Theory of magnetic polarons in antiferromagnetic semiconductors

L. Liu
Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60201
(Received 30 March 1987; revised manuscript received 26 May 1987)

In magnetic semiconductors, a charge carrier is dressed with a cloud of lattice spins due to the strong exchange coupling between the carrier and the local moments, and forms a so-called magnetic polaron. We formulate a theory of the ground state of magnetic polarons in antiferromagnets for electrons from the conduction band as well as those bound to impurity centers. We discuss how the orbital motion of the electron is influenced by its magnetic interaction with the lattice. We also determine the structure of the lattice-spin cloud surrounding the electron.

I. INTRODUCTION

In magnetic semiconductors, the exchange coupling between the charge carrier and the lattice spin is often strong in comparison with either the carrier kinetic energy or the lattice-lattice exchange interaction responsible for the long-range magnetic order. Through this coupling the conduction electron is capable of polarizing the lattice spins. In analogy with an ordinary polaron, one refers to an electron dressed with lattice spins as a magnetic polaron. If the electron is not in the conduction band but bound to an impurity center, it is specifically called a bound magnetic polaron.

Because of this strong carrier-lattice exchange, the magnetic, optical, and transport properties of a magnetic semiconductor may be altered. Let us cite a few random examples. In Eu-rich EuO, which is a ferromagnet, the electric conductivity suddenly increases by 10^{13}-fold as the temperature is lowered through the magnetic transition temperature.[1] It is believed[2] that this insulator-metal transition is caused by a sudden decrease in the ionization energy of the bound magnetic polaron centered at the oxygen vacancy site. In antiferromagnetic substances, the magnetic polarons manifest themselves in the form of ferromagnetic spin clusters which were experimentally detected in EuSe and EuTe.[3,4] In dilute magnetic semiconductor alloys,[5] such as $Cd_{1-x}Mn_xSe$ or $Cd_{1-x}Mn_xTe$, new features in the magnetooptical spectra have been observed which are attributable to bound magnetic polarons in the sample.

To trace the development of the polaron theory, one probably should begin with Zener[6] who first recognized the importance of the carrier-lattice exchange interaction. It is through this coupling that conduction electrons in metals are capable of collectively mediating an indirect exchange between local moments embedded in the lattice, thus forming a subject of intensive research by itself. At the same time, the question of how properties of a charge carrier from the conduction band are affected by its strong magnetic coupling with the lattice was considered.[7-13] As to the concept of the bound magnetic polaron,[2] it was first proposed as the underlying mechanism responsible for the insulator-metal transition in EuO cited above, and was further pursued by a number of authors.[14-18] Instead of giving an extensive reference list on the past theory of polarons, we refer the reader to a recent review article,[19] and in addition mention a few recent contributions to the theory of carrier-lattice exchange interaction in ferromagnetic and antiferromagnetic materials. For ferromagnets, the magnetic polaron plays an important role around the ferromagnetic transition temperature and in the paramagnetic region, where its property is expected to be strongly influenced by thermal fluctuations of the lattice moments. This was studied by several authors.[20-23] For antiferromagnets, on the other hand, magnetic-polaron effects exist even at absolute-zero temperature. Accordingly, the ground-state properties of the magnetic polaron[24,25] have been investigated. A dynamic study[26] of polarons in antiferromagnets has also been made.

The present work is an extension of our previous theory on the ground state of the magnetic polaron in antiferromagnets.[25] Although that work represents a first quantum theory in the field, its validity is limited to the case of weak coupling between the spin of the charge carrier and the lattice moment. We now present a quantum theory valid not only in the weak-coupling case but also in the more realistic strong-coupling limit where the carrier-lattice exchange is much stronger than the lattice-lattice coupling. The theory is based on the variation method. Regarding the exchange coupling constants of the electron with various lattice moments as given parameters, we first obtain the ground-state magnetic energy by a variational procedure in Sec. II. In Sec. III we again use the variation method to discuss how the electron orbital should adjust itself to take advantage of its magnetic coupling with the lattice spins. Both electrons from the conduction band and those bound to impurity centers are included in the discussion. For conduction electrons, the question of whether or not they can be self-trapped in the potential well created by their magnetic interaction with the lattice is addressed. For bound electrons, we discuss how their binding energy is influenced by the magnetic interaction. In Sec. IV the total lattice spin carried by the electron is calculated. In Sec. V we make a brief remark in concluding the paper.

