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Jahn-Teller resonance states in the V*b* metal hydrides: A model calculation*

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A simple tight-binding model representing hydrogen in the V*b* metals and including a special electron-phonon interaction is shown to give a molecular Jahn-Teller resonance state for physically reasonable values of the various energy parameters. This unusual resonance state is pinned to the shell of metal atoms adjacent to hydrogen by an effective Coulombic attraction that exists because of the nearly equal but opposite electron displacements on that shell, caused by the direct interaction of hydrogen on the one hand and by the Jahn-Teller interaction on the other. The mutual orthogonality of these two interactions implies that the Jahn-Teller state is an intrinsic feature of the host metal.

I. INTRODUCTION

The properties of the bcc hydrides of V, Nb, and Ta reveal a surprising complexity given the simplicity of the hydrogen atom. The most striking feature is the coexistence of an apparently cubic lattice distortion and a matrix of hydrogen vibrations that has tetragonal symmetry. If these two properties are determined by direct interaction of the hydrogen atomic s state with tight-binding states (d orbitals) of the nearest-neighbor metal atoms, then they should *both* reflect the tetragonal symmetry of the tetrahedral interstitial site occupied by hydrogen. Any attempt to explain the cubic lattice distortion in terms of long-range interactions (of unexplainably large magnitude) must show why these same interactions do not also impart cubic symmetry to the hydrogen vibration matrix.

In fact, the paradox described above seems to require a more radical explanation—that the interactions determining lattice distortion on the one hand and hydrogen vibrations on the other are *distinct* from one another. It was essentially this idea that led to the proposition[1] that interstitial hydrogen stabilizes a peculiar Jahn-Teller distorted molecular resonance state made up of t_{2g} d orbitals on the metal atoms closest to interstitial hydrogen. It was shown in I that most of the important puzzles concerning the behavior of hydrogen in the V*b* metals could be nicely rationalized in terms of both static and dynamic aspects of this Jahn-Teller resonance state. An important highlight was the development of a striking mechanism for hydrogen diffusion involving the interplay of Jahn-Teller reorientation with coherent tunneling of hydrogen on hexagonal rings. Supporting this idea was the argument that Jahn-Teller reorientation relaxation qualitatively explains the existence of a temperature-independent dispersion step in the phonon branch corresponding to the C' elastic constant.[2] Experimentally, this relaxation correlates with hydrogen diffusion, a result predicted by the notion that Jahn-Teller reorientation limits hydrogen diffusion.

While the basic ideas of I are firmly anchored in experimental fact, their connection to fundamental principles is no more than tenuous; indeed, the very question of plausibility remains open. The present article attempts to settle that question by showing the essential reasonableness of the idea of a quasimolecular Jahn-Teller resonance state. The basic approach here is not a frontal attack on the problem of hydrogen in the V*b* metals, but rather a highly simplified representation of that problem by a model amenable to exact solution.

II. MODEL OF INTERSTITIAL HYDROGEN IN THE V*b* METALS

The model we have chosen to represent interstitial hydrogen in the V*b* metals is illustrated in Fig. 1. Hydrogen is located symmetrically between four atoms on the (100) surface of a simple cubic (sc) semi-infinite lattice. The lattice is represented by an s-band tight-binding Hamiltonian and hydrogen by a strongly localized s state. The tight-binding orbitals for the impurity cluster are schematically indicated in Fig. 1. A direct interaction V_H couples the hydrogen state to the four nearest-neighbor metal states, and for simplicity we take $V_H \gg T$, where T is a positive number with $-T$ the hopping energy connecting nearest-neighbor metal atoms. Finally, the model includes a special electron-phonon interaction to be described in Sec. III.

Our primary reasons for choosing the above model are twofold: (i) It is perhaps the simplest model that includes enough features to mimic the indirect Jahn-Teller response described in I; (ii) the problem of the direct interaction has already been solved for this model by Green's-function techniques[3] which are easily extended to the pres-

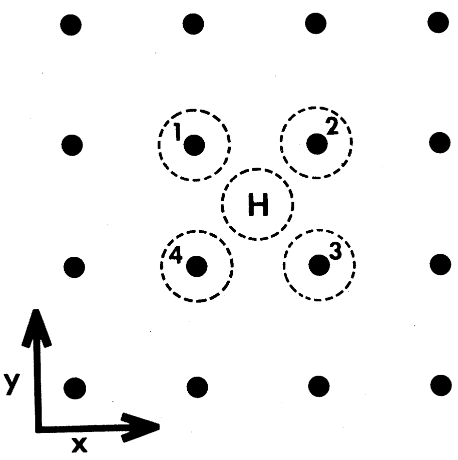

FIG. 1. Hydrogen in centered configuration on (100) surface of a simple cubic lattice. Dashed circles show tight-binding orbitals on impurity cluster atoms.

