Theory of the bound magnetic polaron in antiferromagnetic semiconductors

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An approximate quantum theory of the ground state of the bound magnetic polaron in antiferromagnetic semiconductors is presented which is valid when the impurity-lattice exchange coupling is weak. In the deduced ground state, various one-magnon states of the lattice are excited through the lattice's exchange interaction with the impurity electron. Due to the same interaction, the effective mass of the impurity electron gets renormalized and its binding energy is correspondingly increased. The total lattice spin carried by the impurity electron is also determined.

I. INTRODUCTION

The concept of magnetic polaron[1-5] has long been used in the study of the electronic transport properties of magnetic semiconductors. In analogy to an ordinary polaron, a magnetic polaron is a charge carrier dressed with a cloud of polarized lattice spins. In case the charge carrier is bound to an impurity center, it is further termed as a bound magnetic polaron (BMP).

The concept of BMP was first introduced in a model[5] to explain the insulator-metal transition in Eu-rich EuO occurring at the ferromagnetic ordering temperature. The observed transition[6] involves a 10^{13}-fold increase in conductivity as the temperature is lowered through the magnetic transition temperature. According to the proposed model, this transition is caused by a sudden change in the binding energy of the impurity electron associated with the oxygen vacancy. When the substance is in the paramagnetic state, there is a lack of perfect long-range order. However, those lattice spins located in the vicinity of the vacancy may be aligned by the impurity electron spin if their exchange interaction with the latter gets sufficiently strong. In this case, since there will be more magnetic energy gained if the impurity orbit gets smaller, the magnetic effect tends to increase the binding energy of the BMP. Below the transition temperature, on the other hand, the lattice spins are already ferromagnetically aligned; the magnetic effect due to the impurity electron is therefore of no particular significance, except that the impurity spin will be aligned along the direction of the lattice magnetization. In other words, the magnetization of the lattice has no bearing at all on the binding energy of the impurity electron. Impurity electrons, if they are loosely bound, will be ionized and contribute to a large extrinsic conductivity. Besides the insulator-metal transition, the BMP mechanism was invoked more recently to analyze certain optical properties of dilute magnetic semiconductors.[7,8] Thermodynamic calculations involving a BMP were also made by several authors.[9,10]

As explained above, the BMP in a ferromagnetic host produces significant effects only near the ferromagnetic transition temperature and only when the exchange interaction between the impurity electron spin and the lattice spin gets stronger than the interatomic exchange responsible for the long-range order. Near the transition temperature, the magnetic order of the lattice is not describable by the spin-wave approximation, and in addition one has to deal with a large local disturbance on the lattice spin. Hence a complete theoretical treatment of the BMP problem would be difficult. On the other hand, if the host lattice is antiferromagnetic, the BMP effect exists at absolute zero temperature and even when the coupling between the impurity and the lattice spin is weak. These are simplifying factors which would help us in formulating a theory of BMP. In addition to an early work,[1] there is a recent report[11] on the theory of BMP in antiferromagnetic substances. But the existing theories are all semiclassical, and a quantum-mechanical approach is still lacking so far. In this paper we present an approximate quantum theory of the ground state of the BMP in antiferromagnetic semiconductors. The BMP theory is done here only in the weak-coupling limit.

Near absolute zero temperature, the low-lying excitations of an antiferromagnetic lattice are spin waves, or magnons, which are subject to a local disturbance due to impurity electrons present in the sample. As the exchange between the impurity electron spin and the lattice spin is weak by assumption, an adiabatic approximation may be invoked, in which the impurity electron spin may be separated from the magnon coordinates of the lattice. Using this approximation, we are able to deduce some properties of the BMP in an assumed ground-state configuration. The deduced results include the magnetic effect on the binding energy of the BMP and the total spin cloud carried by the BMP. In order to make our quantum treatment physically more transparent, we precede its presentation with a classical picture of a BMP in an antiferromagnetic lattice in the next section.

II. CLASSICAL PICTURE

It is well known that the magnetic property of an antiferromagnetic insulator (or semiconductor) may be

analyzed in terms of a two-sublattice structure. At perfect alignment, the spins localized at one sublattice, which all point to the same direction, are exactly opposite to that of spins localized at the other sublattice. The fact that this is a stable configuration may be seen by considering the torque experienced by each sublattice due to its exchange interaction with the other. Since the torque is proportional to the vector product between the interacting spins, it vanishes when the two spins are aligned along the same axis. This static classical ground state has to be replaced in quantum mechanics by two sublattices partaking in zero-point motion consisting of spin-wave modes with certain minimal amplitudes. The spin wave may be pictured as a wave of precessional motion of lattice spins around the sublattice magnetization axis.

