Amplitude solitons in systems with a spin-density wave

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Soliton states in systems with a spin density wave are considered. The profile, charge, and spin of solitons in a system with a linearly polarized spin-density wave are obtained. Possible types of solitons in systems with a helicoidal spin-density wave are described.

There are many known compounds with the ground state in the form of a spin-density wave (for reviews see Refs. 1–3). The experience gained in investigations of systems with charge-density waves (for a review see Ref. 4) shows that topological solitons with a split-off local electron level can be expected for systems with spin-density waves. The structure of solitons for systems with spin-density and charge-density waves may generally be different because of the difference between the spaces of degeneracy of the order parameter for these systems. For example, commensurate and incommensurate charge-density waves are characterized by a double degeneracy of the real parameter $\pm\Delta$ and a phase degeneracy of the complex parameter $\Delta\exp(i\varphi)$. On the other hand, in the case of a linearly polarized sinusoidal spin-density wave (SDW) the degeneracy space is a sphere of real vectors $\mathbf{\Delta}$ and for a helicoidal SDW it is a set of orthogonal pairs of vectors $\mathbf{\Delta}_1\perp\mathbf{\Delta}_2$: $\mathbf{\Delta}=\mathbf{\Delta}_1+i\mathbf{\Delta}_2$.

The problem of solitons and soliton lattices in a model of the Peierls–Fröhlich type in the case of SDWs is exactly soluble, as already found for charge-density waves. In view of the complexity of the task of investigating this problem completely, we shall limit ourselves to the determination of the possible types of solitons with one split-off electron level. We can therefore consider analogs of kinks in charge-density waves, but we shall not discuss analogs of polarons. We shall show that in the case of a linearly polarized SDW the soliton profile is exactly the same as of a kink of a charge density wave. In the case of a helicoidal SDW the soliton profile may be more complex if the conditions for the existence of the SDW are satisfied.

We shall consider the model of interacting electrons in a chain with a Fermi spectrum linearized near the surface. In the self-consistent field approximation a system of this kind is described by the effective Hamiltonian (see, for example, Ref. 4)

$$H=\int dx\Big[\psi_{+\sigma}^{+}\Big(-i\frac{\partial}{\partial x}\Big)\psi_{+\sigma}+\psi_{-\sigma}^{+}\Big(i\frac{\partial}{\partial x}\Big)\psi_{-\sigma} -\Delta_{\sigma\sigma'}^{+-}\psi_{+\sigma}^{+}\psi_{-\sigma}-\Delta_{\sigma\sigma'}^{-+}\psi_{-\sigma}^{+}\psi_{+\sigma'}+\frac{1}{g}\Delta_{\sigma\sigma'}^{+-}\Delta_{\sigma'\sigma}^{-+}\Big],\qquad(1)$$

where $\psi_{\pm\sigma}^{+}$ is the electron creation operator with a spin $\sigma=\uparrow,\downarrow$ and a wave vector which does not differ greatly from $\pm p_F$; g is the effective interaction constant. The case of an SDW corresponds to the selection $\Delta^{+-}=\boldsymbol{\sigma}\mathbf{\Delta}$, $\mathbf{\Delta}=\mathbf{\Delta}_1+i\mathbf{\Delta}_2$, where $\mathbf{\Delta}_1$ and $\mathbf{\Delta}_1$ are three-dimensional real vectors. The arbitrary nature of the selection of the phase $\mathbf{\Delta}$ corresponds to the possibility of a spatial shift of an SDW. In the case of a double commensurability (half-filled energy band) the phase is fixed. Two situations are possible: $\mathbf{\Delta}_1\|\mathbf{\Delta}_2$ or $\mathbf{\Delta}_1\perp\mathbf{\Delta}_2$. The first case corresponds to a sinusoidal SDW and the second to a helicoidal one. It should be pointed out that the selection of the order parameter Δ^{+-} in the form $\Delta_{\sigma\sigma'}^{+-}=\delta_{\sigma\sigma'}\Delta$ corresponds to a charge-density wave.

