Dynamic symmetry breaking in mixed-valence systems

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The precise mechanism which allows the hybridization between nearly degenerate localized $4f$ and $(6s,5d)$-conduction-band states of a mixed-valent rare earth (RE) is investigated in detail. We propose that a dynamic symmetry breaking, generated by coupling the displacement of the RE ion from its equilibrium position to the mixing term of the Anderson Hamiltonian, induces the hybridization of the opposite-parity f and sd states. The model is solved under the assumption that the degeneracy of the $4f$ level, N_f, is large, which yields exact results in the $N_f \to \infty$ limit. Also, only one Einstein phonon mode is retained. Both a semiclassical and a full quantum-mechanical treatment are presented. Finally, we apply our model to the metal-insulator transition of SmS.

I. INTRODUCTION

In spite of the elapsed time and the significant efforts that have been devoted to the understanding of intermediate valence,[1,2] several important issues remain open. An area of special importance, with many ambiguities and unanswered questions, is the full description of the electron-phonon interaction in fluctuating-valence systems. The aim of this paper is to discuss and clarify one outstanding problem in this area: the precise mechanism which induces the hybridization between the nearly degenerate $(6s,5d)$-band states and the $4f$ electrons localized on the rare-earth (RE) ion.

While the earlier efforts to understand the intermediate valence phenomenon were developed within the framework of the Ramîrez-Falicov model,[3] most recent work is based on the Anderson Hamiltonian,[4] or generalizations of it.[5] The latter include a coupling term between localized and band states with the phonon field.[6] However, with few exceptions,[7] only breathing modes of the fluctuating valence RE are incorporated. These modes do not break the local inversion symmetry at the RE lattice site, which is present in many physical systems of interest.

In this paper we investigate the dynamical symmetry breaking at the RE site. It is induced by coupling the displacement of the ion from its equilibrium position to the mixing term of the Anderson Hamiltonian. The relevance of the latter, in the context of intermediate valence, was first recognized by Alascio, López, and Olmedo.[8] In our formulation, band and localized states hybridize through this dynamic Jahn-Teller mechanism, thus allowing the mixing of opposite parity states.

This paper is organized as follows. After this introduction the model is formulated analytically and solved in Sec. II. Next, in Sec. III its application to SmS is briefly discussed. In Sec. IV a summary is given and conclusions are drawn.

II. MODEL AND SOLUTION

In the analytic formulation of our model we limit ourselves to the simplest case which nevertheless incorporates most of the essential physical elements. That is, to a single impurity Anderson Hamiltonian with degenerate f states which hybridize with sd-band states. This mixing is induced by a local distortion that breaks the inversion symmetry at the impurity site. For simplicity we do retain just a single local phonon mode.

The Hamiltonian, in the partial-wave representation and with use of the notation of Ref. 6, reads

$$H = H_{\rm el} + H_B + H_{\text{el-}B} \ , \tag{1}$$

where

$$H_{\rm el} = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_{\nu=1}^{N_f} \varepsilon_f f_\nu^\dagger f_\nu + U \sum_{\nu,\nu'=1}^{N_f} \hat{n}_{f\nu} \hat{n}_{f\nu'} \ , \tag{2a}$$

$$H_B = \hbar\omega b^\dagger b \ , \tag{2b}$$

$$H_{\text{el-}B} = \left[\frac{\hbar}{2M\omega} \right]^{1/2} (b + b^\dagger) \sum_k (V_k c_k^\dagger f_\nu + V_k^* f_\nu^\dagger c_k) \ . \tag{2c}$$

Above, $c_k^\dagger$ (c_k) creates (destroys) a conduction electron in state k, where $k=(\mathbf{k},\nu)$ is a collective index denoting both the wave vector $\mathbf{k}$ and the z component of the total angular momentum ν; ε_k and ε_f are the energies of the conduction and f electrons, respectively. The operator $f_\nu^\dagger$ creates a $4f$-electron state, $\hat{n}_{f\nu} = f_\nu^\dagger f_\nu$; U is the Coulomb integral between different f states on the impurity; $b^\dagger$ creates the Einstein phonon mode of frequency ω; and V_k is the strength of the s-f mixing matrix element. Obviously, the c and f operators obey Fermi commutation relations, while the b operators obey Bose rules.