Suppose there exists an extra electron bound to an impurity center. We ask then for its effect on the antiferromagnetic ordering of the host due to its exchange interaction with the lattice spin. Let us begin by assuming that the electron spin is somehow fixed at a transverse direction relative to the magnetization axis of the sublattice (say by an external field). A stable configuration would be established if the lattice spins in the vicinity of the impurity assume a canted antiferromagnetic arrangement while the impurity electron spin stays in its original direction, as shown in Fig. 1. The impurity spin is not expected to change its direction because the torque acting on it by one sublattice is always cancelled by that due to the other. On the other hand, each sublattice is now interacting with two exchange fields, one from the other sublattice and one from the impurity electron. A lattice spin should then change its direction until it lies along the resultant of the two vector fields mentioned above so that there is no more torque acting on it. From Fig. 1 it is seen that the cosine of the angle of inclination θ is proportional to the ratio of the two exchange fields, i.e.,

$$\cos\theta \sim \frac{J(R)}{I} ,$$

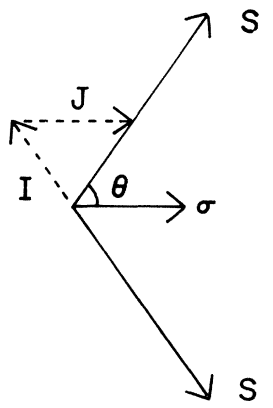

FIG. 1. Ground-state configuration for two neighboring lattice spins S and the impurity spin σ. Although the two lattice spins start from the same point in the drawing, they are actually centered at different lattice sites. Dotted line J represents the impurity-lattice exchange field, and dotted line I represents the total exchange field due to all the neighboring lattice spins belonging to the other sublattice.

where $J(R)$ and I denote impurity-lattice and lattice-lattice exchange coupling constant, respectively. Since J varies with the distance R from the impurity center, the angle of inclination is spatially nonuniform. In this final canted equilibrium configuration, a lattice magnetization is induced along the direction of the impurity electron spin and a BMP is thus formed. In the next section we shall derive such a ground state quantum mechanically.

III. MAGNETIC GROUND STATE

Our model system consists of an antiferromagnetic semiconductor containing dilute impurities, each capable of donating one electron. To consider the magnetic interaction in such a system, we assume two sublattices of identical localized spins properly aligned at temperature $T=0$. Each lattice spin, by assumption, only interacts with its nearest neighbors, in addition to its exchange interaction with the impurity electron. As the impurity concentration is dilute, we may consider only one isolated impurity center, which is chosen as the origin of the lattice space. The part of the Hamiltonian representing the magnetic interaction in our model system may be assumed to be of Heisenberg form:

$$\begin{aligned} H_M &= H_L + H_I , \\ H_L &= I \sum_{(\mu,\nu)} \mathbf{S}_\mu \cdot \mathbf{S}_\nu , \\ H_I &= -\tfrac{1}{2} \sum_\mu J(\mathbf{R}_\mu) \sigma \cdot \mathbf{S}_\mu - \tfrac{1}{2} \sum_\nu J(\mathbf{R}_\nu) \sigma \cdot \mathbf{S}_\nu , \end{aligned} \tag{3.1}$$

where $\mathbf{S}_\mu$ and $\mathbf{S}_\nu$ denote the lattice spin localized at the two sublattices labeled by μ and ν, and σ is the Pauli spin operator for the impurity electron. The interatomic exchange constant I in H_L for lattice spins is positive, and the sum there is restricted to nearest neighbors. The exchange interaction between the impurity electron and the local spin as described by H_I is assumed ferromagnetic, and hence the exchange coupling constant J is also positive. Its value is determined by the following exchange integral involving the impurity electron orbital ϕ and the magnetic electron orbital ψ localized at a lattice site $\mathbf{R}$:

$$J(\mathbf{R}) = \int d^3 r_1 \int d^3 r_2 \, \Phi^*(\mathbf{r}_1) \psi^*(\mathbf{r}_2 - \mathbf{R}) \frac{e^2}{r_{12}} \times \psi(\mathbf{r}_1 - \mathbf{R}) \Phi(\mathbf{r}_2) . \tag{3.2}$$

As the wave function for the bound impurity electron decays with distance, the coupling constant J for local spins further away from the impurity center decreases in value correspondingly.