II. MAGNETIC GROUND STATE

For antiferromagnetic semiconductors containing a charge carrier, either free or bound to an impurity center, a model Hamiltonian representing the magnetic interaction may be written as

$$H_M = I \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{2} \sum_i J(\mathbf{R}_i) \boldsymbol{\sigma} \cdot \mathbf{S}_i \ , \tag{2.1}$$

where $\mathbf{S}_i$ denotes a lattice spin localized at the i site and the Pauli spin operator $\frac{1}{2}\boldsymbol{\sigma}$ represents the spin of the charge carrier. The interaction between localized moments responsible for the antiferromagnetic order is denoted by the first term. By assumption, this interaction is confined to nearest neighbors and is of Heisenberg form with a positive and site-independent coupling constant I. The second term represents the interaction between the spin of the charge carrier and the lattice spins. This interaction, also in Heisenberg form, is assumed to be ferromagnetic. Hence, the coupling constant J is positive, whose value may vary with the lattice position $\mathbf{R}_i$. The actual functional form of $J(\mathbf{R}_i)$ depends on the spatial distribution of the charge carrier; it is through this interdependence that the orbital motion of the charge carrier may be altered by its magnetic coupling with the local moments.

If, for the time being, we regard the coupling constants J as given parameters and if we further neglect the spin-orbit coupling of the charge carrier, the Hamiltonian H_M in (2.1) may be treated as an independent unit separate from the orbital part of the total Hamiltonian for the charge carrier. In this way the ground state energy of H_M (or more precisely, its upper bound) is first obtained by using the variation method. The magnetic-polaron orbital is then adjusted so as to minimize the total energy (i.e., the orbital plus the magnetic energy).

In constructing a trial ground-state wave function of H_M, we invoke the adiabatic approximation. This approximation was also used in our weak-coupling theory.[25] In the strong-coupling limit where $J \gg I$, the lattice moments precess around the carrier spin rapidly while they adjust to each other at a much slower rate. The adiabatic approximation is then again valid. In other words, a product-type wave function may be assumed:

$$\theta(s, S_1, \ldots, S_N) = \psi(s) \Omega(S_1, \ldots, S_N) \ , \tag{2.2}$$

where ψ depends on the spin coordinates of the charge carrier and Ω on the lattice spins. Let us use the sublattice magnetization direction of the antiferromagnet as the quantization z axis. Referring to this axis, we assume that ψ is a equal admixture of up and down spinors, representing a carrier spin fixed along the transverse x direction (say, by an external magnetic field). Explicitly,

$$\psi = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} . \tag{2.3}$$

For the lattice part, we take a trial function which is a product of spin functions associated with various lattice points labeled by i:

$$\Omega = \prod_i \mathcal{R}(\alpha_i, \beta_i, \gamma_i) \phi_{SS}^i \ , \tag{2.4}$$

where $\mathcal{R}$ is the rotation operator for angular-momentum eigenfunctions. When $\mathcal{R}$ is applied to ϕ_{SM}, an eigenfunction of the spin operators S^2 and S_z, it results in the transformed spin function under a rotation of coordinates through Euler angles α, β, and γ. Note that in the trial wave function attached to each lattice site the magnetic quantum number M assumes its maximum possible value of S representing the quantum number of the lattice spin. The physical meaning of the trial function is transparent; it represents an arrangement of spins on the lattice with their orientations varying from site to site in a manner favored by the magnetic Hamiltonian in (2.1). The Euler angles specifying the orientation of the local spin at each site are the variation parameters to be determined by minimizing the expectation value of the magnetic Hamiltonian H_M.

To calculate the expectation value of the ground-state energy according to (2.1) and (2.2), we note that, with ψ given in (2.3),

$$\langle \psi \mid \boldsymbol{\sigma} \mid \psi \rangle \cdot \langle \Omega \mid \mathbf{S}_i \mid \Omega \rangle = \langle \Omega \mid S_{ix} \mid \Omega \rangle \ .$$

Thus we can eliminate the spin coordinates of the charge carrier from the expectation value and obtain

$$\langle \theta \mid H_M \mid \theta \rangle = I \sum_{i,j} \langle \Omega \mid \mathbf{S}_i \cdot \mathbf{S}_j \mid \Omega \rangle - \tfrac{1}{2} \sum_i J(\mathbf{R}_i) \langle \Omega \mid S_{ix} \mid \Omega \rangle \ . \tag{2.5}$$

Let us first consider the matrix element $\langle \Omega \mid \mathbf{S}_i \cdot \mathbf{S}_j \mid \Omega \rangle$ representing the interaction between two neighboring lattice spins. In our model Hamiltonian, the lattice spin S_i stands for the sum of the spin of all electrons localized at the i site, each having a spin of $\hbar/2$. The wave function ϕ_{SS}^i in (2.4) may be expressed as a product of up spinors, and the effect of applying the rotation operator to ϕ_{SS}^i is equivalent to the product of rotated up spinors. It is obvious then

$$\langle \Omega \mid \mathbf{S}_i \cdot \mathbf{S}_j \mid \Omega \rangle = S^2 \langle \mathcal{R}_i v_i \mathcal{R}_j v_j \mid \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \mid \mathcal{R}_i v_i \mathcal{R}_j v_j \rangle \ , \tag{2.6}$$

where $\mathcal{R}_i$ is an abbreviated notation for the rotation operator at the i site which acts on the up spinor v_i, and $\boldsymbol{\sigma}_i$ is the Pauli spin operator associated with an electron localized at the i site.