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A. Semiclassical approach

In order to obtain a qualitative understanding of our model, without the intricacies of a full quantum-mechanical treatment, we start providing a semiclassical approach. In the Born-Oppenheimer approximation Eqs. (2) reduce to

$$H=H_{\rm el}+H_{\text{el-}B}(x)+p^2/2M+M\omega^2x^2/2\ , \tag{3}$$

where

$$H_{\text{el-}B}=\sum_k x(V_k c_k^\dagger f_\nu+V_k^* f_\nu^\dagger c_k)\ , \tag{4}$$

and p and x are the canonical momentum and displacement of the Einstein oscillator. The kinetic energy term is negligible in the large-M limit. The adiabatic electronic eigenstates $|\psi_n(x)\rangle$ are obtained from

$$(H_{\rm el}+H_{\text{el-}B})|\psi_n(x)\rangle=E_n(x)|\psi_n(x)\rangle\ , \tag{5}$$

and following Born and Huang[9] the ground state of the system reads

$$\langle x|E_0\rangle=\sum_n \phi_n(x)|\psi_n(x)\rangle\cong\phi_0(x)|\psi_0(x)\rangle\ , \tag{6}$$

where $\phi_0(x)$ satisfies the Schrödinger equation

$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dx^2}+E_0(x)+kx^2/2\right]\phi_0(x)=\varepsilon_0\phi_0(x)\ . \tag{7}$$

To obtain $|\psi_0(x)\rangle$ we employ the variational *ansatz* of Varma and Yafet,[10] which in the large N_f limit, and for infinite U, yields

$$|\psi_0(x)\rangle=a(x)\left[|\phi_F\rangle+\sum_{k\le k_F}\frac{xV_k}{\Delta E-\varepsilon_f+\varepsilon_k}|\phi_k\rangle\right]\ , \tag{8}$$

where

$$a(x)=\left[1+\sum_{k\le k_F}\frac{x^2|V_k|^2}{(\Delta E-\varepsilon_f-\varepsilon_k)^2}\right]^{-1/2} \tag{9a}$$

is a normalization factor, $|\phi_F\rangle$ denotes the full Fermi sea and

$$|\phi_k\rangle=(N_f)^{-1/2}\sum_\nu f_\nu^\dagger c_k|\Phi_F\rangle\ . \tag{9b}$$

The shift $\Delta E\equiv E_0(x)-E_F$, with E_F being the ground-state energy of the full Fermi sea, is given by

$$\Delta E=\sum_{k\le k_F}\frac{x^2|V_k|^2}{\Delta E-\varepsilon_f-\varepsilon_k}\ . \tag{10}$$

The f-level occupation can now be evaluated as

$$n_f\equiv\left\langle\psi_0(x)\left|\sum_\nu f_\nu^\dagger f_\nu\right|\psi_0(x)\right\rangle=1-a^2(x)\ . \tag{11}$$

For a half-full conduction band, of width $2D$ $\gg|\Delta E(x)-\varepsilon_f|$ and constant density of states $\rho=1/(2D)=(2D)^{-1}$, one obtains

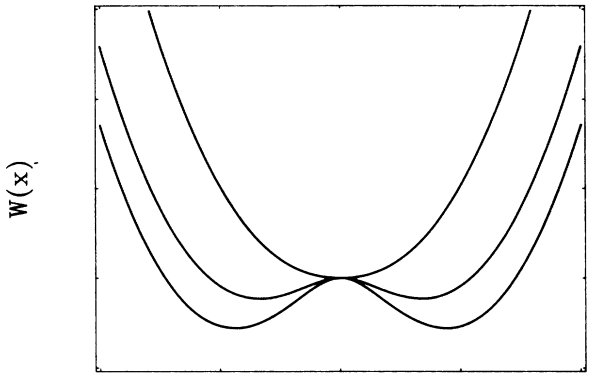

FIG. 1. Effective potential $W(x)$ in the semiclassical approximation, plotted for three values of the parameter $\rho\langle|V_k|^2\rangle$. The upper curve corresponds to the smallest value of $\rho\langle|V_k|^2\rangle$ and the lowest one to the largest. Arbitrary units are used. The change in character of the potential, from single to double well as $\rho\langle|V_k|^2\rangle$ increases, is clearly seen.

