Magnetic polarons in one-dimensional antiferromagnetic chains

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We study magnetic polarons in antiferromagnetic chains by using the one-dimensional Anderson-Hasegawa double-exchange discrete model, and find analytically different families of *magnetic polaron compactons*. To study stability and nontrivial dynamics of the self-trapped magnetic polarons, we generalize the Anderson-Hasegawa model to allow for a finite spin of the lattice, and investigate different types of stationary states with collinear and canted spin structure, revealing the existence of stable nonmobile collinear solutions as well as *stable mobile magnetic polarons* having a canted structure.

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Currently there is a common belief that the concept of phase separation plays a crucial role in the determination of physical properties of manganites and related compounds,[1,2] being especially relevant to the remarkable colossal magnetoresistance phenomenon. The self-trapping of charge carriers is the most widely discussed type of phase separation, first predicted by Nagaev almost 40 years ago[3] and still being actively studied.[4–8] A *self-trapped magnetic polaron* is formed when an itinerant carrier induces inhomogeneous deformation of the magnetic lattice [due to a strong coupling between a doped electron (hole) and the lattice localized spins], thus creating a domain of the metallic ferromagnetic (FM) or (perhaps) canted or mixed state inside the insulating antiferromagnetic (AFM) matrix. Then the carrier becomes trapped by this effective self-induced potential.

As was first pointed out by de Gennes,[9] the self-trapping of the carrier may stipulate not a local but rather a weakly decaying distortion of the magnetic ordering, thus producing a *canted state* of the magnetic subsystem, being quite different from the simple picture of a ferron as a local confined FM domain inside the perfect AFM.[10] The type of magnetic ordering resulting from the self-trapping of the carrier was recently readdressed for both isotropic[6] and anisotropic[5,7,8] types of 1D magnetic lattices. While for the anisotropic case one may naturally expect that the presence of a second spatial scale (magnetic length[11]), being inherently related to the anisotropy strength, should emanate in the smoothing and spreading of the ordering deviations (the same as occurs for the simple domain walls), in the case of the isotropic system the situation is not so obvious, although Pathak and Satpathy[6] predicted the existence of extended states in this case as well. So, the first question raised in this paper concerns the structure and classification of self-trapped states for the *isotropic* AFM lattice: we present a systematic analysis of different types of strongly localized magnetic polarons and, for the first time to our knowledge, demonstrate a link between the magnetic polarons of the Anderson-Hasegawa (AH)[12] model and so-called *compactons*, spatially localized nonlinear modes with a finite extent.[13]

The second topic addressed in the current paper is the *stability and mobility* of the self-trapped states in the isotropic AFM lattice. Although the question of "thermal" stability, i.e., whether magnetic polarons may exist in thermal equilibrium at nonzero temperatures, was studied long ago[14] (see Ref. 15 for recent studies of that type), we, for the first time to our knowledge, consider *dynamical* (linear) stability of magnetic polarons as nonequilibrium excitations (or, alternatively, stability in the limit of zero temperature). Even though the magnetic polarons found may not be thermally stable at higher temperatures, a great deal of important physical processes are nonequilibrium ones, and linear (dynamical) stability is expected to give a necessary condition for an excitation to be sufficiently long lived to participate in nonequilibrium transport if the temperature of the surroundings is low enough. To carry out the linear stability analysis we *generalize* the AH model to include a finite value of the localized spins, and derive coupled nonlinear dynamical equations for the two fields describing the carrier wave function and the classical spin-field component for the AFM and/or FM distribution of the background lattice, respectively.

Magnetic polaron compactons. When the conduction bandwidth is much less than the strength of the coupling of the itinerant carrier to the localized spins of the magnetic lattice, which is just the case for strongly correlated systems such as manganites, etc., one can describe the system in the framework of the AH double-exchange spin Hamiltonian[6,12] (see also Ref. 16). This model describes an itinerant carrier coupled to the AFM isotropic (in the case we consider) classical spin chain

$$\mathcal{H}=\sum_n\left(-\alpha\psi_n^*\psi_{n+1}\cos\frac{\chi_n}{2}+\text{c.c.}+\cos\chi_n\right), \qquad (1)$$

where χ_n is the relative angle between the (classical) lattice d-spins localized at the neighboring sites n and $n+1$, ψ_n is the carrier wave function at site n with the normalization $\Sigma_n|\psi_n|^2=1$, $\alpha=t/J$ is the electron-magnon coupling constant, t is the hopping integral, and J describes the spin exchange within the lattice; these quantities are assumed to be positive with the typical values $t\sim 0.1$ eV and $J\sim 10$ meV, such that $\alpha\sim 10$. Equations for the field components ψ_n can be found as $i\hbar\dot{\psi}_n=\partial\mathcal{H}/\partial\psi_n^*$, and the spin distribution is found by mini-