Let us first discuss the lattice part H_L in (3.1). The ground state for H_L was derived by Anderson,[12] and his approximate quantum-mechanical treatment is presented here in terms of creation and annihilation operators for magnons. Let us designate the sublattice magnetization axis as the z axis, and rewrite the Hamiltonian H_L as

$$H_L = I \sum_{(\mu,\nu)} [S_{\mu z} S_{\nu z} + \tfrac{1}{2}(S_\mu^+ S_\nu^- + S_\mu^- S_\nu^+)] \tag{3.3}$$

with raising operators S^+ and lowering operators S^-.

We recall the definition of these operators as

$$S^+ = S_x + iS_y \ , \qquad S^- = S_x - iS_y \ . \tag{3.4}$$

To find the approximate eigenstates of H_L, we incorporate Anderson's assumption for an antiferromagnetic magnon state into the Holstein-Primakoff transformation[13] as follows:

$$\begin{aligned} S_{\mu z} &= S - a_\mu^\dagger a_\mu \ , \\ S_{\nu z} &= -S + a_\nu^\dagger a_\nu \ , \\ S_\mu^+ &= \sqrt{2S}\, a_\mu^\dagger \ , \\ S_\nu^+ &= \sqrt{2S}\, a_\nu \ , \\ S_\mu^- &= \sqrt{2S}\, a_\mu \ , \\ S_\nu^- &= \sqrt{2S}\, a_\nu^\dagger \ . \end{aligned} \tag{3.5}$$

Here $a^\dagger$ and a are boson creation and annihilation operators associated with a lattice site, and S is the quantum number for the lattice spin. Using this transformation and keeping only terms quadratic in the a's and $a^\dagger$'s, we obtain the linearized H_L as

$$H_L = -\tfrac{1}{2}NZIS^2 + ZIS\left[\sum_\mu a_\mu^\dagger a_\mu + \sum_\nu a_\nu^\dagger a_\nu\right] + IS\sum_{(\mu,\nu)}(a_\mu^\dagger a_\nu^\dagger + a_\mu a_\nu) \ , \tag{3.6}$$

where N is the total number of lattice spins in the system and Z is the number of nearest neighbors to each spin.

To obtain the normal modes for the lattice spin system, we go to the reciprocal $\mathbf{k}$ space with the following transformation:

$$a_{\mu(\nu)} = N^{-1/2}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_{\mu(\nu)}} a_{\mathbf{k}} \ . \tag{3.7}$$

Expressed in terms of $\mathbf{k}$-space boson operators, the Hamiltonian H_L in (3.6) becomes

$$H_L = -\tfrac{1}{2}NZIS^2 + ZIS\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \tfrac{1}{2}IS\sum_{\mathbf{k}}(\gamma_{\mathbf{k}}^* a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + \gamma_{\mathbf{k}} a_{\mathbf{k}} a_{-\mathbf{k}}) \ . \tag{3.8}$$

The quantity $\gamma_{\mathbf{k}}$ above stands for the following sum over nearest neighbors:

$$\gamma_{\mathbf{k}} = \sum_{n=1}^{Z} e^{i\mathbf{k}\cdot\mathbf{R}_n} \ , \tag{3.9}$$

where $\mathbf{R}_n$ is a vector connecting any spin with any of its Z nearest neighbors. From the definition of $\gamma_{\mathbf{k}}$ it is obvious that $\gamma_{\mathbf{k}}^* = \gamma_{-\mathbf{k}}$. As the spins are arranged on a Bravais lattice with inversion symmetry, it is further noted that $\gamma_{\mathbf{k}} = \gamma_{-\mathbf{k}}$. In other words, $\gamma_{\mathbf{k}}$ is a real even function of $\mathbf{k}$.

The Hamiltonian H_L in (3.8) may be diagonalized by making the following Bogoliubov transformation[14] to magnon operators:

$$\begin{aligned} a_{\mathbf{k}} &= (\cosh u_{\mathbf{k}})b_{\mathbf{k}} + (\sinh u_{\mathbf{k}})b_{-\mathbf{k}}^\dagger \ , \\ a_{\mathbf{k}}^\dagger &= (\cosh u_{\mathbf{k}})b_{\mathbf{k}}^\dagger + (\sinh u_{\mathbf{k}})b_{-\mathbf{k}} \ . \end{aligned} \tag{3.10}$$