The matrix element on the right-hand side of (2.6) may be evaluated using the explicit form of the rotation matrix,[27]

$$\mathcal{R}(\alpha, \beta, \gamma) = \begin{bmatrix} \cos(\beta/2) e^{-i(\alpha+\gamma)/2} & -\sin(\beta/2) e^{i(\gamma-\alpha)/2} \\ \sin(\beta/2) e^{-i(\gamma-\alpha)/2} & \cos(\beta/2) e^{i(\alpha+\gamma)/2} \end{bmatrix} , \tag{2.7}$$

in a representation in which

$$v = \begin{bmatrix} 1 \\ 0 \end{bmatrix} . \tag{2.8}$$

After some straightforward algebra we obtain

$$\langle \mathcal{R}_i v_i \mathcal{R}_j v_j \mid \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \mid \mathcal{R}_i v_i \mathcal{R}_j v_j \rangle = \cos\beta_i \cos\beta_j + \sin\beta_i \sin\beta_j \cos(\alpha_i - \alpha_j) \ . \tag{2.9}$$

The remaining matrix element, $\langle \Omega \mid S_{ix} \mid \Omega \rangle$, in (2.5) may be similarly evaluated. First,

$$\langle \Omega \mid S_{ix} \mid \Omega \rangle = S \langle \mathcal{R}_i v_i \mid \sigma_{ix} \mid \mathcal{R}_i v_i \rangle \ . \tag{2.10}$$

We obtain then

$$\langle \Omega \mid S_{ix} \mid \Omega \rangle = S \sin\beta_i \cos\alpha_i \ . \tag{2.11}$$

In the limit of strong carrier-lattice coupling, the term involving matrix elements (2.11) is the dominating one in the magnetic Hamiltonian. Minimization of this part of the interaction energy with respect to the angles α_i gives

$$\alpha_i = 0 \ . \tag{2.12}$$

In a two-sublattice model for the antiferromagnet, the i site and its neighboring j site belong to different sublattices. Accordingly we assume that

$$\beta_j = \pi - \beta_i \ . \tag{2.13}$$

Under these conditions we have

$$\langle \Omega \mid \mathbf{S}_i \cdot \mathbf{S}_j \mid \Omega \rangle = -S^2 \cos(2\beta_i) \ . \tag{2.14}$$

From (2.5), (2.11), (2.12), and (2.14) we then get

$$\langle \theta \mid H_M \mid \theta \rangle = -\tfrac{1}{2} \sum_i [zIS^2 \cos(2\beta_i) + J(\mathbf{R}_i) S \sin\beta_i] \ , \tag{2.15}$$

where z is the number of nearest neighbor to each lattice spin, and the summation is over the entire lattice. The angles β_i constitute the set of variation parameters. It is noted that the result in (2.15) may be interpreted in terms of the classical vector model for spins; indeed, it coincides with the corresponding semiclassical result obtained by previous authors.[24] This is so because the solution in (2.12) suppresses all quantum fluctuations of lattice spins around the carrier-spin direction.

Now we come to determine the variation parameters β_i which will minimize the energy expectation value in (2.15). The solutions are

$$\beta_i = \begin{cases} \pi/2 & \text{if } J(\mathbf{R}_i) \geq 4zSI \ , \\ \sin^{-1}\left[\dfrac{J(\mathbf{R}_i)}{4zSI}\right] & \text{otherwise} \ . \end{cases} \tag{2.16}$$

Based on a vector model for spins, the case $\beta_i = \pi/2$ means that the lattice spin at the i site is fully aligned with the carrier spin. The structure of the magnetic polaron as given by the solutions in (2.16) may be visualized as one consisting of a ferromagnetic core surrounded by a halo of enhanced but not fully aligned lattice spins. Of course, if there is no site for which $J(\mathbf{R}_i) \geq 4zSI$, the ferromagnetic core is then absent.

Substituting (2.16) into (2.15), one obtains an upper bound of the ground-state magnetic energy as

$$E_m = -\tfrac{1}{2} zNS^2 I + \Delta E_m \ , \tag{2.17}$$

$$\Delta E_m = -\frac{S}{2} \sum_i^{N_c} [J(\mathbf{R}_i) - 2zSI] - \frac{1}{16zI} \sum_i^{N-N_c} [J(\mathbf{R}_i)]^2 \ ,$$

where N denotes the total number of lattice spins and N_c the number of lattice spins contained inside the ferromagnetic core. The first term in E_m denotes the magnetic energy of the unperturbed antiferromagnetic lattice. The interaction energy between the carrier spin and the local moments is denoted by ΔE_m. As indicated, the summation in the first term in ΔE_m runs over all lattice points inside the core while the second term involves a sum over the rest of lattice points situated outside the core.