Variation of the functional of Eq. (1) with respect to Δ yields the following self-consistency condition

$$\Delta_{\alpha\beta}^{+-}=g\langle\psi_{+\alpha}\psi_{-\beta}^{+}\rangle=(\Delta_{\alpha\beta}^{-+})^{+}=\mathbf{\Delta}\boldsymbol{\sigma}_{\alpha\beta}.$$

Variation of Eq. (1) with respect to the wave functions ψ yields the equations for the eigenvalues:

$$\begin{pmatrix}-i\dfrac{\partial}{\partial x} & \boldsymbol{\sigma}\mathbf{\Delta}\\ \boldsymbol{\sigma}\mathbf{\Delta}^{*} & i\dfrac{\partial}{\partial x}\end{pmatrix}\begin{pmatrix}\psi_{+\uparrow}\\ \psi_{+\downarrow}\\ \psi_{-\uparrow}\\ \psi_{-\downarrow}\end{pmatrix}=E\begin{pmatrix}\psi_{+\uparrow}\\ \psi_{+\downarrow}\\ \psi_{-\uparrow}\\ \psi_{-\downarrow}\end{pmatrix}.\qquad(2)$$

The order parameter Δ is found from the minimum condition of the energy of the system

$$W=\sum_{E<\mu}E+\frac{|\mathbf{\Delta}|^2}{g},\qquad(3)$$

where μ is the chemical potential.

In the ground state ($\Delta=\text{const}$) we find that the electron spectrum is described by

$$E^2=k^2+|\mathbf{\Delta}_1|^2+|\mathbf{\Delta}_2|^2,\quad \mathbf{\Delta}_1\|\mathbf{\Delta}_2,$$
$$E^2=k^2+(|\mathbf{\Delta}_1|\pm|\mathbf{\Delta}_2|)^2,\quad \mathbf{\Delta}_1\perp\mathbf{\Delta}_2.\qquad(4)$$

The spectrum of a helocoidal SDW consists of two branches corresponding to states with different polarizations. In the case when $|\mathbf{\Delta}_1|=|\mathbf{\Delta}_2|$, one of the branches of the spectrum has a zero gap. We can easily see that the energy of a state of an SDW with a linear polarization is less than the energy of a state with a helicoidal polarization, i.e., the ground state of the model under discussion is a linearly polarized SDW.

It is known that the model of Eq. (2) is exactly integrable in the class of finite-band potentials.[5] The Bloch function $\psi(E)$ is meromorphic on a Riemann surface and has $\tau+3$ poles (τ is a certain type of a four-sheet surface). The branching points of this surface are unrelated to the spectrum of the periodic or antiperiodic problem. We shall find the soliton solution of the system by following the method of Krichever.[6] The wave function $\psi(E,x)$ of a one-soliton solution is meromorphic on the algebraic Riemann surface described by

$$E(Z)=\sum_{i=1}^{4}\frac{\alpha_i}{Z-Z_i},\qquad \sum_{i=1}^{4}\alpha_i=0,\qquad(5)$$

where Z_i and α_i are parameters governed by the coupling and self-consistency conditions discussed below. In the case under discussion the wave function has four poles and four zeros, and can be written in the form

$$\psi_i(x,Z)=C_i(x)e^{ipx}\prod_{j\neq i}(Z-Z_j)[Z-a_i(x)]\Big/\prod_{k=1}^{4}(Z-\gamma_k), \tag{6}$$

where $i = 1, 2, 3$, and 4, the quasimomentum is

$$p(Z)=\sum_{i=1}^{4}\frac{f_k\alpha_k}{Z-Z_k},\qquad f_k=(1,1,-1,-1),$$

$\gamma_k = \text{const}$, and the coefficients $C_i(x)$ are found from the asymptotic form of ψ in the limit $E\to\infty$:

$$C_i(x)=\frac{\exp(-i\lambda_i x)}{Z_i-a_i(x)}\prod_{j=1}^{4}(Z_i-\gamma_j)\Big/\prod_{k\neq i}(Z_i-Z_k),$$

$$\lambda_k=\sum_j\frac{(f_j-f_k)\alpha_j}{Z_k-Z_j},\quad \psi_1=\psi_{+\uparrow},\quad \psi_2=\psi_{+\downarrow},\quad \psi_3=\psi_{-\uparrow},\quad \psi_4=\psi_{-\downarrow}.$$

The wave functions ψ_i satisfy an additional condition

$$\psi_i(x,\varkappa)=\psi_i(x,\varkappa'), \tag{7}$$

where $\varkappa$ and $\varkappa'$ are found from the condition $E(\varkappa)=E(\varkappa')=E_0$ (E_0 is the energy of a local level).

