New field model of a one-dimensional spin density wave

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A new model is offered for a spin density wave in a quasi-one-dimensional magnetic conductor. This model is amenable to exact solution. Deep self-trapping states of charge carriers, similar to those which exist in charge density waves, are predicted in a magnetic system.

The physics of quasi-one-dimensional conducting compounds has recently attracted much interest. In particular, the deep self-trapping states of large radius, which are typical of the systems, are extremely interesting. Some examples of these states are solitons and polarons of the order parameter of a charge density wave in conducting polymers.[1] Self-trapping in a charge density wave results from an interaction of conduction electrons with lattice vibrations (a Peierls dielectric). We know that in magnetic conductors an instability arises and gives rise to a spin density wave (e.g., Ref. 2). In contrast with the situation in a charge density wave, the electron density in a spin density wave is spatially uniform, while the distribution of the magnetic moment is modulated. The spontaneous magnetic moment of a spin density wave determines the gap in the spectrum of conduction electrons, and in the phase of a spin density wave a one-dimensional metal becomes an insulator. The existence of a spin density wave is usually linked with electron-electron Coulomb correlations, but in the one-dimensional case a new approach to the description of spin density waves can be proposed for several systems. This approach is analogous to the Peierls approach and uses the so-called *s-f* model.[3] A description based on the *s-f* model is convenient in that it allows one to construct an exactly solvable continuum model in the spirit of Ref. 1 and to study the nature of the self-trapping states. These are our purposes in the present letter.

We consider a ferromagnetic metal below the Curie point T_C, described by the

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Hamiltonian

$$H = \sum_{n,\alpha} J^\alpha S_n^\alpha S_{n+1}^\alpha + A \sum_{n,\tau,\tau'} a_{n\tau}^+ (\mathbf{S}\vec{\tau})_{\tau\tau'} a_{n\tau'}$$

$$+ t \sum_{n,\tau} (a_{n\tau}^+ a_{n+1\tau} + \text{H.a.}). \tag{1}$$

The first term is the Heisenberg Hamiltonian ($\alpha = x, y, z$); the operator $\mathbf{S}_n$ represents the spin of an atom at lattice site n; the operator $a_{n\tau}^+$ creates an s-electron with a spin projection τ; $\vec{\tau}$ is the set of Pauli matrices; A is the s-f exchange constant; and t is the electron-transport integral along sites. It turns out that ferromagnetic state (1), characterized by the values $\langle S_n^z \rangle = S$ and $\langle S_n^{x,y} \rangle = 0$ and by a metallic conductivity, is unstable below a certain temperature $T_{\text{SDW}} < T_C$ with respect to the formation of a spin density wave—a condensation of magnons with momenta $\pm 2k_F$—and the simultaneous appearance of an energy gap in the spectrum of the s-electrons. Since the temperature T_{SDW} is determined by three-dimensional interactions, we consider a one-dimensional structure of a spin density wave at $T \ll T_{\text{SDW}}$.

To describe the spin density wave, it is convenient to use the Holstein-Primakov representation, introducing the quasiaverage magnon operators $C_{2k_F} = \Delta \exp(i\varphi)$, $C_{-2k_F} = \rho \exp(-i\theta)$. In terms of the order parameters of the spin density wave, the spontaneous components of a site spin are

$$\begin{aligned} \langle S_n^x \rangle &= \sqrt{2S}(\Delta\cos(2k_F na + \varphi) + \rho\cos(2k_F na + \theta)) \\ \langle S_n^y \rangle &= \sqrt{2S}(\rho\sin(2k_F na + \theta) - \Delta\sin(2k_F na + \varphi)), \\ \langle S_n^z \rangle &= S - 2(\Delta^2 + \rho^2), \end{aligned} \tag{2}$$

where a is the lattice constant.

Following Ref. 4, we can easily write the Lagrangian of the continuum model of the spin density wave:

$$L = i\bar{\psi}\gamma_\mu D_\mu \psi + i\bar{\chi}\gamma_\mu D_\mu^* \chi - \bar{\psi}\bar{\Delta}\exp(-i\gamma_5\varphi)\psi$$

$$- \bar{\chi}\bar{\rho}\exp(-i\gamma_5\theta)\chi - g_1^{-2}(\bar{\Delta}^2 + \bar{\rho}^2) - g_2^{-1}\bar{\Delta}\bar{\rho}\cos(\varphi - \theta), \tag{3}$$

where ψ, χ are two-component spinors which differ in the direction of the spin of the electrons and holes:

$$\psi = \begin{pmatrix} u\uparrow \\ v\downarrow \end{pmatrix}, \quad \chi = \begin{pmatrix} u\downarrow \\ v\uparrow \end{pmatrix}.$$