III. MAGNETIC-POLARON ORBITAL

As stated before, the orbital motion of the charge carrier may be affected by its magnetic interaction with the lattice spins. This is the focus of our discussion in this section.

Under the effective-mass approximation, the one-particle Hamiltonian for the charge carrier can be written as

$$H = \frac{P^2}{2m^*} + V + E_m \ . \tag{3.1}$$

Here the effect of the crystalline potential has been incorporated into the effective-mass parameter m^*. The potential energy V stands for that due to impurities, defects, etc., which may be present in the sample. To obtain the ground-state energy for the total Hamiltonian in (3.1), we again rely on the variation method. We adopt a trial orbital wave function which is localized and hydrogenlike,

$$\phi = (\pi r_0^3)^{-1/2} \exp(-r/r_0) \ , \tag{3.2}$$

using r_0 as a variation parameter adjusted to minimize the total energy. We use such a localized function to represent an electron either in the conduction band or bound to an impurity center. For the former case, using a localized function enables us to test whether or not a band electron will be self-trapped in a potential well created by the magnetic interaction; if no solution for a real r_0 exists in the variation calculation, it is an indication that self-trapping is not possible.

With the trial function in (3.2) we first evaluate the exchange coupling constant J between the charge carrier and the lattice spins. As the magnetic electrons responsible for the lattice spin are highly localized at the lattice site, we may approximate the exchange integral by a contact interaction. In terms of Dirac's δ function, it is expressed as

$$J(R) = 4\pi A \Delta \int dr \, \phi^*(r) \phi(r) \delta(r - R) \ , \tag{3.3}$$

where A, a material parameter, denotes the exchange

coupling strength between the carrier, normalized within a unit cell of volume Δ, and the lattice spin localized at the same cell. With the wave function ϕ in (3.2), one gets

$$J(R)=4A\Delta r_0^{-3}\exp(-2R/r_0)\ . \tag{3.4}$$

Next, we determine the size of the ferromagnetic core, within which the lattice spins are fully aligned along the direction of the carrier spin. According to (2.16) and (3.4), the radius of the spherical core, R_c, is given by

$$R_c=\begin{cases} 0 \ \text{ if } A<\dfrac{r_0^3}{\Delta}zSI\ , \\ \dfrac{r_0}{2}\ln\left[\dfrac{\Delta}{r_0^3}\dfrac{A}{zSI}\right] \ \text{ if } A>\dfrac{r_0^3}{\Delta}zSI\ . \end{cases} \tag{3.5}$$

The number of lattice spins contained inside the core is written as

$$N_c=b(R_c^3/\Delta)\ , \tag{3.6}$$

where b stands for the geometric factor $4\pi/3$ if the core is spherical and each unit cell contains only one lattice spin.

In order to simplify the task of performing the lattice sum in (2.17), we assume specifically a simple cubic lattice with lattice constant R_0. For the same reason, we also assume that the ferromagnetic core, if it exists, is cubic in shape. The latter assumption amounts to altering the value of the geometric factor b in (3.6) to 8. The essential physics of magnetic polarons contained in our results, however, will not be changed by these assumptions. The two lattice sums in (2.17), one over the saturated core and one over the lattice space outside the core, are approximately evaluated in the Appendix.

From (A7) and (A9), we can calculate the magnetic energy ΔE_m in (2.17). The result for the case where the polaron has a ferromagnetic core is different from that when the core is absent. Both cases are discussed below.

(1) Type I: Polaron without a core $[A<(r_0^3/\Delta)zSI]$. Here we have adopted the same classification as used in Ref. 24, and name a polaron without a core a type-I polaron. It is to be noted that the condition above for the absence of a ferromagnetic core contains not only material parameters but, in addition, depends on the spatial extent of the polaron itself, i.e., on r_0. The parameter r_0 is yet to be determined in the present work. In any case, this type of polaron is likely to occur in the weak-coupling limit where the carrier-lattice exchange is weak in comparison with the lattice-lattice exchange.

In this case, the core radius $R_c=0$, and the only lattice sum which enters the magnetic energy calculation is S_2 in (A9). Under the condition $r_0>R_0$, this term becomes

$$S_2\approx 16\frac{\Delta}{r_0^3}A^2\ .$$

The magnetic energy is then given by

$$\Delta E_m^{\mathrm{I}}=-\left[\frac{\Delta}{r_0^3}\right]\frac{A^2}{zI}\ . \tag{3.7}$$

(2) Type II: Polaron with a core $[A>(r_0^3/\Delta)zSI]$. Again we note that the condition for a type-II polaron depends on r_0. Materials with a strong carrier-lattice exchange coupling are more favorable for the formation of this type of polaron.