ent case. One may well object to the use of an sc surface to represent a bcc bulk effect; but we note that (in a perfect vacuum) a metal atom on a (100) sc surface differs only slightly from one in the bulk, having five nearest neighbors instead of six. Besides, while it is true that a bcc bulk metal atom couples strongly to eight nearest neighbors and six next-nearest-neighbors, an individual atomic *d* orbital will participate strongly in perhaps half of these couplings. A discussion of localized molecular effects must necessarily focus on interatomic interactions of individual *d* orbitals rather than total averaged interactions between neighbor atoms. For these reasons, use of an *s*-band tight-binding Hamiltonian corresponding to a bulk bcc metal would *not* improve the present model. In any case, we emphasize that our model represents the real problem more by analogy than in any literal sense.

Before proceeding to the Green's-function resolution of the direct interaction, it will be useful to treat the impurity cluster (hydrogen plus four nearest neighbors) as a separate molecule interacting with the semi-infinite lattice (*sans* cluster) and to develop symmetrized molecular orbitals (MO's) that transform according to the representations of the appropriate C_{4v} point group. This is more than a conceptual artifice—it is the extra orbital limit and provides an alternative point of departure for the discussion of resonances localized on the cluster. Such an approach has been fully justified and exploited to great advantage for atomic impurity states, primarily by Anderson.[4] In terms of the cluster metal atom orbitals labeled in Fig. 1, we obtain the following symmetrized orbitals:

$$\begin{aligned} |A_1\rangle &= \tfrac{1}{2}(|1\rangle + |2\rangle + |3\rangle + |4\rangle)\,, \\ |B_2\rangle &= \tfrac{1}{2}(|1\rangle - |2\rangle + |3\rangle - |4\rangle)\,, \\ |E_\pm\rangle &= \tfrac{1}{2}(|1\rangle \mp |2\rangle - |3\rangle \pm |4\rangle)\,, \end{aligned} \tag{1a}$$

which are labeled by the corresponding representation using chemical notation. The states belonging to the doubly degenerate E representation are further labeled according to whether they are symmetric (+) or antisymmetric (−) under σ_v^y (plane of reflection normal to y axis). Taking the one-center metal atom matrix elements (the atomic-orbital self-energies) as defining zero energy, we obtain one-electron energies (the MO self-energies) corresponding to the MO's of Eq. (1a):

$$\begin{aligned} \epsilon(A_1) &= -2T\,, \\ \epsilon(E_\pm) &= 0\,, \\ \epsilon(B_2) &= 2T\,. \end{aligned} \tag{1b}$$

Taking $V_{\text{H}} = 0$ and turning on the interaction between cluster and depleted lattice gives back the perfect (semi-infinite) lattice; so we may also characterize the cluster orbitals in the perfect lattice representation by projecting the total density of states (DOS) onto the corresponding orbitals. To do this, we introduce the lattice Green's function

$$G(z) = \sum_k \frac{|k\rangle\langle k|}{z - E(k)}\,, \tag{2}$$

where $|k\rangle$ and $E(k)$ are, respectively, the eigenfunctions and eigenvalues of the appropriate tight-binding Hamiltonian, and $z \equiv \epsilon - i\delta$ is restricted to the lower half-plane near the real (energy) axis.[5] In the tight-binding representation, the matrix elements are $G_{lm}(z) = \langle l|G(z)|m\rangle$, so that the projection of $G(z)$ onto the cluster orbitals of Eq. (1) gives

$$\begin{aligned} G_A^0(z) &\equiv \langle A_1|G(z)|A_1\rangle = G_{11} + 2G_{12} + G_{13}\,, \\ G_B^0(z) &\equiv \langle B_2|G(z)|B_2\rangle = G_{11} - 2G_{12} + G_{13}\,, \\ G_\pm^0(z)) &\equiv \langle E_\pm|G(z)|E_\pm\rangle = G_{11} - G_{13}\,. \end{aligned} \tag{3}$$