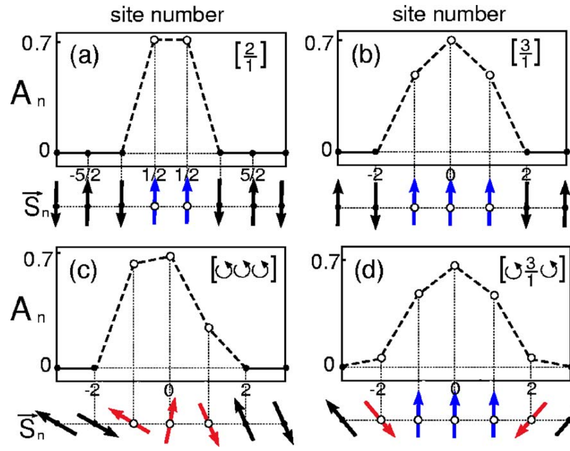

FIG. 1. (Color online) Examples of localized magnetic polarons. Shown are the amplitudes of the wave functions A_n and spin subsystem $\mathbf{S}_n$ for (a) MF $[\frac{2}{1}]$; (b) MF $[\frac{3}{1}]$; (c) SCP $[\circlearrowleft\circlearrowleft\circlearrowleft]$ for $\alpha=3.5$, $\gamma=0.25$; (d) SCF $[\circlearrowleft\frac{3}{1}\circlearrowleft]$ for $\alpha=12$.

mizing Eq. (1) with respect to χ_n, $\partial\mathcal{H}/\partial\chi_n=0$.

Looking for stationary solutions in the form $\psi_n=A_n\exp(i\omega t)$ with real amplitudes A_n, we obtain

$$\sin\frac{\chi_n}{2}\left(\alpha A_nA_{n+1}-2\cos\frac{\chi_n}{2}\right)=0, \tag{2}$$

$$\omega A_n-\alpha\left(A_{n+1}\cos\frac{\chi_n}{2}+A_{n-1}\cos\frac{\chi_{n-1}}{2}\right)=0, \tag{3}$$

where dimensionless ω is measured in units of $\hbar/J$.

The simplest localized solution of Eqs. (2) and (3) is obtained for the Mott polaron or *Mott ferron* (MF)[10] that describes a local domain of the FM state with K collinear spins embedded into an AFM chain: inside the FM region we have $\chi_n=0$ and $A_n\neq 0$. Examples of such MFs are shown in Figs. 1(a) and 1(b). For these localized solutions, the linear modes of the field ψ_n become trapped by an effective infinite potential well created by the spin state in the magnetic system. The MF solutions are characterized by the quantum number N that can be either integer (for odd K) or half-integer (for even K), i.e., $N=\frac{1}{2}(K-1)$. Then, the localized field ψ_n describing MF can be presented in the form

$$\psi_n(t)=\mathrm{e}^{\mathrm{i}\omega_m t}\sqrt{\frac{2}{K+1}}\begin{cases}\cos k_mn, & \text{odd } m,\\ \sin k_mn, & \text{even } m,\end{cases} \tag{4}$$

where $n\in[-N;N]$ (for a half-integer N the "site number" n also takes half-integer values with the unit step), and the parameters are coupled through the dispersion relation, $\omega_m=2\alpha\cos k_m$, where $k_m=\pi m/(K+1)$, and the mode index is $m\in[1;K]$. The MF energy is negative only for positive frequencies, $\delta E_m=-\omega_m(\alpha)/2+2(K-1)$, and smaller m ("long-wave" ferrons) correspond to larger negative energies. For convenience of the classification, we introduce a fractional index $[K/m]$ for each solution. In general, there exist also multiharmonic MF solutions described by linear combinations of single-harmonic modes given by Eq. (4): $[K/(m_1+m_2+\cdots)]$. Uncompensated magnetization for MF is $M=K$, and the total rotation of the spin vector for such a solution is $\Gamma=\Sigma_{n=-N}^{N-1}\chi_n=0$.