$$\Delta E=-\frac{\Delta(x)}{\pi}\ln\left[\frac{D}{|\Delta E-\varepsilon_f|}\right]\ , \tag{12}$$

$$n_f=\left[1-\frac{\pi(\Delta E-\varepsilon_f)}{\Delta(x)}\right]^{-1}\ , \tag{13}$$

where $\Delta(x)\equiv\pi\rho x^2\langle|V_k|^2\rangle$. Consequently, the RE ion oscillates in the effective potential

$$W(x)=E_0(x)+kx^2/2\ , \tag{14}$$

which is displayed in Fig. 1 for several values of the parameter $\rho\langle|V_k|^2\rangle$. It is observed that $W(x)$ has either one or three extrema; they can be evaluated by means of the Hellman-Feynman theorem. One readily obtains an implicit equation for these extrema which reads

$$x_0^2=\frac{2}{k}[n_f(x_0)-1]\Delta E(x_0)\ . \tag{15}$$

Thus, in close analogy with the results of Ref. 6, Eq. (15) has either one or three solutions. This implies the existence of a critical value of $\rho\langle|V_k|^2\rangle$ above which spontaneous symmetry breaking does occur. In the latter case the system gains more electronic energy than the elastic one required to distort the high symmetry equilibrium configuration. On the other hand, when there is no distortion, no hybridization is induced and the RE remains in an integral valence electronic configuration. Conversely, distortion implies mixing and nonintegral valence; as the first increases so does the latter.

B. Quantum-mechanical approach

Up to this point our treatment only allows for static solutions; quantum tunneling between the minima of the potential well of Fig. 1 was excluded. Below, a full quantum-mechanical calculation of the fluctuations of an

Einstein oscillator coupled to a correlated electron gas, is provided. Our treatment yields a dynamical symmetry breaking due to the Jahn-Teller effect. The analysis is closely related to the calculation scheme developed by Schönhammer and Gunnarson[6] to treat the breathing ion case.

Consider again the Hamiltonian H of Eq. (1) and define the ground state $|E_0\rangle$ and its energy E_0 by

$$H|E_0\rangle = E_0|E_0\rangle \ . \tag{16}$$

This state belongs to the product space $H_{\rm el} * H_B$ and thus is is natural to adopt the following *ansatz* as the variational trial function:

$$|E_0\rangle = \sum_e a_e |e\rangle * |B_e\rangle \ , \tag{17}$$

where $\{|e\rangle\}$ is a complete orthonormal set of states of $H_{\rm el}$, chosen as eigenstates of the operator $\hat{n}_f = \sum f_\nu^\dagger f_\nu$. On the other hand, $\{|B_e\rangle = \langle e|E_0\rangle\}$ is a complete set of boson states. Thus, Eq. (16) can be rewritten as

$$\sum_{e'} \langle e|H_{\rm el}+H_B+H_{\text{el-}B}|e'\rangle \, |B_{e'}\rangle = E_0|B_e\rangle \tag{18}$$

and in the $N_f \to \infty$ limit, in which the Hilbert space splits into two disjoint parts, a substantial simplification does occur. In fact, the states $|\phi_F\rangle$ and $\{|\phi_k\rangle\}$ of Eq. (8) do not mix with the rest of the electronic states and consequently, electron-hole pairs and double f occupancy do not enter our description in the large N_f limit. From (18) we thus obtain the following set of variational equations:

$$a_0(E_\phi + \hbar\omega b^\dagger b)|B_0\rangle + \left[\frac{\hbar}{2M\omega}\right]^{1/2} \sum_{k\le k_F} a_k v_k (b+b^\dagger)|B_k\rangle = a_0 E_0 |B_0\rangle \ , \tag{19a}$$

$$a_0 \left[\frac{\hbar}{2M\omega}\right]^{1/2} v_k^*(b+b^\dagger)|B_0\rangle + a_k(E_\phi - \varepsilon_k + \varepsilon_f + \hbar\omega b^\dagger b)|B_k\rangle = a_k E_0 |B_k\rangle \ , \tag{19b}$$

where E_ϕ is the full Fermi sea energy, ε_k the energy of a conduction electron with wave vector $\mathbf{k}$, and $v_k \equiv V_k/\sqrt{N_f}$. The combination of Eqs. (19) yields

$$\{\hbar\omega b^\dagger b + (b+b^\dagger)[\Gamma(\varepsilon_f + \hbar\omega b^\dagger b - \Delta E)](b+b^\dagger)\}|B_0\rangle = \Delta E|B_0\rangle \ , \tag{20}$$

where $\Delta E \equiv E_0 - E_\phi$ is the energy shift of the ground state relative to the noninteracting Fermi sea and

$$\Gamma(z) \equiv -\frac{\hbar}{2M\omega} \sum_{k\le k_F} \frac{|v_k|^2}{z-\varepsilon_k} \ . \tag{21}$$

