(V_0\Theta)^{1/2}\int\limits_0^\infty \frac{{\rm d}z}{e^{\sigma+z^2}+1}\,, \tag{9}$$

$$\Omega = -\Theta\left(\frac{\Theta}{\eta-a_3}\right)^{1/2}\int\limits_0^\infty \ln\left[1+e^{-(\sigma+z^2)}\right]{\rm d}z\,. \tag{10}$$

In formulae (9), (10) the following notation is used: $L$ is the length of the chain, $V_0=\mu_n B$, $\Theta = k_{\rm B}T/V_0$ is the renormalised temperature, $\eta=\mu/V_0$, $\sigma=(a_3-\eta)/\Theta$. In our model we assume that the "Fermi level" is in the middle of the third Brillouin zone ($a_3$ is at the bottom of the zone and it depends on $\Delta'$).

By numerical integration of (9) and (10), we find that the particle free energy $F_{\rm p}$ decreases with the parameter of distortion $\Delta'$. On the other hand, the phonon free energy $F_{\rm ph}$ increases with the parameter of the distortion. Minimizing the total free energy $F=F_{\rm ph}+F_{\rm p}$ of the distortion parameter $\partial F/\partial\Delta'=0$, we obtain a self-consistent equation of the parameter of distortion as a function of temperature. Results of numerical calculations for various values of phonon frequency and polarization (spin up $s\uparrow$ and spin down $s\downarrow$) are shown in fig. 3*a*), *b*).

The diagram shows that the distortion state is stable for all temperatures without point of phase transition. The behaviour of the parameter of distortion is similar to the magnetization of a one-dimensional Ising antiferromagnet in the magnetic field [12]. However, in the zero-temperature limit the parameter of distortion has a value between 0 and 1, depending on the

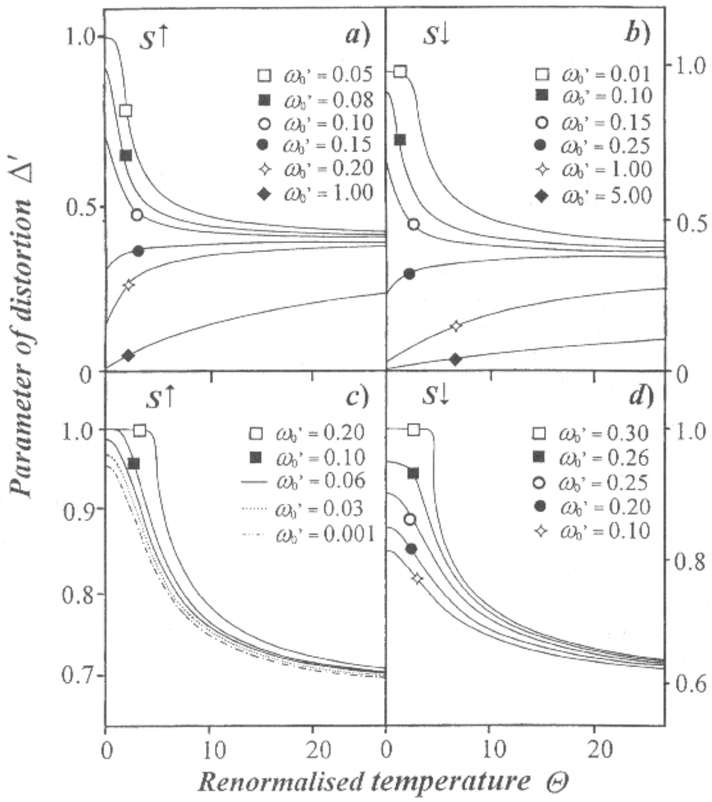


Fig. 3. – Plots of the parameter of distortion as a function of temperature for various values of the phonon frequency and polarization of spin in the case of rectangular magnetic barriers ($a$), $b$)) and magnetic delta-function ($c$), $d$)).

phonon frequency. We find nothing which looks like a critical magnetic field as in the case of Ising antiferromagnet.

Repeating the previous procedure for an infinite chain of magnetic barriers, one can determine the band structure of the system of magnetic delta-functions. Namely, if instead of the Hamiltonian (1) we consider the Hamiltonian

$$\widehat{H} = -\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2} - \mu_n \widehat{\sigma}_z B \sum_{j=-\infty}^{\infty} \left[ \delta(x - \frac{b}{2} - jl) + \delta(x - \frac{b}{2} - c - jl) \right] , \tag{11}$$

where the period of lattice is $l = b + c$, we obtain new matrix elements of the $M$ matrix and a new form of energy bands which depend on the parameter of distortion $\Delta' = v_0(c-b)/2$. In the single-phonon approximation one can get the self-consistent equation for $\Delta'$. After the numerical integration and differentiation we obtain the dependence $\Delta' = \Delta'(\Theta)$, where $\Theta$ is the renormalized temperature (fig. 3$c$), $d$)). Again it is evident that the distorted state is stable at all temperatures.

In conclusion, we have shown that a periodic magnetic potential (of the form of rectangular barriers or delta-functions) as a result of a quantum "interaction" with an ensemble of neutral particles of spin-(1/2), exhibits an instability of the Peierls type. We think that this mechanism can be important in explaining the processes followed by structural transformations.

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