In deriving these expressions, we have made full use of the symmetry of the $G_{lm}(z)$ as described by Einstein and Schrieffer.[3] The particular $G_{lm}(z)$ on the right-hand side of Eq. (3) have been evaluated and are available in tabular form.[6] Using these quantities to determine the cluster Green's functions of Eq. (3) allows an exact solution for any perturbing potential whose range is limited to the cluster of Fig. 1. Of particular interest in such problems will be the local DOS given by

$$\rho_\Gamma(\epsilon) = \frac{1}{\pi}\text{Im}G_\Gamma(\epsilon)\,, \tag{4}$$

which is the projection of $\rho(\epsilon)$ onto the cluster orbital belonging to the Γ representation. Figure 2 shows the unperturbed ρ_Γ and reveals the following significant features: (i) the MO self-energies in Eq. (1b) retain their significance when the "interaction" between the "extra orbitals" and the extended states is switched on, and (ii) the ρ_Γ are considerably sharper than ρ_{tot} (all normalized to one electron). The location (Fig. 2) of the various cluster DOS peaks within the band justifies the intuitive arguments advanced in I concerning the relative location of the various MO's associated with the impurity polyhedra of hydrogen on tetrahedral interstitial sites in the V*b* hydrides. In chemical parlance, the bonding state ($|A_1\rangle$) lies in the lower half, the nonbonding state ($|E_\pm\rangle$) in the center, and the antibonding state ($|B_2\rangle$) in the upper half of the band. The relative sharpness of the molecular states reflects the fact that of the five nearest neighbors coupled to a given atom within a cluster state, only three of these are external to that state, resulting in a ratio[7] of approximately $\sqrt{3}:\sqrt{5}$ for molecular state bandwidth to atomic state bandwidth (the latter being identical to the bandwidth of ρ_{tot}).

We turn now to the direct interaction of hydrogen with the cluster metal atoms. This problem involves only the fully symmetric (A_1) subspace and has already been studied in connection with chemisorption.[8] Because our primary interest is with indirect effects, we take for the direct interaction a very simple limiting case which fortunately, is a good representation of the actual effect in many transition metal hydrides, including the V*b* hydrides.[9] We have chosen the molecular limit, which results when V_{H} is the dominant energy parameter of the problem. In this limit the interaction gives two localized states straddling the band.[8] For the C_{4v} cluster, these states are

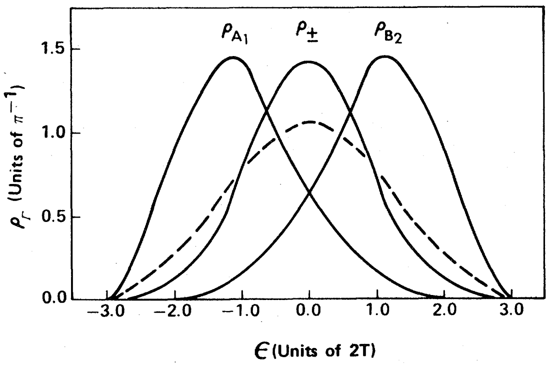

FIG. 2. Cluster-projected DOS [Eq. (4)] for $V_{\text{H}}=0$. The dashed curve gives the total DOS. All DOS curves are normalized to one electron. The unit of energy throughout is $2T$.

$$\begin{aligned}\psi_B &= (|\text{H}\rangle + |A_1\rangle)/\sqrt{2}\,,\\ \psi_A &= (|\text{H}\rangle - |A_1\rangle)/\sqrt{2}\end{aligned} \tag{5}$$

($|\text{H}\rangle$ represents the hydrogen *s* orbital), where ψ_B is a fully occupied bonding state and ψ_A is antibonding and empty. But the problem cannot be considered resolved at this point because the solution given by Eq. (5) is not self-consistent. This is due to a significant charge depletion localized on the metal atom cluster. The Fermi level (ϵ_F, see Fig. 4) for our model was chosen to give a fractional band occupancy (0.4) matching that of the *d* band in the V*b* metals. With this value of ϵ_F, Eq. (5) gives local neutrality for the impurity hydrogen atom, but for the metal cluster the result is a local depletion of electrons given by $\Delta n_A = [n_A(V_{\text{H}}) - n_A(0)]$, where

$$n_A(V_{\text{H}}) = 2\int_{-\infty}^{\epsilon_F} \rho_{A_1}(\epsilon;\, V_{\text{H}})\,d\epsilon\,. \tag{6}$$