The ground state $|E_0\rangle$ is thus

$$|E_0\rangle = a_0 \left[|\phi_F\rangle + \left[\frac{\hbar}{2M\omega}\right]^{1/2} \sum_{k\le k_F} \frac{v_k^*}{(\Delta E - \varepsilon_f - \hbar\omega b^\dagger b + \varepsilon_k)} (b+b^\dagger)|\phi_k\rangle \right] * |B_0\rangle \ . \tag{22}$$

To obtain ΔE, Eqs. (20) and (21) have to be solved self-consistently. Introducing the basis set $\{|n\rangle\}$, defined by $b^\dagger b|n\rangle = n|n\rangle$ and expanding $|B_0\rangle = \sum B_n|n\rangle$, a tridiagonal matrix equation for the coefficients β_n is derived

$$[n\hbar\omega + (n+1)\Gamma_{n+1} + n\Gamma_{n-1}]\beta_n + \sqrt{n(n-1)}\Gamma_{n-1}\beta_{n-2} + \sqrt{(n+1)(n+2)}\Gamma_{n+1}\beta_{n+2} = \Delta E \beta_n \ . \tag{23}$$

Assuming again a half-full conduction band of width $2D$ and a constant density of states $\rho = 1/(2D) = (2D)^{-1}$, one has

$$\Gamma_n = \frac{\hbar\langle |v_k|^2\rangle}{4M\omega D} \ln \left| \frac{\varepsilon_f - \Delta E + n\hbar\omega}{D + \varepsilon_f - \Delta E + n\hbar\omega} \right| \ . \tag{24}$$

The simplicity of Γ_n and the tridiagonal form of the matrix of Eq. (23), make the numerical solution both simple and efficient.

C. Wave function, probability density, and f-level occupation

Once the set $\{\beta_n\}$ is known, the vibrational wave functions can readily be evaluated using

$$\langle x|B_0\rangle = \sum_n \beta_n \langle x|n\rangle = \sum_n \beta_n \varphi_n(x) \ , \tag{25}$$

where

$$\varphi_n(x) = \left[\frac{M\omega}{\pi\hbar}\right]^{1/4} (2^n n!)^{-1/2} \times \exp(-M\omega x^2/2\hbar) H_n(\sqrt{M\omega/\hbar}\, x) \tag{26}$$

and H_n are the Hermite polynomials.[11] By the same token

$$\langle x \mid B_k \rangle = \frac{a_0}{a_k}\sqrt{\hbar/2M\omega}\,v_k^* \times \sum_n \beta_n \left[\frac{\sqrt{n}\,\varphi_{n-1}(x)}{\Delta E-\varepsilon_f-(n-1)\hbar\omega+\varepsilon_k} + \frac{\sqrt{n+1}\,\varphi_{n+1}(x)}{\Delta E-\varepsilon_f-(n+1)\hbar\omega+\varepsilon_k} \right] . \tag{27}$$

Notice that only coefficients β_n with the same parity in the n index are coupled through Eq. (23). Since the eigenfunctions $\varphi_n(x)$ of Eq. (26) are even (odd) when n is even (odd), the vibrational wave functions $\langle x \mid B_0 \rangle$ and $\langle x \mid B_k \rangle$ have definite parity; furthermore, Eqs. (25) and (27) imply that the parity of $\langle x \mid B_0 \rangle$ is opposite to that of $\langle x \mid B_k \rangle$. The full ground state $\mid E_0 \rangle$ instead, according to Eq. (22), is given by a linear superposition of even and odd functions. The relative weight of each of them is determined by the model parameters, mainly by v_k and ε_f.