We also find more general localized solutions for magnetic polarons characterized by *canted spin structure*, i.e., those corresponding to the condition $\Gamma=\Gamma(\alpha)\neq 0$. The simplest solution of this kind describes a *small canted polaron* (SCP) with three canted spins (e.g., located at the sites $k-1$, k, and $k+1$), as shown in Fig. 1(c), with nonvanishing amplitudes A_{k-1}, A_k, and A_{k+1}. We find that this solution is degenerated, and it can be parametrized by a continuous parameter γ as follows: $A_k=2^{-1/2}$, $A_{k-1}=(1/2-\gamma^2)^{1/2}$, and $A_{k+1}=\gamma$, so that $\chi_i=2\cos^{-1}(\alpha/2)A_iA_{i+1}$ and $\omega=\alpha^2/4$. For $\alpha<4$, the parameter γ changes within the existence domain $\gamma\in[0;1/\sqrt{2}]$; and for $\alpha>4$ the existence domain becomes narrower, $0\leq\sqrt{1/2-8/\alpha^2}\leq\gamma\leq 2\sqrt{2}/\alpha\leq 1/\sqrt{2}$, with the upper border at $\alpha=4\sqrt{2}$. A single SCP changes the energy of the chain by the amount $\delta E=-\alpha^2/8$, and the corresponding uncompensated magnetization is $M(\alpha)=\Sigma_{i=k-1}^{k}\cos(\chi_i/2)$.

Introducing the special notation $\circlearrowleft$ for each site with a canted spin, we can present such localized solutions in the form: $[\circlearrowleft\circlearrowleft\circlearrowleft]$. As can be shown using Eqs. (2) and (3), localized solutions with more than three canted neighboring spins without either FM or AFM domains are not possible. A symmetric structure of MFs and SCPs describes canted spins at the edges of the FM region; we call these solutions *symmetric canted ferrons* (SCF), see Fig. 1(d). In our notations, these solutions can be presented in the form: $[\circlearrowleft\frac{K}{m}\circlearrowleft]$. The minimum number of FM sites involved, K, is two, and the mode number $m\leq\mathrm{int}(K/2)$. The wave function amplitudes A_n for this solution with odd m can be found in an explicit analytical form,

$$A_n=\frac{\sqrt{2\omega}}{\alpha\cos kN}\cos kn,\quad n\in[-N,N],$$
$$A_{\pm(N+1)}=\sqrt{\frac{2\omega}{\alpha^2}-\frac{2}{\alpha}\frac{\cos[k(N-1)]}{\cos kN}}, \tag{5}$$

and the similar solution for even m where in Eq. (5) the cosines should be replaced by the sines. The angle between the canted spins at the edges of the FM domain is defined by the relation $\cos(\chi/2)=(\alpha/2)A_NA_{N+1}$. The parameter k for the solution $[\circlearrowleft\frac{K}{m}\circlearrowleft]$ belongs to the interval $k_m\in[\frac{\pi m}{K+3};\frac{\pi m}{K+1}]$, and the frequency ω is given by the expression $\omega_m=2\alpha\cos k_m(\alpha)$. The existence domain and the wave number $k_m(\alpha)$ are determined by the normalization condition for the field ψ; the total magnetization for a single SCF is $M=K+2\cos\chi/2$. We also find asymmetric combinations of MFs and SCP, where the FM domain has a canted spin only at one of the edges: in our notations these states can be presented as $[\circlearrowleft\frac{K}{m}]$ or $[\frac{K}{m}\circlearrowleft]$.