The real parameter $u_{\mathbf{k}}$ above, which satisfies $u_{\mathbf{k}} = u_{-\mathbf{k}}$, must be chosen properly to diagonalize the Hamiltonian H_L in (3.8). It is straightforward to find the required $u_{\mathbf{k}}$; it satisfies

$$\tanh 2u_{\mathbf{k}} = -\gamma_{\mathbf{k}}/Z \ . \tag{3.11}$$

The diagonalized H_L is then

$$H_L = -\tfrac{1}{2}NZIS(S+1) + \sum_{\mathbf{k}}(b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \tfrac{1}{2})\hbar\omega_{\mathbf{k}} \tag{3.12}$$

with

$$\hbar\omega_{\mathbf{k}} = ZIS(1-\gamma_k^2/Z^2)^{1/2} \ . \tag{3.13}$$

The physical meaning of H_L in (3.12) is rather obvious. The original system of interacting lattice spins has been replaced by a collection of free magnons, each carrying a quantum of energy $\hbar\omega_k$ associated with the spin-wave motion. The eigenvalues of the operator $b_{\mathbf{k}}^\dagger b_{\mathbf{k}}$ are integers $n_{\mathbf{k}}$, denoting the number of magnons excited in the mode with wave vector $\mathbf{k}$. At $T=0$, the number $n_{\mathbf{k}}$ for any mode is equal to zero, and there exist no magnons but only zero-point modes.

In the presence of an impurity electron, the system is subject to an additional interaction H_I in (3.1). Due to this interaction, magnons will be excited even at $T=0$. We proceed now to deduce a ground state for H_M in (3.1) with the assumption that the Pauli spin vector is along the x direction, transverse to the sublattice magnetization axis. Using (3.5), we may rewrite H_I in (3.1) as

$$H_I = -\tfrac{1}{2}(S/2)^{1/2}\sigma_x\sum_i J(R_i)(a_i^\dagger + a_i) \ , \tag{3.14}$$

where the sum i is over all lattice sites (i.e., on both sublattices). When transformed to the reciprocal space, this becomes

$$H_I = -\tfrac{1}{2}(S/2N)^{1/2}\sigma_x\sum_{\mathbf{k}}(J_{\mathbf{k}}^* a_{\mathbf{k}}^\dagger + J_{\mathbf{k}} a_{\mathbf{k}}) \ , \tag{3.15}$$

with

$$J_{\mathbf{k}} = \sum_i J(\mathbf{R}_i)e^{i\mathbf{k}\cdot\mathbf{R}_i} \ . \tag{3.16}$$

As $J(\mathbf{R}_i)$ is expected to have spherical symmetry relative to the impurity center, it is concluded that $J_{\mathbf{k}}^* = J_{-\mathbf{k}} = J_{\mathbf{k}}$. In other words, $J_{\mathbf{k}}$ is a real even function of $\mathbf{k}$. The Hamiltonian H_I in (3.15) is further expressed in terms of magnon operators by using the Bogoliubov transformation in (3.10).

At this stage, we assume that the impurity-lattice exchange is weak as compared with the interaction between lattice spins, so that we may invoke the adiabatic approximation. In other words, the eigenfunction of H_M in (3.1) is, by this approximation, expressible in terms of the product of a magnon wave function and a spinor function for the impurity electron. We further assume that the impurity spinor function describes an eigenstate of the σ_x operator consisting of an equal admixture of up and down spi-

nors. In this case, the operator σ_x in (3.15) may simply be replaced by its eigenvalue of unity.

The total magnetic Hamiltonian H_M, which contains both quadratic (H_L) and linear (H_I) terms of the magnon operator b and $b^\dagger$, may be brought into a diagonal form by shifting the origin of the magnon operator. Let us introduce the following transformation:

$$b'_{\mathbf{k}}=b_{\mathbf{k}}-\alpha_{\mathbf{k}} ,$$
$$(b'_{\mathbf{k}})^\dagger=b^\dagger_{\mathbf{k}}-\alpha^*_{\mathbf{k}} , \tag{3.17}$$

where $\alpha_{\mathbf{k}}$ is a parameter to be determined presently. It should be chosen such that, after the transformation, the Hamiltonian H_M no longer contains any linear term in $b'_{\mathbf{k}}$ or $(b'_{\mathbf{k}})^\dagger$. The choice is

$$\alpha_{\mathbf{k}}=\tfrac{1}{2}(S/2N)^{1/2}(J_{\mathbf{k}}/\hbar\omega_k)\exp(u_{\mathbf{k}}) . \tag{3.18}$$