While the ground-state expectation values of the displacement $\langle E_0 \mid x \mid E_0 \rangle = 0$, the probability of finding the RE ion at $x=0$ is finite. Actually, this probability as a function of x can be evaluated using

$$p(x) = \mid \langle x \mid E_0 \rangle \mid^2 = a_0^2 \mid \langle x \mid B_0 \rangle \mid^2 + \sum_{k \le k_F} a_k^2 \mid \langle x \mid B_k \rangle \mid^2 , \tag{28}$$

which can be expanded in the basis set $\{\varphi_n(x)\}$ of Eq. (26) as

$$\begin{aligned} p(x) = a_0^2 \Bigg[& \sum_n \beta_n^2 [n\Gamma'_{n-1}\varphi^2_{n-1}(x) + \varphi_n^2(x) + (n+1)\Gamma'_{n+1}\varphi^2_{n+1}(x)] \\ & + \beta_n\beta_{n+1}\sqrt{(n+1)(n+2)}\,\Gamma'_{n+1}\varphi^2_{n+1}(x) + \beta_n\beta_{n-2}\sqrt{n(n+2)}\,\Gamma'_{n-1}\varphi^2_{n-1}(x) \\ & + \sum_{\substack{n,m \\ (n\neq m)}} \frac{\beta_n\beta_m}{\hbar\omega} \left[\frac{\sqrt{nm}}{n-m}(\Gamma_{n-1}-\Gamma_{m-1})\varphi_{n-1}(x)\varphi_{m-1}(x) + \frac{\sqrt{(n+1)(m+1)}}{n-m}(\Gamma_{n+1}-\Gamma_{m+1})\varphi_{n+1}(x)\varphi_{m+1}(x) \right] \\ & + \sum_{\substack{n,m \\ (n\neq m+2)}} \frac{\beta_n\beta_m}{\hbar\omega}\frac{\sqrt{n(m+1)}}{n-m-2}(\Gamma_{n-1}-\Gamma_{m+1})\varphi_{n-1}(x)\varphi_{m+1}(x) \\ & + \sum_{\substack{n,m \\ (n\neq m-2)}} \frac{\beta_n\beta_m}{\hbar\omega}\frac{\sqrt{m(n+1)}}{n-m+2}(\Gamma_{n+1}-\Gamma_{m-1})\varphi_{n+1}(x)\varphi_{m-1}(x) \Bigg] . \end{aligned} \tag{29}$$

Above we have used the definition

$$\Gamma'_n \equiv \frac{\partial \Gamma_n(z)}{\partial z} , \tag{30}$$

which under the same assumptions that led to Eq. (24) yields

$$\Gamma'_n = \frac{\hbar\langle \mid v_k \mid^2 \rangle}{4M\omega D}\frac{D}{(\Delta E-\varepsilon_f-n\hbar\omega)(\Delta E-\varepsilon_f-n\hbar\omega-D)} . \tag{31}$$

Plots of the probability density $p(x)$ versus x are given in Fig. 2, for various values of v_k. As the latter increases so does the probability p for finding the ion displaced from its static equilibrium position. However, in sharp contrast with the semiclassical results, there is always a non-negligible probability for finding the atom in the neighborhood of $x=0$. In Fig. 3 we also plot $p(x)$ versus x, but now for various values of ε_f (the distance between the bare f level and the Fermi energy). It is apparent that v_k and ε_f have a competing effect on $p(x)$. The larger ε_f, the smaller the mixing between localized and band states and the smaller also the consequent symmetry breaking. In fact, the similarity between Fig. 2(a), plotted with parameters $V \equiv (\langle \mid v_k \mid^2 \rangle)^{1/2} = 1$ and $\varepsilon_f = 1$, and Fig. 3(c) with $V=5$ and $\varepsilon_f = 20$, is quite apparent. Moreover, the sets $V=1$, $\varepsilon_f = 1$ [Fig. 2(a)] and $V=5$, $\varepsilon_f = 100$ (not shown) yield identical results, as far as the probability density $p(x)$ is concerned.

On the other hand, the similarity between Figs. 2(b) and 3(a) is quite obvious. It is due to the fact that reducing the value of ε_f below a single quantum of energy of the Einstein phonon (which we did choose as our unit of energy) has no effect on the admixture of localized and band states.