It follows from Eqs. (6) and (7) that

$$a_i(x)=\frac{\varkappa A_i\exp(-p_0x)-\varkappa'}{A_i\exp(-p_0x)-1},$$

$$ip_0=p(\varkappa)-p(\varkappa'),\qquad A_i=\prod_{j\neq i}\frac{\varkappa-Z_j}{\varkappa'-Z_j}\prod_{k=1}^{4}\frac{\varkappa'-\gamma_k}{\varkappa-\gamma_k}. \tag{8}$$

In the limit $x\to\pm\infty$, we find from Eq. (8) that

$$a_i\to\begin{cases}\varkappa', & x\to+\infty\\ \varkappa, & x\to-\infty\end{cases}. \tag{9}$$

The Schrödinger equation (2) expanded in the vicinity of $E\to\infty$, yields

$$\psi_i|_{Z\to Z_k}=\left(\delta_{ik}+\frac{\xi_{ik}}{E}\right)e^{\pm iEx},\qquad \xi_{ik}=\begin{pmatrix}0 & \sigma\Delta\\ \sigma\Delta^* & 0\end{pmatrix}. \tag{10}$$

A comparison of the expansion of the wave function in the form of Eqs. (6) and (10) shows that

$$\xi_{ik}=\alpha_k\Big[\prod_{j\neq i,k}(Z_k-Z_j)\Big/\prod_{j\neq i}(Z_i-Z_j)\Big]$$
$$\times\frac{Z_k-a_i(x)}{Z_i-a_i(x)}\Big[\prod_{m=1}^{4}(Z_i-\gamma_m)\Big/\prod_n(Z_k-\gamma_n)\Big]\exp[i(\lambda_k-\lambda_i)x],$$

$$\xi_{13}=\xi_{31}^*=\Delta_z=-\xi_{24}=-\xi_{42}^*,\qquad \xi_{14}=\xi_{41}^*$$
$$=\Delta_-=\Delta_x-i\Delta_y,\ \xi_{23}=\xi_{32}^*=\Delta_+=\Delta_x+i\Delta_y. \tag{11}$$

Equations (6)–(8) and (11) considered allowing for the self-consistency solution of Eq. (3) define uniquely the nature of the wave function with the order parameter $\Delta(x)$.

We shall consider soliton states against the background of the ground state with a linearly polarized SDW. In the limit $x\to+\infty$ we select $\Delta_x=\Delta_y=0$, $\Delta_z\neq0$, i.e., $\xi_{14}=\xi_{23}=0$. It follows from Eq. (11) that in the limit $x\to+\infty$ we can expect the conditions $a_4(x)\to Z_1$, and $a_3(x)\to Z_2$ to be satisfied, or subject to Eq. (9), we can expect $\varkappa'=Z_1=Z_2$. The last condition may not be true because it follows from Eqs. (5) and (7) that $E(\varkappa')=E_0$ and $E(Z_i)=\infty$. Therefore, in order to satisfy conditions of the $\xi_{14}\to0$ type, we must ensure that the constant coefficient in front of $Z_4-a_1(x)$ in Eq. (11) vanishes. Consequently, the requirement that $\xi_{14}\to0$ or $\xi_{23}\to0$ in the limit $x\to+\infty$ yields the condition $\xi_{14}(x)=0$ or $\xi_{23}(x)=0$ for all x. Therefore, in the case of a soliton against the background of a linearly polarized SDW we have the condition $\Delta_x=\Delta_y=0$, i.e., the soliton is linearly polarized.