As $J_{\mathbf{k}}$, $\omega_{\mathbf{k}}$, and $u_{\mathbf{k}}$ are all real, the parameter $\alpha_{\mathbf{k}}$ is real also. It is noted that the transformation in (3.17) preserves the boson commutation relations and hence is unitary. The transformed H_M is

$$H_M=-\tfrac{1}{2}NZIS(S+1)+\sum_{\mathbf{k}}[(b'_{\mathbf{k}})^\dagger b'_{\mathbf{k}}+\tfrac{1}{2}]\hbar\omega_{\mathbf{k}} - \sum_{\mathbf{k}}\alpha^2_{\mathbf{k}}\hbar\omega_{\mathbf{k}} . \tag{3.19}$$

As $(b'_{\mathbf{k}})^\dagger$ and $b'_{\mathbf{k}}$ are boson creation and annihilation operators, the eigenvalues of $(b'_{\mathbf{k}})^\dagger b'_{\mathbf{k}}$ are integers $n'_{\mathbf{k}}$. The ground state then is characterized by $n'_{\mathbf{k}}=0$ for any mode $\mathbf{k}$. Comparing the new ground state with the zero-magnon state of H_L in (3.12), we see that the energy is lowered by an amount equal to $\sum_{\mathbf{k}}\alpha^2_{\mathbf{k}}\hbar\omega_{\mathbf{k}}$ due to the impurity-lattice exchange interaction. The magnon part of the new ground-state wave function can be constructed from a product of new zero-point normal mode solutions as

$$|G'\rangle=\prod_{\mathbf{k}}|n'_{\mathbf{k}}=0\rangle , \tag{3.20}$$

where $|n'_{\mathbf{k}}=0\rangle$ satisfies

$$b'_{\mathbf{k}}|n'_{\mathbf{k}}=0\rangle=0 . \tag{3.21}$$

It is easily verified that the following state satisfies (3.21) to first order of $\alpha_{\mathbf{k}}$:

$$|n'_{\mathbf{k}}=0\rangle=|n_{\mathbf{k}}=0\rangle+\alpha_{\mathbf{k}}|n_{\mathbf{k}}=1\rangle . \tag{3.22}$$

The unprimed states on the right-hand side of the above equation are the magnon states of H_L in (3.12). It is seen that the new ground state $|G'\rangle$ contains one-magnon excitations.

IV. BINDING ENERGY OF THE BMP

Let us now consider the orbital motion of the impurity electron. Using the effective-mass approximation[15] and assuming a potential due to a singly charged impurity center, we write the impurity electron Hamiltonian as

$$H_B=\frac{P^2}{2m^*}-\frac{e^2}{\epsilon r}-E_m , \tag{4.1}$$

with

$$E_m=\sum_{\mathbf{k}}\alpha^2_{\mathbf{k}}\hbar\omega_{\mathbf{k}} ,$$

where m^* is the effective mass for the conduction-band edge assumed to be nondegenerate and isotropic, and ϵ is the dielectric constant of the semiconductor host. The last term in (4.1) represents the lowering of the electron's energy due to its magnetic interaction with the localized lattice spins as derived in (3.19). The magnetic term E_m should have a bearing on the impurity electron orbit because the exchange coupling constant $J_{\mathbf{k}}$ (contained in $\alpha_{\mathbf{k}}$) depends on the impurity orbital wave function, as can be seen explicitly from (3.16) and (3.2).

We evaluate the ground-state energy of H_B by a variational procedure. We take as our trial impurity wave function the hydrogenic orbital

$$\phi=(\pi a_0^3)^{-1/2}\exp(-r/a_0) \tag{4.2}$$

with the orbital radius a_0 as the variational parameter.

We first evaluate E_m with this trial function. Let us begin by considering the exchange coupling constant J. Since the magnetic electrons are highly localized at lattice sites while the impurity electron orbit is expected to extend over many lattice points, we may approximate the exchange integral $J(R)$ in (3.2) by the following:

$$J(R)=4\pi A'\Delta\int dr\,\phi^*\phi\,\delta(r-R) , \tag{4.3}$$

where Δ is the volume of the unit cell. Then

$$J(R)=4A'\Delta a_0^{-3}\exp(-2R/a_0) . \tag{4.4}$$

In order to obtain an explicit form for $J_{\mathbf{k}}$ defined in (3.16), we assume a simple-cubic lattice with lattice constant R_0 and perform the required summation over such a lattice. This is done in the Appendix. Using (A3), we obtain an approximate $J_{\mathbf{k}}$ as follows:

$$J_{\mathbf{k}}=32A'(R_0/a_0)^3\frac{1-\exp(-2R_0/a_0)\cos(k_zR_0)}{1+\exp(-4R_0/a_0)-2\exp(-2R_0/a_0)\cos(k_zR_0)} \times\frac{1-\exp(-2R_0/a_0)\cos(k_xR_0)}{1+\exp(-4R_0/a_0)-2\exp(-2R_0/a_0)\cos(k_xR_0)}\,\frac{1-\exp(-2R_0/a)\cos(k_yR_0)}{1+\exp(-4R_0/a_0)-2\exp(-2R_0/a_0)\cos(k_yR_0)} . \tag{4.5}$$