The f-level occupation n_f is the most relevant physical quantity in the study of intermediate valence. A procedure quite similar to the one used to obtain Eq. (29) yields

$$\begin{aligned} n_f \equiv \langle \hat{n}_f \rangle = \left\langle E_0 \left| \sum_{\nu=1}^{N_f} \varepsilon_f f_\nu^\dagger f_\nu \right| E_0 \right\rangle = a_0^2 \sum_n \{ & \beta_n^2 [n\Gamma'_{n-1} + (n+1)\Gamma'_{n+1}] \\ & + \beta_n\beta_{n-2}\sqrt{n(n-1)}\,\Gamma'_{n-1} + \beta_n\beta_{n+2}\sqrt{(n+1)(n+2)}\,\Gamma'_{n+1} \} \end{aligned} \tag{32}$$

and also $a_0=(1+n_f)^{-1/2}$.

In Fig. 4 we display plots of the RE valence n_f versus ε_f for different values of v_k. As expected, for a given value of the hybridization v_k, the f-level occupancy decreases rapidly as the energy ε_f moves away from the Fermi level. On the other hand, for fixed ε_f the f level becomes more and more populated as the hybridization v_k grows. Finally, it is noticed that quantum fluctuations enhance the f-level occupation relative to the semiclassical results.

III. THE METAL-INSULATOR TRANSITION OF SmS

At ambient temperature and pressure SmS is a semiconductor[12] with a 0.2 eV energy gap. Its crystal structure is of the NaCl type. The Sm^{2+} ion has six $4f$ electrons forming a nonmagnetic $^7F_0$ ground state, which lies

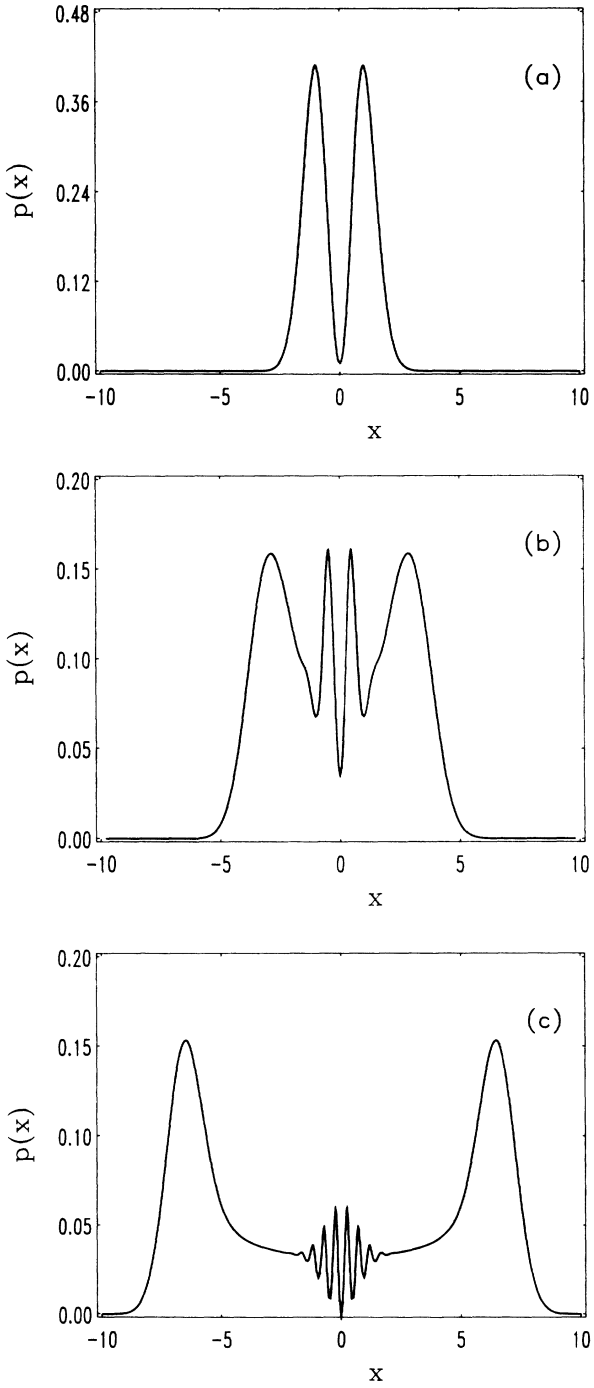

FIG. 2. Probability density $p(x)$ vs x for fixed $\varepsilon_f=1$ and $V\equiv[\langle\,|\,v_k\,|^2\rangle]^{1/2}=1$ (a), $V=5$ (b), and $V=7.5$ (c). Energies are measured in units of $\hbar\omega$ and lengths in units of $(\hbar/2M\omega)^{1/2}$.