We calculate $n_A(0) = 1.34$ and $n_A(V_{\text{H}} \to \infty) = 1.00$ giving $\Delta n_A = -0.34$, which is a moderately large Coulomb hole. A trivial accomodation of this perturbation consists of small phase shifts of the various non-A_1 cluster-projected DOS (Fig. 2); for sufficiently small phase shifts, this essentially free-electron response can be described in first Born approximation.[10]

III. JAHN-TELLER ELECTRON-PHONON INTERACTION

In this section we consider an alternate response to the Coulomb perturbation—a peculiarly *molecular* response. To describe the effect, we temporarily adopt Anderson's extra orbital point of view,[4] treating the impurity cluster as a separate molecule. If this molecule is open shell with the degenerate state ($|E_\pm\rangle$) of Eq. (1a) partially occupied, the celebrated Jahn-Teller theorem[11] tells us that some distorted configuration which splits the electronic degeneracy will be energetically favored. For molecules with a fourfold symmetry axis, Hougen[12] has described the Jahn-Teller effect in detail, including dynamic and static aspects (both being pertinent here). The particular symmetry discussed therein was D_{4h}, but the results apply also to C_{4v} *and to* D_{2d}. Because the latter is the relevant point group for hydrogen in the V*b* metals, isomorphism is an important feature of the present model. Figure 3 shows the Jahn-Teller active normal modes for C_{4v} symmetry. Here we are implicitly applying the extra orbital point of view also to the vibrational part of the total Hamiltonian for our model. There should be no objection to this given the widespread use of the tight-binding formalism for the

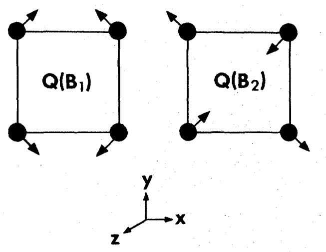

FIG. 3. Jahn-Teller active normal modes for the C_{4v} metal-atom cluster.

phonon field and the experimental reality of phonon resonances. In fact, we will argue that a Jahn-Teller effect sufficiently strong to produce a sharp electronic resonance necessarily produces a sharp phonon resonance corresponding to the appropriate normal mode which, after all, is just the other side of the same interaction.

Returning now to the electronic problem, it is clear from Fig. 3 that through first order only the B_1 mode can modify nearest-neighbor distances and thus affect $\epsilon(E_\pm)$ (by changing the overlap integral T). This conclusion also applies, at least approximately, to hydrogen in the V*b* metals as described in I. But this fact leads to an important simplification: *The two electronic states* $|E_\pm\rangle$ *and also their associated vibrational states can be considered independently.* We have here an accidental Born-Oppenheimer case where the complete vibronic state is to a good approximation a simple product state (i.e., $|\phi_{ev}\rangle \cong |\phi_e \phi_v\rangle$), in spite of the vibronic Jahn-Teller interaction.[12] The net result is two harmonic oscillator potentials, each displaced laterally in coordinate space and downward in energy relative to the unperturbed values, but with unchanged vibrational quanta. The oscillator associated with $|E_+\rangle$ ($|E_-\rangle$) corresponds to a displacement of the potential minimum to a negative (positive) value of $Q(B_1)$. Thus, we have two kinds of Jahn-Teller centers, called x and y types, labeled according to the direction of enlongation for the stabilized center. At sufficiently high temperature, a given center will undergo thermally activated transitions between the two types, giving a very simple dynamic Jahn-Teller reorientation process.

The total electronic stabilization relative to the undistorted configuration is given by

$$\Delta E = -(n_+ - n_-)^2 E_{\rm JT} \ , \tag{7}$$

where n_+ and n_- are the occupation numbers for $|E_+\rangle$ and $|E_-\rangle$, respectively, and

$$E_{\rm JT} = V^2/2K \, , \tag{8}$$

where

$$V = \frac{\partial \epsilon(E_\pm)}{\partial Q(B_1)} \, , \tag{9}$$

and K is the force constant associated with $Q(B_1)$. Equation (7) is derived by minimizing $E(Q) = \frac{1}{2}KQ^2 - (n_+ - n_-)VQ$ with respect to Q. The quantity V can be written in terms of the overlap integral T. First, $Q(B_1)$ is expressed in terms of displacements between nearest neighbors:

$$Q(B_1) = -\Delta r_{12} + \Delta r_{23} - \Delta r_{34} + \Delta r_{14} \, , \tag{10}$$

where $\Delta r_{12} = r_{12} - r_{12}^0$, the latter quantity representing the undistorted separation. Now we write

$$\frac{\partial \epsilon}{\partial Q} = \frac{\partial \epsilon}{\partial r_{12}} \left(\frac{dQ}{dr_{12}} \right)^{-1} + \frac{\partial \epsilon}{\partial r_{23}} \left(\frac{dQ}{dr_{23}} \right)^{-1} + \cdots \, . \tag{11}$$