For the sake of simplicity, we further neglect the $\mathbf{k}$ dependence of $J_{\mathbf{k}}$ and replace it by its value at $k=0$ given below:

$$J_0 = A(R_0/a_0)^3[1-\exp(-2R_0/a_0)]^{-3} \tag{4.6}$$

with $A=32A'$. Due to this approximation, $J_{\mathbf{k}}$ is overestimated for large values of $\mathbf{k}$. The a_0^{-3} dependence of J_0 which comes from the normalization of the impurity electron wave function accounts for the fact that the electron's coupling with each lattice spin should get stronger if it is distributed over a smaller region in space. On the other hand, a smaller orbit encloses a smaller number of lattice points, and hence J_0, which is equal to $\sum_i J(R_i)$, should decrease accordingly. This effect is contained in the remaining a_0-dependent factor in (4.6). It is noted that the two factors mentioned above compensate each other to a large extent so that J_0 is a slowly decreasing function of a_0. When $a_0 \gg R_0$, J_0 becomes essentially independent of a_0.

We are now ready to evaluate E_m according to (4.1). Since the allowed spin-wave modes characterized by wave vectors $\mathbf{k}$ are densely distributed over the first Brillouin zone (BZ), we may replace the summation over $\mathbf{k}$ by an integral:

$$\sum_{\mathbf{k}} \rightarrow \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k$$

with V denoting the volume of the crystal. Then, using (4.1), (3.18) and (3.13), we have

$$E_m = \frac{VJ_0^2}{8(2\pi)^3 NZI}\int_{\mathrm{BZ}} d^3k \exp(2u_{\mathbf{k}})(1-\gamma_{\mathbf{k}}^2/Z^2)^{-1/2} .$$

From (3.11) we have

$$2u_{\mathbf{k}} = -\tanh^{-1}(\gamma_{\mathbf{k}}/Z) .$$

The integrand above may be simplified based on the following formula:

$$\tanh^{-1}x = \tfrac{1}{2}\ln\left(\frac{1+x}{1-x}\right) .$$

Finally, we have

$$E_m = \frac{VJ_0^2}{8(2\pi)^3 NZI}\int_{\mathrm{BZ}} d^3k(1+\gamma_{\mathbf{k}}/Z)^{-1} . \tag{4.7}$$

To proceed further we assume again a simple-cubic lattice. According to its definition in (3.9), $\gamma_{\mathbf{k}}$ in this case is explicitly

$$\gamma_{\mathbf{k}} = 2[\cos(k_x R_0)+\cos(k_y R_0)+\cos(k_z R_0)] .$$

For a simple-cubic lattice $Z=6$, and the integral in (4.7) becomes

$$\int_{\mathrm{BZ}} d^3k(1+\gamma_{\mathbf{k}}/Z)^{-1} = \eta(2\pi/R_0)^3 \tag{4.8}$$

with

$$\eta = (2\pi)^{-3}\int_{-\pi}^{\pi}dx\int_{-\pi}^{\pi}dy\int_{-\pi}^{\pi}dz[1+\tfrac{1}{3}(\cos x+\cos y+\cos z)]^{-1} .$$

The above multiple integral can be found in a mathematical table.[16] It is evaluated to be $\eta=1.5$. The magnetic energy is given then as follows:

$$E_m = \frac{\eta J_0^2}{8ZI} . \tag{4.9}$$

Let us analyze the result in (4.9) a little further. Certain qualitative features of (4.9) may be predicted by simple arguments. As discussed in Sec. II, the cosine of the angle between the lattice spin and the impurity spin is proportional to $J(R)/I$. Therefore, the magnetic energy which is equal to the scalar product of the lattice spin and the exchange field of the impurity should be proportional to $[J(R)]^2/I$ and indeed E_m in (4.9) contains a factor J_0^2/I. However, simple arguments would predict a total magnetic energy proportional to $n[J(R)]^2/I$, where n is the total number of lattice points in the vicinity of the impurity. As J_0 itself is proportional to n, the energy E_m in (4.9) is actually proportional to n^2. Although the magnetic energy E_m as given in (4.9) has been overestimated due to our replacement of all $J_{\mathbf{k}}$'s by J_0, the extra power in n accounts for the extra energy gained due to correlation among lattice spins not contained in an independent-particle model. Another point which one should emphasize is that (4.9) is not valid in the strong-coupling limit where $J(R)>I$. In this case, the impurity-lattice exchange may be strong enough to align all lattice spins in the vicinity of the impurity. Beyond this saturation point, further increase in $J(R)$ should not cause any corresponding increase in the magnetic energy so long as the impurity orbit stays the same. Equation (4.9), which is the result of a linear theory, obviously does not contain such a saturation point.

After obtaining the magnetic energy, we come to consider the kinetic- and the potential-energy term in the Hamiltonian in (4.1). Their expectation values with respect to the trial wave function in (4.2) can be trivially evaluated. The results are given in the following:

$$\langle\phi\,|\,-\frac{\hbar^2}{2m^*}\nabla^2\,|\,\phi\rangle = \frac{\hbar^2}{2m^*a_0^2} ,$$

$$\langle\phi\,|\,\frac{e^2}{\epsilon r}\,|\,\phi\rangle = \frac{e^2}{\epsilon a_0} .$$

Now the orbital radius a_0 must be chosen to minimize the energy of the BMP given by

$$\langle\phi\,|\,H_B\,|\,\phi\rangle = \frac{\hbar^2}{2m^*a_0^2} - \frac{e^2}{\epsilon a_0} - \frac{\eta A^2}{8ZI}(R_0/a_0)^6[1-\exp(-2R_0/a_0)]^{-6} . \tag{4.10}$$

If the magnetic energy is small as compared with the kinetic or potential energy, the orbital radius should not be too different from the effective Bohr radius $a_B=\epsilon\hbar^2/m^*e^2$. Based on this assumption we can solve for a_0 which minimizes the energy expectation value in (4.10). The result accurate to first order in the magnetic energy is given below:

$$a_0=(1-f)a_B$$

with

$$f=\frac{3\eta A^2 m^* R_0^6}{4ZI\hbar^2 a_B^4}[1-\exp(-2R_0/a_B)]^{-6} \times\left[1-\frac{2R_0\exp(-2R_0/a_B)}{a_B[1-\exp(-2R_0/a_B)]}\right] . \quad (4.11)$$

The shrinking of the BMP orbit may be interpreted as being equivalent to its mass renormalization. Due to the magnetic interaction, the mass of the BMP increases from the conduction-band-edge effective mass m^* to a value $m_{\rm BMP}$ given by

$$m_{\rm BMP}=(1+f)m^* . \quad (4.12)$$

Correspondingly, the binding energy of the BMP increases from one effective Ryderberg by the same fraction:

$$E_{\rm BMP}=(1+f)\frac{e^2}{2\epsilon a_B} . \quad (4.13)$$

V. SPIN CLOUD CARRIED BY THE BMP

As discussed in the classical model in Sec. II, the BMP carries with it a cloud of lattice spins in the transverse direction. The total spin associated with the impurity electron may be determined by calculating the following matrix element:

$$S_{\rm BMP}=\langle G'|\sum_i S_{ix}|G'\rangle , \quad (5.1)$$

where G' is the ground state given in (3.20), and the summation is over all lattice points. From (3.4) we have

$$S_{ix}=\tfrac{1}{2}(S_i^+ +S_i^-) .$$

The S_i^+ and S_i^- operators, in turn, may be expressed in terms of magnon operators $b_{\mathbf{k}}^\dagger$ and $b_{\mathbf{k}}$. Using (3.5), (3.7), and (3.10), we have

$$S_{ix}=(S/2N)^{1/2}\sum_{\mathbf{k}}\exp(u_{\mathbf{k}})(e^{-i\mathbf{k}\cdot\mathbf{R}_i}b_{\mathbf{k}}^\dagger+e^{i\mathbf{k}\cdot\mathbf{R}_i}b_{\mathbf{k}}) . \quad (5.2)$$

We substitute (5.2) into (5.1) and perform the lattice sum first. Only the $k=0$ mode is projected out because of the well-known result in the following:

$$\sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i}=N\delta_{\mathbf{k},0} .$$