In general, we can construct different families of combined states of magnetic polarons in the form

$$\left[\cdots\frac{K_1}{m_1}\circlearrowleft\underbrace{\ldots}_{i_1}\circlearrowleft\frac{K_2}{m_2}\circlearrowleft\underbrace{\ldots}_{i_2}\circlearrowleft\frac{K_3}{m_3}\cdots\right], \tag{6}$$

which include FM domains of arbitrary length K_n with i_n canted spins. Such localized solutions have a finite extent being embedded into a perfect AFM chain, because in the AH model the carrier hopping is allowed only in the inhomogeneity region. In fact, such finite-extent solutions represent a specific realization of the concept of *compactons*, introduced earlier for other continuous and discrete models with nonlinear dispersion.[13]

Generalized Anderson-Hasegawa model. In the AH model described by Eq. (1), the energy change due to the carrier hopping to the neighboring site with opposite spin is infinite, and the absolute value of the background lattice spins, S, is formally infinite as well. This means that this model does not allow to describe the nontrivial *dynamics* of magnetic polarons, and both polaron (dynamical) stability and mobility remain ill-defined in the framework of this model. In order to study the polaron dynamics utilizing the Landau-Lifshitz (LL) equations[11] for the dynamics of classical spins, our model should be modified to allow for a finite value of the lattice spins. This can be achieved if we include into the model the terms beyond the leading series expansion in the powers of $1/S$, which are omitted in Eq. (1) with the $\cos \chi/2$ factor in the carrier hopping amplitude.[12] The corresponding generalized Hamiltonian can be written in the form

$$\mathcal{H} = \sum_n \left(-\frac{\alpha}{2}\psi_n^*\psi_{n+1}|\mathbf{S}_n + \boldsymbol{\sigma}_n + \mathbf{S}_{n+1}| + \text{c.c.} + \mathbf{S}_n \cdot \mathbf{S}_{n+1}\right), \tag{7}$$

where $\alpha = t/JS$ is the coupling parameter, $\mathbf{S}_n$ is the classical spin with the absolute value S for all sites, and $\boldsymbol{\sigma}_n$ stands for the effective spin of the itinerant carrier. As in the original AH model, we assume that the effective spin has the same direction as the lattice spin $\mathbf{S}_n$, so that $\boldsymbol{\sigma}_n = \mathbf{S}_n/2S$ and $|\boldsymbol{\sigma}_n| = 1/2$. In this model, the value of the lattice spin S is finite and, consequently, carriers can now penetrate in the AFM region because the required energy is finite as well. In the limit $S \to \infty$ the hopping amplitudes transform to the form of that in the AH model (1).

Using the generalized model (7) we can describe the dynamics of the classical lattice spins by means of the discrete LL equation,[11] $\hbar \dot{\mathbf{S}}_n = -\mathbf{S}_n \times \mathbf{h}_{\text{eff}}$, where the symbol $\times$ stands for the vector product, and the effective field acting on the site magnetization is defined as $\mathbf{h}_{\text{eff}} = -\partial\mathcal{H}/\partial\mathbf{S}_n$. Thus, the equations of motion are

$$\dot{\mathbf{S}}_n = \sum_\delta \left(1 - \frac{\alpha C}{2}\frac{\psi_n\psi_\delta^* + \text{c.c.}}{|C\mathbf{S}_n + \mathbf{S}_\delta|}\right)[\mathbf{S}_n \times \mathbf{S}_\delta], \tag{8}$$

$$\mathrm{i}\dot{\psi}_n = -\sum_\delta \frac{\alpha}{2}\psi_\delta |C\mathbf{S}_n + \mathbf{S}_\delta|, \tag{9}$$

where $\delta = n\pm 1$, $C = 1 + 1/2S$, the overdot stands for the time derivative, and time is measured in units of $J/\hbar$.

Using Eqs. (8) and (9), we find stationary localized solutions for magnetic polarons that generalize the localized solutions obtained above for the AH model. The arrangement of the spin subsystem in each MF coincides with that found earlier for the AH model, see Figs. 1(a) and 1(b); the dependencies on α and S for MF $\left[\frac{2}{1}\right]$ change to become $\omega = \alpha[1 + 4S + 1/(1+4S)]/4$ and $A_l = 2\sqrt{S(1+2S)}/(1+4S)^{l+1}$, where l is the absolute distance from the right (left) edge of MF. The analytical expressions for the fields ψ_n of large MFs can be found but they are too involved to be shown here.