But

$$\frac{\partial \epsilon}{\partial r_{12}} = -\frac{1}{4} \frac{\partial}{\partial r_{12}} (\langle 1 | \mathcal{H}_{\rm el} | 2 \rangle + {\rm H.c.}) = \frac{1}{2} \frac{dT}{dr}$$

($\mathcal{H}_{\rm el}$ is the electronic Hamiltonian) and similarly for the other derivatives giving

$$\frac{\partial \epsilon}{\partial r_{34}} = \frac{1}{2} \frac{dT}{dr} \, , \quad \frac{\partial \epsilon}{\partial r_{23}} = \frac{\partial \epsilon}{\partial r_{14}} = -\frac{1}{2} \frac{dT}{dr} \, .$$

For the derivative of the overlap integral, we take the result of Barišić *et al.*[13]:

$$\frac{dT}{dr} = -q_0 T \, ,$$

where q_0 is the coefficient describing the exponential decrease of the d function ($q_0 \sim 1$ Å^{-1}). The dQ/dr are taken directly from Eq. (10), and putting the various quantities back into Eq. (11) gives by use of Eq. (9) the result $V = 2q_0 T$. But this quantity is essentially related to $\langle I^2 \rangle$, the average of the square of the electron-phonon matrix element, which appears in McMillan's strong-coupling definition[14] of the phonon-induced effective coupling constant that determines the superconducting transition temperature. A recent study[15] using a nonorthogonal tight-binding interpolative scheme with a full complement of atomic valence orbitals to calculate $\langle I^2 \rangle$ for Nb, demonstrated that t_{2g} d orbitals give by far the strongest contribution. This is highly significant to the present study, because the Jahn-Teller state proposed for the V*b* metal hydrides is based entirely on t_{2g} orbitals. Thus we take $V \simeq (\langle I^2 \rangle)^{1/2}$ and for Nb this gives $V \simeq 3$ eV/Å. Treating V as the Kanzaki force that distorts the lattice and allowing it to act only along one of the four $\langle 111 \rangle$ bonds of the V*b* hydride D_{2d} impurity cluster (consistent with the hypothesis of I) gives a force dipole tensor that agrees closely with experiment.[16] This is an indication of the internal consistency of our model.

To determine the force constant K, we note that $K = \mu\omega^2$, where μ is the effective mass appropriate to the normal mode $Q(B_1)$ and $\hbar\omega$ is the vibrational quanta for that mode. Now, if the separate molecule limit is physically reasonable, then $\mu = M$ (atomic mass of a cluster atom).[17] Moreover, this limit implies a strong separation of the harmonic oscillator corresponding to $Q(B_1)$ from the phonon continuum of the macroscopic crystal. Thus if a Jahn-Teller distortion driven by $Q(B_1)$ is sufficiently strong, *there should be a sequence of essentially dispersionless phonon resonances corresponding to transitions between the $Q(B_1)$ harmonic oscillator levels*. In fact, such a sequence has been observed in a recent neutron scattering study of $NbH_{0.82}$ and $NbD_{0.85}$ with isotope and temperature-independent excitations at 10.8 and 18.4 meV.[18] Furthermore, the linewidth of these excitations correlate with hydrogen diffusion. Taking the smaller excitation as the $Q(B_1)$ vibrational quanta gives a value $K = 2.5$ eV/Å^2 for NbH_x which, combined according to Eq. (8) with the value for V derived earlier, gives $E_{JT} \simeq 1.8$ eV. To express E_{JT} in units of $2T$ we use the relation appropriate for the present model, $12T = B$ (bandwidth) which for the Vb hydrides is about 10 eV. Thus for Nb, $E_{JT} \simeq 1.1$ in units of $2T$.