We have then

$$S_{\rm BMP}=(NS/2)^{1/2}\exp(u_0)\langle G'|(b_0^\dagger+b_0)|G'\rangle . \quad (5.3)$$

From (3.20), (3.18), and (3.22) we obtain immediately,

$$S_{\rm BMP}=\frac{J_0}{2ZI}\exp(2u_0)[1-(\gamma_0/Z)^2]^{-1/2} .$$

Following the same procedure for obtaining the integrand in (4.7), we can simplify the above and obtain

$$S_{\rm BMP}=\frac{J_0}{2ZI}(1+\gamma_0/Z)^{-1} . \quad (5.4)$$

For a simple-cubic lattice, $\gamma_0/Z=1$, and

$$S_{\rm BMP}=\frac{J_0}{4ZI} .$$

This is indeed an obvious result. We will not comment on it any further, except to remind the reader that the result does not hold if the lattice spins in the vicinity of the impurity are saturated.

VI. CONCLUDING REMARKS

In this paper we have formulated a theory of BMP at $T=0$ in antiferromagnetic semiconductors. On the experimental side, evidence for the magnetic effect due to charge carriers exists in antiferromagnetic substances. For example, large ferromagnetic spin clusters have been detected in antiferromagnetic EuTe,[17] which were attributed to the magnetic polaron effect. We do not attempt here to make a quantitative comparison of our theory with these measurements. The reason is that while our theory is valid only in the weak-coupling limit, in reality the impurity-lattice exchange is often stronger than the interatomic exchange which is usually due to an indirect mechanism.[18] Quantitative interpretation of experimental data in EuTe has been made by Mauger and Mills[11,19] based on their semiclassical theory valid for the entire range of impurity-lattice coupling strength. The observed ferromagnetic cluster was attributed by them to the formation of BMP consisting of a saturated ferromagnetic core surrounded by a large halo of enhanced but not saturated lattice spins.

After considering the weak-coupling case, we may speculate a little about the behavior of the charge carrier in the strong-coupling limit where all lattice spins in the vicinity of the impurity are saturated and the magnetic energy is larger than the kinetic and the Coulomb potential energy. When the lattice spins are already saturated, the impurity electron could gain more magnetic energy only be expanding its orbit to enclose more saturated lattice spins within it. Thus, quite opposite to the weak-coupling case, the impurity electron now tends to delocalize instead of having its binding strengthened. Then, a question arises as to whether a delocalized electron can be self-trapped in a potential well produced by the magnetic interaction. This point has been included in the recent study of Mauger and Mills[19] and in earlier works by other authors.[4,20] According to Ref. 19, in the weak-coupling limit, ferrons (i.e., self-trapped polarons) do not exist, at least not in a three-dimensional system. In the strong-coupling limit, all authors concluded that the stability of ferrons depends on the actual values of material parameters involved. Considering EuTe specifically, Mauger and Mills predicted no ferrons, in agreement with Umehara[20] but in contradiction with Kasuya.[4] It should be interesting to investigate the problem quantum mechanically.

APPENDIX: EVALUATION OF $J_{\mathbf{k}}$

To get an explicit $J_{\mathbf{k}}$ defined in (3.16), we perform the sum on a simple-cubic lattice of lattice constant R_0. When the direct-space $J(R)$ is of the form given in (4.4), the lattice sum involved is as follows:

$$S_{\text{lattice}}=\sum_{n_1,n_2,n_3}\exp(-2nR_0/a_0)\exp[i(n_1k_x+n_2k_y+n_3k_z)R_0]\ , \tag{A1}$$

where

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

with integers n_1,n_2,n_3, each running from $-(N_1/2)$ to $(N_1/2)$. (Here we assume that the total number of lattice points is equal to N_1^3.) We further approximate the number n by a positive integer:

$$n\rightarrow|n_1|+|n_2|+|n_3|\ .$$

Then the sum in (A1) can be factored into the product of three similar sums. Each one is like

$$S_1=\sum_{n_1=-N_1/2}^{N_1/2}\exp(-2|n_1|R_0/a_0+in_1k_xR_0)\ . \tag{A2}$$

This is a simple geometric series which can be easily summed. As N_1 is a very large number and as each term in the series carries an exponential damping factor, the sum S_1 becomes independent of N_1 and is equal to

$$S_1=\frac{2[1-\exp(-2R_0/a_0)\cos(k_xR_0)]}{1+\exp(-4R_0/a_0)-2\exp(-2R_0/a_0)\cos(k_xR_0)}\ . \tag{A3}$$

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