In addition, $D_\mu = (\partial_0, \partial_1 - iAS/2v_F)$, $\gamma_\mu = (\sigma_1, -iv_F\sigma_2)$, $\gamma_5 = \sigma_3$, σ_i are the Pauli matrices, $\bar{\psi} = \psi^+\sigma_1$; $\bar{\Delta}, \bar{\rho} = (\Delta, \rho)A\sqrt{S/2}$, and

$$g_1^{-2} = \frac{(J^x + J^y)\cos(2k_F a) - 2J^z}{A^2}, \quad g_2^{-1} = 2\frac{J^x - J^y}{A^2}\cos(2k_F a).$$

The fermion part of Lagrangian (3) is the same as the Gross-Neveu chiral model.[5]

Kinetic terms resulting from the dynamics of f-electrons (and containing $\dot{S}^{\alpha}$) were omitted in Ref. 3. Here we will study only static solutions of the model, assuming that the adiabatic approximation in the small parameter $t_f/t \ll 1$, is valid, where t_f is the width of the f-electron band.

The model in (3) describes a so-called spin density wave when the quantity $k_F a/\pi$ is not a rational number. In complete analogy with the Peierls model, a special case is that of a twofold commensurability, $k_F a = \pi/2$, in which Δ, ρ, φ, and θ are no longer dynamic degrees of freedom, and a combination of these variables serves as order parameter:

$$\Phi = \Delta\cos\varphi + \rho\cos\theta, \qquad \langle S_n^x \rangle = \sqrt{2S}(-1)^n \Phi(n), \quad \langle S_n^y \rangle = 0. \tag{4}$$

The Lagrangian corresponds to the $N = 2$ Gross-Neveau model with the real order parameter Φ:

$$L = i\bar{\psi}_s \gamma_\mu D_\mu \psi_s - \bar{\psi}_s \Phi \psi_s - g_3^{-2}\Phi^2, \qquad s = 1, 2 \tag{5}$$
$$g_3^{-2} = 4(J^x + J^z)/A^2$$

In the ground state, the order parameter is uniform:

$$\bar{\Delta}_0 = \bar{\rho}_0 = 2\left(\epsilon_F^2 - \frac{A^2 S^2}{4}\right)^{1/2} \exp\left(-\frac{1}{N(0)}(g_1^{-2} - \frac{1}{2}|g_2|^{-1})\right), \tag{6}$$
$$\Phi_0 = 2\left(\epsilon_F^2 - \frac{A^2 S^2}{4}\right)^{1/2} \exp(-1/g_3^2 N(0)),$$

where $N(0)$ is the state density at the Fermi level. According to (6), the conditions for the existence of the phase of a spin density wave are $2g_1^{-2} > |g_2|^{-1}$ and $\epsilon_F > AS/2$. In our model, the spin density wave is always linearly polarized: At $g^2 > 0$ we have $\langle S^x \rangle = 0$, and at $g_2 \leqslant 0$ we have $\langle S^y \rangle = 0$. In the isotropic case, the polarization is determined by a commensurability effect, i.e., by higher-order flipping processes.

Since the gap in the spectrum is an order parameter, it depends on external fields. An electric field directed along the chains suppresses the gap[6] and interacts with the phase of the spin density wave, $\varphi + \theta$, by virtue of the chiral anomaly[4,7]: i.e., the spin density wave is electrically active. A magnetic field H acts on the electron and spin subsystem, but the contribution of H to the electron subsystem is important only in very strong fields, $\mu H \sim \bar{\Delta}_0$, and the effect of H on the spin subsystem reduces to a renormalization of the coefficient of the exponential function in (6) and of the coupling constants. The single-ion anisotropy plays a similar role.

A study of inhomogeneous solutions of model (3) shows that they agree with the self-trapping states of the Gross-Neveau $U(1) \otimes U(1)$ chiral model. Specifically, there is only a nontopological order-parameter soliton with an energy $2/\pi\bar{\Delta}_0$ and with a singly filled electron level, lying in the middle of the energy gap. The Lagrangian in (5) corresponds to two types of inhomogeneous solutions: a topological soliton with a triply degenerate electron level in the middle of the gap, with an energy $2/\pi\bar{\Delta}_0$, and a polaron with an energy $2\sqrt{2}/\pi\overline{\Delta}_0$ with a singly filled level $\omega_0 = \pm\overline{\Delta}_0/\sqrt{2}$ (Refs. 1 and 8). The anomalous spin-charge coupling applies to the topological soliton.

The model proposed here can be used to describe systems containing atoms of rare-earth metals. Such systems should exhibit two magnetic-ordering temperatures, T_C and $T_{\rm SDW}$: below $T_{\rm SDW}$, the spiral structure in (2) arises, accompanied by the transition of the conductor into an insulator. The trapped electron states in the energy gap can be observed in optical or IR spectra.

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