The radius of the core, R_c, if it exists, is given in (3.5). Substituting this expression for R_c into (A7), we have

$$S_1=32A\Delta r_0^{-3}\left[\frac{1-(zSIr_0^3/A\Delta)^{1/2}}{\exp(R_0/r_0)-1}\right]^3\ .$$

As $zSIr_0^3/A\Delta<1$ and the extent of the polaron, r_0, is expected to be larger than the lattice constant R_0, the sum S_1 is roughly

$$S_1\approx 32A\ .$$

Using the same procedure we estimate S_2 in (A9) to be

$$S_2\approx 48zSIA\ .$$

The magnetic energy is then obtained as

$$\Delta E_m^{\mathrm{II}}=zbS^2\frac{R_c^3}{\Delta}I-19SA\ . \tag{3.8}$$

The last term represents the magnetic-energy gain due to the carrier-lattice exchange. Within our approximation, this energy is a constant independent of the spatial extent of the polaron. The numerical coefficient, 19, for this term should be regarded as an order-of-magnitude estimate only. We obtained this particular value by assuming a specific lattice and core structure as shown in the Appendix. In any case, this term should be close in value to S times $4\pi A$, which, according to (3.3), represents the carrier-lattice exchange energy for a carrier normalized to one unit cell. The first term in (3.8) represents the energy loss as the lattice spins outside the core are drawn away from their original antiferromagnetic alignment by the carrier spin. This term has a rather strong r_0^3 dependence; the total number of lattice spins inside the core increases as R_c^3 which is roughly proportional to r_0^3.

It is noted that the magnetic interaction term in (3.7) is different in form from that in (3.8); while in (3.7) it is proportional to A^2, it depends on A in (3.8). Let us explain this difference by recalculating (3.7) through a qualitative and classical argument. With the electron spin pointing along the x direction, the lattice moment becomes canted, making an angle θ with respect to the sublattice magnetization z axis. The total magnetic interaction between the electron and the lattice is then equal to $-AS\sin\theta$. The angular factor $\sin\theta$ should be equal to the ratio of the carrier-lattice to lattice-lattice exchange coupling strength. On the average, the coupling constant of the carrier with one lattice moment is equal to $A(\Delta/r_0^3)$. With

$$\sin\theta\sim\frac{A}{zSI}\frac{\Delta}{r_0^3}\ ,$$

we have reproduced (3.7). On the other hand, if there exists a ferromagnetic core, the angle θ is equal to a constant $(\pi/2)$. Hence in this case the magnetic energy is proportional to A and becomes independent of r_0.

With the magnetic energy calculated for type-I and type-II polarons, we can proceed to complete the variation calculation and determine the polaron localization radius r_0 if it exists. We consider two cases: one for electrons in the conduction band, and one for electrons bound to impurity centers.

A. Magnetic polaron

We consider the case of a carrier in the conduction band, for which the impurity potential $V=0$ in (3.1). Using the trial function in (3.2), one obtains the expectation value of the kinetic energy as

$$\langle \phi \mid \frac{P^2}{2m^*} \mid \phi \rangle = \frac{\hbar^2}{2m^* r_0^2} \ . \tag{3.9}$$

Since the magnetic energy has a different dependence on r_0 for the two types of polaron discussed above, it is more convenient to investigate the two cases separately.

(1) Type-I polaron. For polaron without a core, the negative magnetic energy as given in (3.7) decreases as r_0^{-3} while the positive kinetic energy decreases more slowly as r_0^{-2}. Hence, there is no minimum in the total energy based on a localized trial wave function. This indicates that excluding the possibility of forming a type-II polaron (to be discussed next), a free carrier cannot be self-trapped in the potential well created by its magnetic interaction with the local moments. In this case, the orbital wave function of the charge carrier is not well represented by (3.2), and the expression for the magnetic energy in (3.7) no longer applies. For an extended conduction electron, its magnetic interaction with one localized moment should be proportional to N^{-2}, N being the total number of lattice points in the crystal. Hence, the total magnetic energy, which is proportional to N^{-1}, approaches zero. The magnetic-polaron effect is then quite unimportant in this case.