The full Jahn-Teller problem, including interaction of the "molecule" with the lattice, can now be solved. To do this, we first need effective one-electron energies for the various Jahn-Teller states. These are obtained by writing $\Delta E = n_+\epsilon_+ + n_-\epsilon_-$ and noting that $\epsilon_- = -\epsilon_+$ giving $\epsilon_\pm = \pm\Delta E/(n_+ - n_-)$ or, using Eq. (7),

$$\epsilon_\pm = \pm(n_+ - n_-)E_{JT}\,. \tag{12}$$

At this juncture, we abandon the extra orbital approach and treat the $\epsilon_\pm$ as localized perturbations affecting the manifold of extended states only through the projection of the latter onto the particular combination of tight-binding states represented by $|E_\pm\rangle$ in Eq. (1a). Considered as such, this perturbation affects only the self-energy of the projected states and is thus diagonal in that subspace. From this perspective the exact solution is straightforward using Green's function techniques[19]; in terms of the unperturbed quantities $G_\pm^0$ of Eq. (3) we have

$$G_\pm(z) = [1/G_\pm^0(z) - \epsilon_\pm]^{-1}\,. \tag{13}$$

In particular, the projected DOS defined by Eq. (4) is just

$$\rho_\pm(\epsilon) = \rho_\pm^0[(1 - \epsilon_\pm \operatorname{Re}G_\pm^0)^2 + (\pi\epsilon_\pm\rho_\pm^0)^2]^{-1} \tag{14}$$

and the corresponding occupation variables (now continuous) are given by

$$n_\pm = 2\int_{-\infty}^{\epsilon_F} \rho_\pm(\epsilon)d\epsilon\,. \tag{15}$$

Thus we have the case first described by Anderson[20] where the $n_\pm$ depend on $\epsilon_\pm$ through Eqs. (15) and (14) while the $\epsilon_\pm$ depend on $n_\pm$ through Eq. (12). The Hartree-Fock solution to this problem is relatively straightforward and shows that a stabilizing distortion exists so long as $\rho_\pm^0(\epsilon_F)E_{JT} \geq \frac{1}{4}$. Figure 4 shows $\rho_\pm$ for several values of E_{JT}, and includes $\rho_\pm^0$ which obtains when $E_{JT} < 0.63$. (As discussed earlier, the location of ρ_+ and ρ_- relative to one another depend on whether the Jahn-Teller center is x or y type.) The effect of the Jahn-Teller stabilization on local charge density is given by $\Delta n_E \equiv \langle n_+ - n_+^0 + n_- - n_-^0\rangle$, which can be calculated using Eqs. (15) and (14) with the result $\Delta n_E = 0.42$ (0.48) for $E_{JT} = 0.92$ (1.15). Thus the Jahn-Teller perturbation acting in the E subspace approximately neutralizes the Coulomb hole of -0.34 generated in the A_1 subspace by the hydrogen direct interaction. *This effective Coulomb attraction pins the Jahn-Teller state to the hydrogen site*. Whether or not stabilization in the Vb metals of this particular state requires the presence of hydrogen is an intriguing question with potentially major ramifications. Experimentally, these states appear to be well camouflaged—even when decorated with hydrogen atoms[1]—so that their existence in the pure metal is at least conceivable.

IV. SUMMARY AND CONCLUSION

The model calculations described above convincingly demonstrate the plausibility of the basic idea advanced in I—that the unusual behavior of hydrogen in the Vb metals is primarily determined by a molecular Jahn-Teller electronic resonance state. The existence of such states in the context of the present model requires only that

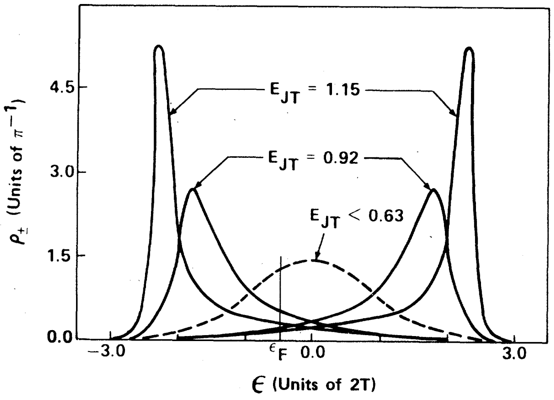

FIG. 4. Jahn-Teller resonance states for several values of E_{JT}. The dashed curve is identical to $\rho_\pm$ of Fig. 2.