In the linear-polarization case under discussion it is convenient to seek the form of the function $\Delta_z(x)=\Delta_1+i\Delta_2$ by applying directly Schrödinger equations of the type described by Eq. (2) which in the $\Delta_x=\Delta_y=0$ case split into equations for $\sigma=\uparrow$ and $\downarrow$. For example, in the case of the $\sigma=\uparrow$ spin, we have

$$-i\frac{\partial}{\partial x}\psi_++\Delta\psi_-=E\psi_+,$$
$$\Delta^*\psi_++i\frac{\partial}{\partial x}\psi_-=E\psi_-. \tag{12}$$

In the variables $U,V=(\psi_+\pm\psi_-)/\sqrt{2}$, the system (12) reduces to

$$U'-\Delta_2U=i(E+\Delta_1)V,$$
$$V'+\Delta_2V=i(E-\Delta_1)U. \tag{13}$$

In the case of the $\sigma=\downarrow$ spin we have to replace Δ with $-\Delta$ and then we find that $U_\downarrow=V_\uparrow$, and $V_\downarrow=U_\uparrow$.

The system (13) was derived earlier[7] for amplitude solitons in Peierls systems with charge-density waves. We can easily see that the self-consistency conditions for spin solitons are also identical with those obtained in Ref. 7. The order parameter is described by $\Delta_z(x)=\Delta_0\tanh(\Delta_0x)$. Moreover, other results obtained for a soliton in a Peierls insulator, particularly for the coupling of the spin to the charge, are retained. In the case of the 1:2 commensurability, the mulitplicity (degree) of occupancy of a level at the center of the band gap can be $\nu_0=0$, 1, or 2. A soliton can have the charge $q=-e$, 0, or e and its spin may be $s=0$, $\frac{1}{2}$, or 0, respectively. In the incommensurate case, we have $\nu_0=1$, $q=0$, and $s=\frac{1}{2}$.

We shall now consider briefly solitons against the background of a helicoidal SDW. An analysis similar to that given above leads from the conditions $\Delta_z\to0$, $\Delta_x=\Delta_1$, $\Delta_y=i\Delta_2$, $\Delta_+=\Delta_1-\Delta_2$, $\Delta_-=\Delta_1+\Delta_2$, in the limit $x\to+\infty$, to the requirement $\Delta_z(x)=0$ for all values of x [if, moreover, $\Delta_1=\Delta_2$ in the absence of a soliton, then in the presence of a soliton the condition $\Delta_+(x)=0$ is also satisfied]. The Schrödinger equations (2) also split into equations describing states with different polarizations. The order parameter is then described by

$$\Delta_{+}=(\Delta_1-\Delta_2)\,\mathrm{th}[(\Delta_1-\Delta_2)x],$$

$$\Delta_{-}=(\Delta_1+\Delta_2)\,\mathrm{th}[(\Delta_1+\Delta_2)x]. \tag{14}$$

We have thus considered possible types of solitons in systems with an SDW. In the model described by Eq. (2) we demonstrated that the ground state is a linearly polarized SDW and the excited states are linearly polarized amplitude solitons of the same type as found in systems with charge-density waves. For a given type of the exchange energy the state with a helicoidal SDW is not the ground state. Without specifying the nature of the exchange energy, we considered the general case and found possible profiles of a soliton against the background of a helicoidal SDW demonstrating that the parameters Δ_1 and Δ_2 in Eq. (14), as well as the charge and magnetic properties of soliton excitations are found by minimization of the functional of the energy of the system.

We can expect a simplified linearly polarized profile to be typical of periodic structures such as soliton lattices. We can then use the results of Ref. 8 and the discussion therein of incommensurate SDWs in chromium alloys. Structure and thermodynamic manifestations of soliton lattices are considered in Refs. 8–10. It is worth noting that in systems with charge-density waves (such as polyacetylene) the main methods for the investigation of soliton structures are optical, electron magnetic resonance, and NMR (for reviews see Refs. 11 and 12). The case of an SDW does not require separate investigation in respect of its optical properties.

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