(2) Type-II polaron. In this case, the lattice-magnetic-energy loss inside the core increases as R_c^3 as shown in (3.8). The dependence of the core radius R_c on the spatial extent r_0 of the polaron is given explicitly in (3.5), which contains a logarithm factor. Since the logarithm function is only slowly varying, we may replace it by a constant. As an order-of-magnitude estimate, we assign a value of 2 to this constant. In other words, we approximate R_c by

$$R_c \approx r_0 \ .$$

Then, with the lattice-magnetic-energy loss increasing as r_0^3 and the kinetic energy decreasing as r_0^{-2}, a stable point can be found at

$$r_{\text{free}}^{\text{II}} = \left[\frac{\hbar^2 \Delta}{3zbm^* S^2 I} \right]^{1/5} \ . \tag{3.10}$$

To be certain that one is dealing with a type-II polaron, one has to check the inequality $A > (r_0^3/\Delta) zsI$, this time solely in terms of material parameters.

We make an order-of-magnitude estimate, using the following parameters appropriate for a typical antiferromagnet like EuTe:

$$z=6, \quad S=\tfrac{7}{2}, \quad \frac{\hbar^2}{m^* R_0^2} \sim 1 \text{ eV} \ ,$$

$$A \sim 0.1 \text{ eV}, \quad I \sim 10^{-4} \text{ eV} \ .$$

The value of r_0 is estimated to be

$$r_{\text{free}}^{\text{II}} \sim R_0 \ .$$

The core radius R_c is then also roughly equal to one lattice constant. With such a small radius it is not too difficult to satisfy the condition of existence of a core as long as $A \gg I$.

Apart from the stability condition, one has to check that the kinetic energy of the carrier at such a small localization distance is not large enough to allow it to escape from the potential well created by its magnetic interaction with the lattice. The result of this comparison is obviously sensitive to material parameters. For the parameters used above, the magnetic energy is indeed larger than the kinetic energy. It seems then that in materials like EuTe, the free electron from the conduction band may be self-trapped to form a tiny magnetic polaron with a ferromagnetic core.

Incidentally, in estimating the kinetic energy of a tiny polaron of the dimension of a few lattice constants, it may be more appropriate to use the free electron mass rather than the effective mass of the carrier. Also, for a polaron with such a small core, it should be possible to obtain a better estimate of the core radius and the magnetic energy than the approximate results obtained here.

B. Bound magnetic polaron

We consider the case of an electron bound to a singly charged impurity center. Based on the effective-mass approximation, the impurity potential V in (3.1) is Coulomb in form and its expectation value with respect to the trial function in (3.2) is

$$\langle \phi \mid V \mid \phi \rangle = -\frac{e^2}{\epsilon r_0} \ , \tag{3.11}$$

where ϵ is the dielectric constant of the material. Again we consider the possibility of forming the two types of polaron separately.

(1) Type-I bound polaron. From (3.7), (3.9), and (3.11) we have the total energy

$$E = \frac{\hbar^2}{2m^* r_0^2} - \frac{e^2}{\epsilon r_0} - \frac{\Delta A^2}{zIr_0^3} \ . \tag{3.12}$$

Without the last term, the energy minimum occurs at $r_0 = a_0^*$, where a_0^* is the effective Bohr radius of the donor electron, i.e.,

$$a_0^* = \frac{\epsilon \hbar^2}{m^* e^2} \ . \tag{3.13}$$

With the magnetic interaction present, the energy minimum exists only if

$$\frac{A^2}{zI} < \frac{1}{12} \frac{\hbar^2 a_0^*}{m^* \Delta} \ . \tag{3.14}$$

When this condition is satisfied, the donor orbit radius will shrink from a_0^* to a value given below:

$$r_{\text{bound}}^{\text{I}} = \frac{a_0^*}{2}\left[1+\left[1-\frac{12m^*\Delta}{\hbar^2 a_0^*}\frac{A^2}{zI}\right]^{1/2}\right] . \tag{3.15}$$

To discuss the effect of the magnetic interaction on the binding energy of the impurity carrier in this case, we note that as the electron orbital radius shrinks, the Coulomb-potential-energy gain is compensated by its kinetic-energy loss. Hence, the increase in the binding energy of the carrier is mainly due to the last term in (3.12). In other words, it is attributable to the fact that there is a change in magnetic energy as the carrier is ionized to the conduction band from the localized state.

When the condition in (3.14) is not satisfied, a stable solution cannot be found with a localized trial wave function. This indicates that the charge carrier may become extended unless there is a possibility of forming a type-II bound polaron (to be discussed next).

(2) Type-II bound polaron. In this case, the total energy is given by

$$E = \frac{\hbar^2}{2m^* r_0^2} - \frac{e^2}{\epsilon r_0} + zbS^2\frac{R_c^3}{\Delta}I - 19SA . \tag{3.16}$$

Again we replace R_c by r_0, and discuss the case when the third term above is smaller than the second one in magnitude, or more precisely

$$\frac{zI}{e^2/\epsilon a_0^*} < \frac{\Delta}{3bS^2 a_0^{*3}} . \tag{3.17}$$

Under this condition, the minimum of the total energy occurs at

$$r_{\text{bound}}^{\text{II}} = a_0^*\left[1-\frac{3\epsilon zbS^2 I a_0^{*4}}{e^2\Delta}\right] . \tag{3.18}$$

The radius of the bound carrier shrinks in order to minimize the lattice-magnetic-energy loss. As discussed before, the increase in the binding energy of the carrier is, for the most part, attributable to the depth of the magnetic potential well.