$E_{JT} \geqslant 1.26T$ (for 40% band occupancy) and does not depend on band idiosyncrasies (such as edge effect, sharp minimum in center of band, etc.).[5] We have estimated a value of $E_{JT} \simeq 2.2T$ for Nb based on (i) an electron-phonon coupling parameter as measured by the superconductivity critical temperature and also by theoretical calculation[15] and (ii) a force constant for the relevant localized phonon resonance mode ("normal" mode) derived from what we claim to be the observed "harmonic oscillator" frequency.[18] We have also argued that, to the extent that the direct interaction V_H falls in the strong-coupling regime, the Jahn-Teller resonance state is pinned to the hydrogen site by an effective Coulomb attraction. Stated differently, the interactions represented by V_H and E_{JT} displace nearly the same amount of electron density, but in opposite directions relative to ϵ_F.

An important shortcoming of the model is the neglect of the Coulomb self-repulsion energy between two electrons in the same orbital.[20] The results are essentially the same so long as $4E_{JT} - U \gtrsim 1/\rho^0$, making it somewhat more difficult to obtain a spontaneous Jahn-Teller resonance distortion. A rough estimate of U for a four-atom molecule is given by $\frac{1}{4}U_{\text{atomic}} \simeq 3$ eV, a value which reduces E_{JT} to the borderline, but which is probably an overestimate due to neglect of molecular correlation effects.

Finally, we wish to stress the fact that the Jahn-Teller resonance states described in this article are not intrinsic to the hydrides of the V*b* metals—*but to the parent metal.* Interstitial hydrogen apparently acts indirectly to stabilize these unusual resonance states to below ϵ_F—the resulting hydrogen "decoration" provides an experimental handle for an otherwise elusive entity. The consequences for pure transition metals of molecular Jahn-Teller resonance states, if indeed they exist, remain to be explored.

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[1] G. C. Abell, Phys. Rev. B 20, 4773 (1979) (hereafter referred to as I).

[2] A. Magerl, W. D. Teuchert, and R. Scherm, J. Phys. C 11, 2175 (1978).

[3] T. L. Einstein and J. R. Schrieffer, Phys. Rev. B 7, 3629 (1973).

[4] P. W. Anderson and W. L. McMillan, in *Theory of Magnetism in Transition Metals, Proceedings of the International School of Physics "Enrico Fermi" Course XXXVII*, Varenna, edited by W. Marshall (Academic, New York, 1967), p. 50.

[5] E. N. Economou, *Green's Functions in Quantum Physics* (Springer, Berlin, 1979).

[6] T. L. Einstein, Univ. of Maryland, College Park (private communication).

[7] R. Haydock and M. J. Kelly, Surf. Sci. 38, 139 (1973).

[8] D. M. Newns, Phys. Rev. 178, 1123 (1969).

[9] A. C. Switendick, in *Hydrogen in Metals* I, Topics in Applied Physics, edited by G. Alefeld and J. Völkl (Springer, Berlin, 1978), Vol. 28; J. P. Muscat and D. M. Newns, Phys. Rev. Lett. 43, 2025 (1979).

[10] F. D. M. Haldane, Phys. Rev. B 15, 2477 (1977).

[11] H. A. Jahn and E. Teller, Phys. Rev. 49, 874 (1936).

[12] J. T. Hougen, J. Mol. Spectrosc. 13, 149 (1964).

[13] S. Barišić, J. Labbé, and J. Friedel, Phys. Rev. Lett. 25, 919 (1970).

[14] W. L. McMillan, Phys. Rev. 167, 331 (1968).

[15] C. M. Varma, E. I. Blount, P. Vashishta, and W. Weber, Phys. Rev. B 19, 6130 (1979).

[16] G. Bauer, E. Seitz, H. Horner, and W. Schmatz, Solid State Commun. 17, 161 (1975).

[17] F. S. Ham, in *Electron Paramagnetic Resonance*, edited by S. Geschwind (Plenum, New York, 1972), Chap. 1.

[18] S. M. Shapiro, Y. Noda, T. O. Brun, J. Miller, H. Birnbaum, and T. Kajitani, Phys. Rev. Lett. 41, 1051 (1978).

[19] H. Callen and V. G. Baryaktar, Phys. Rev. B 6, 1010 (1972).

[20] P. W. Anderson, Phys. Rev. 124, 41 (1961).