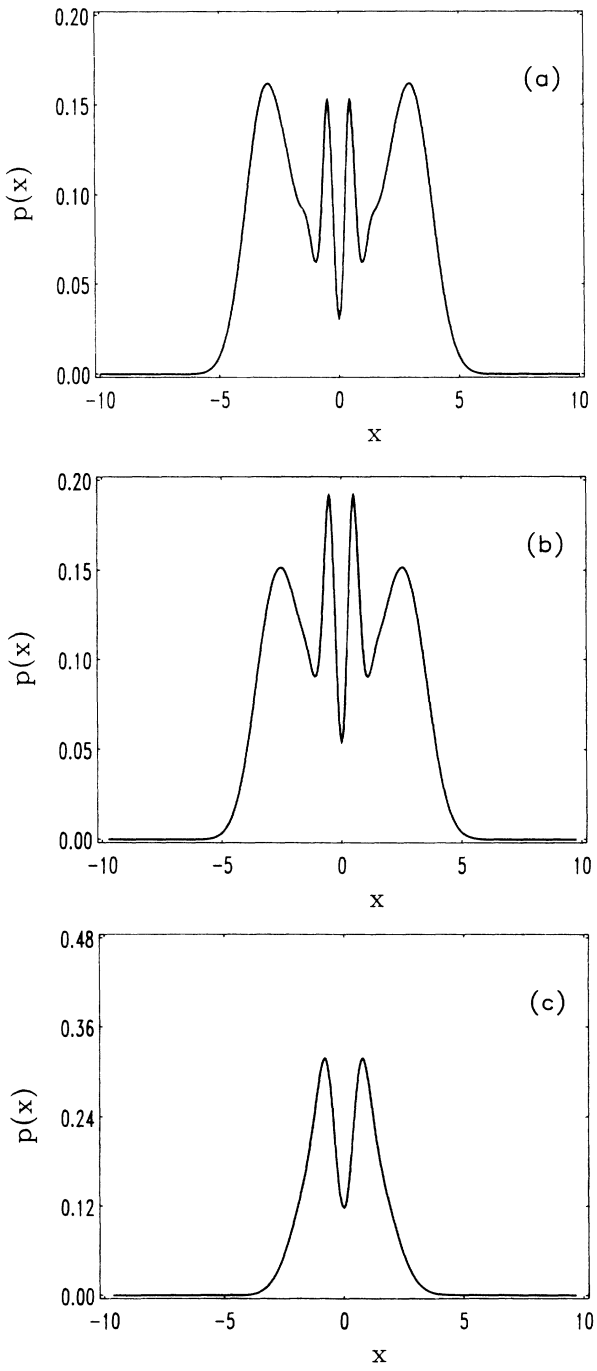

FIG. 3. Probability density $p(x)$ vs x for fixed $V=5$ and $\varepsilon_f=0.01$ (a), $\varepsilon_f=10$ (b), and $\varepsilon_f=20$ (c). The units are the same as in Fig. 2.

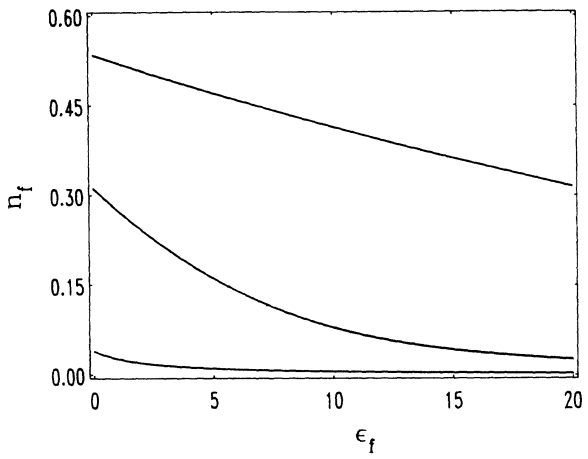

FIG. 4. Occupation n_f vs energy ε_f of the bare f level, relative to the top of the Fermi sea. The uppermost curve corresponds to $V=7.5$, the middle one to $V=5$ and the lowest one to $V=2.5$. Energies are measured in units of $\hbar\omega$.