IV. LATTICE SPINS CARRIED BY THE POLARON

From (2.11) and (2.16) we may calculate the total lattice moment carried by the polaron:

$$S_{\text{polaron}} = N_c S + \frac{1}{4zI}\sum_i^{N-N_c} J(\mathbf{R}_i) . \tag{4.1}$$

The first term evidently represents the total spin of the ferromagnetic core, and the second term comes from the halo of enhanced spins outside the core. The lattice sum in the second term is evaluated in the Appendix. From (A12) we have

$$S_{\text{polaron}} = N_c S + \frac{8A\Delta r_0^{-3}}{zI}\frac{1-[1-\exp(-R_c/r_0)]^3}{[\exp(R_0/r_0)-1]^3} . \tag{4.2}$$

For a type-I magnetic polaron, both N_c and R_c are equal to zero. Since the conduction electron is not localized, its spatial extent, r_0, is much larger than R_0. Then

$$S_{\text{polaron}}^{\text{I}} = \frac{8A}{zI} . \tag{4.3}$$

This result also applies to a type-I bound magnetic polaron so long as its spatial extent is large, containing many lattice points inside.

For a type-II magnetic polaron, R_c is given in (3.5). Substituting this into (4.2) gives

$$S_{\text{polaron}}^{\text{II}} = N_c S + \frac{8A\Delta r_0^{-3}}{zI}\frac{1-\left[1-\left[\frac{zSIr_0^3}{A\Delta}\right]^{1/2}\right]^3}{[\exp(R_0/r_0)-1]^3} . \tag{4.4}$$

In the limit of strong coupling where $A \gg I$, the second term representing the total lattice spin contained in the halo surrounding the ferromagnetic core may become much larger than the moment of the core itself.

V. CONCLUDING REMARKS

We have presented a quantum theory of magnetic polarons in antiferromagnets. The ground-state properties are deduced based on the variation method. Very often this method cannot account for some finer effects due to quantum fluctuations, and the present work is no exception. Consequently, our ground-state magnetic energy agrees with that deduced by previous authors based on a classical treatment of the spins. Nevertheless, the present work is still different from the previous semiclassical theory; while the absence of quantum fluctuations is a deduced result in the present framework, it is assumed from the very beginning in a classical theory. In addition, the influence of magnetic interactions on the carrier orbitals has been discussed in a quantitatively more explicit manner.

APPENDIX: EVALUATION OF LATTICE SUMS

In evaluating the magnetic energy E_m in (2.17), the following two lattice sums are involved:

$$S_1 \equiv \sum_i^{N_c} J(\mathbf{R}_i) , \tag{A1}$$

$$S_2 \equiv \sum_i^{N-N_c} [J(\mathbf{R}_i)]^2 . \tag{A2}$$

We evaluate them on a simple cubic lattice with lattice constant R_0. For this lattice,

$$R_i = nR_0 , \tag{A3}$$

where

$$n = (n_1^2+n_2^2+n_3^2)^{1/2} , \tag{A4}$$

and n_1, n_2, and n_3 are integers representing the coordinates of the lattice vector $\mathbf{R}_i$.

To make it possible for us to evaluate the lattice sums S_1 and S_2 explicitly, we approximate n in (A4) by a positive number

$$n \to \tfrac{1}{2}(\,|n_1|+|n_2|+|n_3|\,)\,. \tag{A5}$$

Since $J(R)$ as given in (3.4) has an exponential dependence on R, the approximation in (A5) allows us to factor S_1 into a product of three lattice sums, each to be carried out along one of the cubic axes. If we further approximate the spherical ferromagnetic core by a cube of side length $2R_c$, the three sums become independent and equal to each other. We then have

$$S_1 = 4A\Delta r_0^{-3}\left[\sum_{n_1}\exp(-|n_1|R_0/r_0)\right]^3, \tag{A6}$$

where the integer n_1 in the summation runs from $-R_c/R_0$ to $+R_c/R_0$. As a simple geometric series, this sum can be evaluated immediately. One obtains

$$S_1 = 32A\Delta r_0^{-3}\left[\frac{1-\exp(-R_c/r_0)}{\exp(R_0/r_0)-1}\right]^3. \tag{A7}$$

As for the sum S_2 in (A2), it is to be evaluated outside the ferromagnetic core, which is a cube in our approximation. Then

$$S_2 = 16A^2\Delta^2 r_0^{-6}\left[\left[\sum_{n_1}\exp(-2|n_1|R_0/r_0)\right]^3 - \left[\sum_{|n_1|<R_c/R_0}\exp(-2|n_1|R_0/r_0)\right]^3\right]. \tag{A8}$$

The first sum is over the entire length of the crystal and the second one is within the cubic core. After evaluating the two geometric series, we obtain

$$S_2 = 128A^2\Delta^2 r_0^{-6}\frac{1-[1-\exp(-2R_c/r_0)]^3}{[\exp(2R_0/r_0)-1]^3}. \tag{A9}$$

This sum is independent of the total number of lattice points, N, in the $N\to\infty$ limit.