The only *mobile* solution of Eqs. (8) and (9) that we find is SCP with a structure similar to that obtained above for the AH model. It describes a three-site domain with canted spins embedded into an AFM chain, and the spin distribution is typically given by Fig. 1(c). It is convenient to parametrize this solution introducing the localization parameter κ expressed through the parameters α and S via the relation $\alpha = \kappa^3/C(\kappa^2-1)$. For given S the parameter κ changes in the interval $\kappa \in [1;4S+1]$. The wave function has the following structure: for the central site $A_c = \sqrt{\kappa/2\alpha C}$, and the amplitudes of left (or right) sites are $A_l = A\kappa^{-l}$ and $A_l = B\kappa^{-l}$, respectively, where l is the distance from the left (right) canted spin, and

$$A = \gamma, \quad B = \left(\frac{\kappa + \kappa^{-1}}{2\alpha C} - \gamma^2\right)^{1/2}. \tag{10}$$

The angles between the three canted spins can be found with the help of the relation: $|C\mathbf{S}_n + \mathbf{S}_{n+1}| = \alpha C A_n A_{n+1}$; the frequency ω vs the localization exponent is found as $\omega = -\alpha(\kappa + \kappa^{-1})/4$. As can be seen from Eq. (10), this solution involves an additional continuous parameter γ, which, for a given value of κ, changes in the interval $\gamma^2 \in [1/2\kappa\alpha C;\kappa/2\alpha C]$. If γ changes from its minimum to maximum value, the solution moves by one site *without any change of its energy*. This property can be explained through the vanishing of the Peierls-Nabarro pinning potential and the existence of mobile polarons. Within the generalized AH model, it is also possible to find the counterparts of the composite solutions presented above for the conventional discrete model, but all such solutions are *immobile*.

To study the dynamical *stability* of the magnetic polarons found, we linearize the system of dynamical equations with respect to small time-dependent perturbations $x_n(t)$, $y_n(t)$ and $w_n(t) = a_n(t) + \mathrm{i}b_n(t)$, near the stationary solutions $S_n^x(t) = S_n^x + x_n(t)$, $S_n^y(t) = S_n^y + y_n(t)$, $\psi_n(t) = [A_n + w_n(t)]\exp(\mathrm{i}\omega t)$; x_n, y_n, $|w_n| \ll 1$; assuming $\Sigma_n A_n a_n = 0$ due to the normalization. Then Eqs. (8) and (9) reduce to a set of linear equations, $\dot{\mathbf{X}} = \hat{\mathbf{M}}X$, where $\mathbf{X} = \{x_n, y_n, a_n, b_n\}$ is a $(4N'-1)$-dimensional vector (N' is the system size) and $\hat{\mathbf{M}}(\alpha,S)$ is a constant matrix. Substituting $\mathbf{X}(t) = \mathbf{X}e^{\lambda t}$ into this system, we obtain a linear eigenvalue problem that determines the dependence of the eigenvalues λ_n on the system parameters. The existence of a nonzero real part of any eigenvalue λ_n indicates the presence of dynamical instability, and it defines the instability growth rate. The results of our stability analysis for MFs of different sizes are summarized in Fig. 2 (for all numerics we use open boundary conditions). We find that MFs $\left[\frac{K}{1}\right]$ have a *stability window for* $K > 2$, see Figs. 2(b) and 2(c), and the stability domain grows with the value of S, see Fig. 2(d). The stability results for the SCP are presented in Fig. 3, where we find that this solution is *stable* for $\kappa > \kappa_c \approx 1.7$, i.e., for *strongly localized* states. In terms of the coupling param-