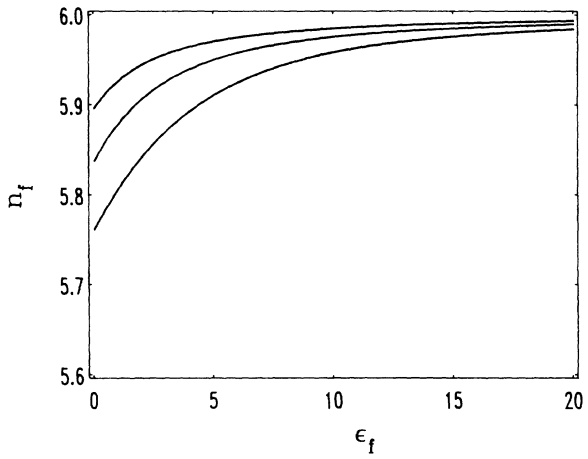

FIG. 5. Samarium f-level occupation vs ε_f. The uppermost curve corresponds to $V=3.5$, the middle one to $V=4$ and the lowest one to $V=4.5$. Energies are measured in units of $\hbar\omega$.

quite close to the bottom of the conduction band. Upon alloying (with Gd, Tm, or Y, for example), or under hydrostatic pressure, the $4f^6$ level is pushed upwards into the conduction band. Hybridization with the latter states tends to further ionize the Sm^{2+}, mixing the $^7F_0$ configuration with the magnetic $^6H_{5/2}$ and $^6H_{7/2}$ configurations of Sm^{3+}. In the context of our theory we propose that this behavior of SmS can be explained in terms of a dynamic shifting of the equilibrium position of the Sm ion, which breaks the high symmetry of its location. The RE is treated as an isolated impurity, due to the small spatial extent of the $4f$ states. In this model the Sm ions fluctuate, independently of each other, between the $4f^6(5d,6s)^0$ and the $4f^5(5d,6s)^1$ configurations.

However, if one just considers a mixing term of the type

$$H=\sum_{i,\delta}(V_{sd-f}c_{i+\delta}^{\dagger}f_i+\text{H.c.})\ , \tag{33}$$

where $c_j^{\dagger}$ creates a Wannier state at site $\mathbf{R}_j$ related to the sd band and δ is a vector connecting $\mathbf{R}_j$ with its nearest neighbors, then for high symmetry no mixing does occur. For example, for cubic symmetry the matrix elements are proportional to

$$[\sin(k_x a)+\sin(k_y a)+\sin(k_z a)]$$

and near the bottom of the band, where the f level is located, the wave vector $\mathbf{k}=0$ and no hybridization can occur.

This proposal constitutes an alternative mechanism to the one put forward by Bilz *et al.*[13] They attributed to a dipolar force, related to the deformation potential of the local charge, the origin of the symmetry breaking which gives rise to a relative displacement between d and f orbitals.

In our formulation we describe the system analytically by means of the following Hamiltonian:

$$\begin{aligned}H=&\sum_k\varepsilon_k c_k^{\dagger}c_k+\sum_\nu\varepsilon_{f^5}|\,^6H_{5/2},\nu\rangle\langle\,^6H_{5/2},\nu\,|\\&+\varepsilon_{f^6}|\,^7F_0\rangle\langle\,^7F_0\,|+\hbar\omega b^{\dagger}b\\&+\left[\frac{\hbar}{2M\omega}\right]^{1/2}(b+b^{\dagger})\\&\times\sum_k(V_k c_k^{\dagger}|\,^7F_0\rangle\langle\,^6H_{5/2},\nu\,|+\text{H.c.})\ ,\end{aligned} \tag{34}$$

where the notation was introduced after Eqs. (2). Applying the formalism of Sec. III one obtains, using reasonable estimates of the pertinent physical parameters, the results displayed in Fig. 5. It is observed that a consistent and plausible physical picture does emerge.

IV. SUMMARY AND CONCLUSION

A detailed study of the mixing mechanism, between f states on RE ions and $(5d,6s)$-conduction-band states, has been presented. The RE ions can be located on highly symmetric lattice points, in particular at sites invariant under inversion symmetry. We propose the Jahn-Teller effect as the mechanism which allows the hybridization to occur. This way, states of opposite parity can mix due to a dynamic symmetry breaking.

Both a semiclassical and a full quantum-mechanical solution have been presented. While its formulation and technical aspects do not differ greatly from previous work,[6] in which the elastic field is coupled to the number of f electrons on the RE, the interpretation we propose is significantly different. Finally, the application of the model to SmS is reasonably successful.

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