For evaluating the lattice-spin cloud carried by the polaron, we also need another lattice sum outside the core:

$$S_3 \equiv \sum_i^{N-N_c} J(\mathbf{R}_i)\,. \tag{A10}$$

With the same assumption about the lattice and the core structure, this sum is equal to

$$S_3 = 4A\Delta r_0^{-3}\left[\left[\sum_{n_1}\exp(-|n_1|R_0/r_0)\right]^3 - \left[\sum_{|n_1|<R_c/R_0}\exp(-|n_1|R_0/r_0)\right]^3\right], \tag{A11}$$

where the sum in the first term is over the entire crystal and the second one is confined within the core. The sum is evaluated to be

$$S_3 = 32A\Delta r_0^{-3}\frac{1-[1-\exp(-R_c/r_0)]^3}{[\exp(R_0/r_0)-1]^3}. \tag{A12}$$

[1] M. R. Oliver, J. A. Kafalas, J. O. Dimmock, and T. B. Reed, Phys. Rev. Lett. **24**, 1064 (1970).
[2] J. B. Torrance, M. W. Shafter, and T. R. McGuire, Phys. Rev. Lett. **27**, 1168 (1972).
[3] J. Vitins and P. Wachter, Phys. Rev. B **12**, 3829 (1975).
[4] N. F. Oliveira, S. Foner, Y. Shapira, and T. B. Reed, Phys. Rev. B **5**, 2634 (1972); Y. Shapira, S. Foner, N. F. Oliveria, and T. B. Reed, *ibid.* **5**, 2647 (1972).
[5] M. Nawrock, R. Planel, G. Fishman, and R. R. Galazka, Phys. Rev. Lett. **46**, 735 (1981).
[6] C. Zener, Phys. Rev. **82**, 403 (1951).
[7] P. C. de Gennes, Phys. Rev. **118**, 141 (1960).
[8] T. Wolfram and J. Callaway, Phys. Rev. **127**, 1605 (1962).
[9] R. M. White and R. B. Woolsey, Phys. Rev. **176**, 908 (1968).
[10] S. Methfessel and D. C. Mattis, *Encyclopedia of Physics* (Springer, Berlin, 1968), Vol. XVIII/I, p. 389.
[11] T. Kasuya, A. Yanase, and T. Takeda, Solid State Commun. **8**, 1543 (1970).
[12] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970).
[13] N. F. Mott and Z. Zinamon, Rep. Prog. Phys. **33**, 881 (1970).
[14] P. Lerowx-Hugon, Phys. Rev. Lett. **29**, 939 (1972).
[15] J. Kubler and D. T. Vigren, Phys. Rev. B **11**, 4440 (1975).
[16] C. E. T. Goncalves da Silva, Solid State Commun. **17**, 677 (1975).
[17] P. Kuivalainen, J. Sinkkonen, K. Kaski, and T. Stubb, Phys. Status Solidi **B94**, 181 (1979).
[18] P. Kuivalainen, J. Sinkkonen, and T. Stubb, Phys. Status Solidi **B104**, 299 (1981).
[19] A. Mauger and C. Godart, Phys. Rep. **141**, 51 (1986).
[20] T. Dietl and J. Spalek, Phys. Rev. Lett. **48**, 355 (1982); Phys. Rev. B **28**, 1548 (1983).
[21] A. Mauger, Phys. Rev. B **27**, 2308 (1983).
[22] D. Heiman, P. A. Wolff, and J. Warnock, Phys. Rev. B **27**, 4848 (1983).
[23] J. Kossut and W. M. Becker, Phys. Rev. B **33**, 1394 (1986).
[24] A. Mauger and D. L. Mills, Phys. Rev. Lett. **53**, 1594 (1984); Phys. Rev. B **31**, 8024 (1985).
[25] L. Liu and J. T. C. Liu, Phys. Rev. B **33**, 1797 (1986).
[26] A. Mauger and D. L. Mills, Phys. Rev. B **34**, 3418 (1986).
[27] See, for example, E. P. Wigner, *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra*, translated by J. Griffin (Academic, New York, 1959).