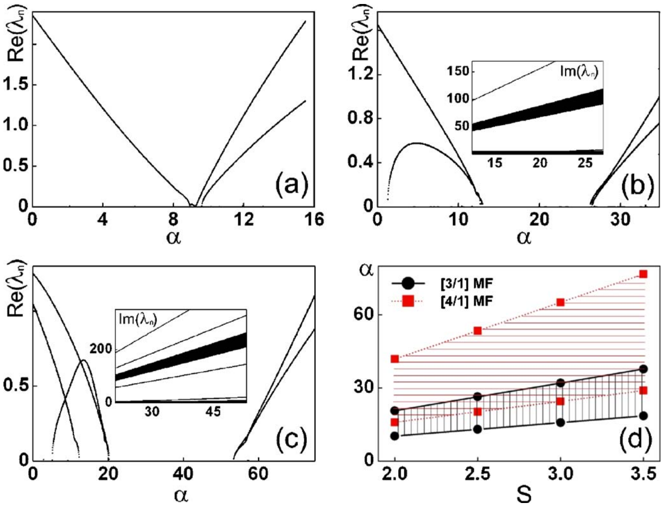

FIG. 2. (Color online) Dependence of the instability growth rate Re(λ) for (a) MF $\left[\frac{2}{1}\right]$, (b) MF $\left[\frac{3}{1}\right]$, (c) MF $\left[\frac{4}{1}\right]$ vs α for $S=5/2$ and $N'=100$. The insets show the stable mode spectrum [Im(λ)] inside the stability window. The panel (d) shows the dependence of the stability window vs S for MFs: the dotted lines (squares) indicate the stability thresholds for $\left[\frac{4}{1}\right]$, the stability area is dashed horizontally; the solid lines (circles) are the same for $\left[\frac{3}{1}\right]$, the stability area is dashed vertically.

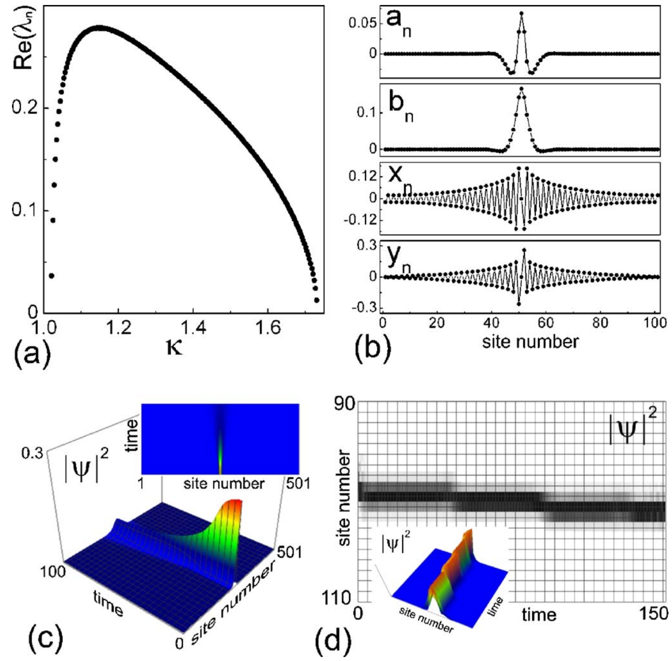

FIG. 3. (Color online) Stability of the SCP ($S=5/2$): (a) instability growth rate vs κ (for $N'=101$); (b) the profiles of the unstable mode ($\kappa=1.2$). Lower panels are the visualization of the dynamics of $|\psi|^2$: (c) evolution of the unstable solution induced by the spin-wave scattering ($\kappa=1.2$, $N'=501$); (d) example of a stable moving SCP ($\kappa=3$, $N'=201$).

eter α, the stable solutions exist for $\alpha_c<\alpha<\alpha_{\max}$, where $\alpha_c=3^{3/2}/2C$ and $\alpha_{\max}=(1+4S)^3/4(1+2S)^2$. Figure 3(c) shows an example of the instability-induced dynamics of unstable SCP under the action of a weak spin wave perturbation. In Fig. 3(d) we show motion of a stable SCP in the field of a wave, which corresponds to the space translation of a symmetric solution.

In conclusion, we have developed a general approach for describing strongly localized magnetic polarons in the framework of the discrete AH model. We have presented a general classification and found different types of exact analytical solutions for magnetic polarons of finite extent, which describe coupled states of electrons and a FM domain of collinear or canted spins embedded into an otherwise perfect AFM chain. We have generalized this model to cover the case of finite spins and performed the linear stability analysis for two classes of magnetic polarons, demonstrating that both types of localized states, with collinear or canted spins, can be dynamically stable. We have found that the AFM polaron with canted spins represents the only stable mobile solution, which can be responsible for the sharp conductivity change of the compounds with colossal magnetoresistance.

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