Spin structure of impurity band in semiconductors in two- and three-dimensional cases

I. V. Ponomarev* and V. V. Flambaum

School of Physics, The University of New South Wales, Sydney 2052, Australia

A. L. Efros

Department of Physics, University of Utah, Salt Lake City, Utah 84112

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The exchange interaction between electrons located at different randomly distributed impurities is studied for small density of impurities. The singlet-triplet splitting $2J(R)$ is calculated for two Coulomb centers at a distance R. Interpolated formulas are found which work for all distances R from zero to infinity. The data from atomic physics are used for the interpolation in the three-dimensional case. For the two-dimensional case the original calculations are performed to find asymptotic behavior of the splitting at large R, the splitting for the ''two-dimensional helium atom'' ($R=0$), and the splitting at $R=a_B$, where a_B is the effective Bohr radius. The spin structure of the impurity band is described by the Heisenberg Hamiltonian. The ground state of a system consists of localized singlets. The new results are obtained for the distribution of the singlet pairs in the ground state. These results are exact at low density. The problem is reduced to a nontrivial geometric problem, which is solved in the mean-field approximation and by computer modeling. The density of free electrons is found as a function of temperature and the distribution function of the singlet-triplet transitions energies is calculated. Both functions are given in an analytical form. [S0163-1829(99)13631-2]

I. INTRODUCTION

The structure of the impurity band of semiconductors has been widely studied during the past two decades both theoretically and experimentally (see Ref. 1). In the early theoretical studies the spin structure of the impurity band was completely ignored. Recent experiments suggest that the spin structure is very important for the variable range hopping conductivity, especially near the metal-nonmetal transition.[2–7]

The exchange interaction must be the main mechanism of the spin-spin interaction in the impurity band. It appears as a result of the overlap of the wave functions of different states. The scale of this interaction decreases exponentially with increasing distance between the states. Thus, this interaction becomes the most important one near the metal-nonmetal transition. In this region the scale of the interaction is of the order of the binding energy of a single impurity.

In this paper we study the spin structure of the impurity band created by Coulomb impurities in both two- and three-dimensional cases in the limit of low density of impurities. In the two-dimensional case the impurities may be located either outside or inside the plane of electron gas. We assume that all impurities are occupied by one electron. In this case we can consider the coordinates of the occupied centers as random variables without any correlations.

Our study of the spin structure is based upon the Heisenberg Hamiltonian, which takes into account the spin-spin interaction of the electrons localized at different randomly distributed impurities,

$$H = \sum_{i \neq k} J_{ik}(I/2 + \mathbf{s_i} \cdot \mathbf{s_k}), \tag{1}$$

where $\mathbf{s}$ is a spin-$\frac{1}{2}$ operator, I is a unit matrix, and i,k denote different impurity atoms. The sum is over all pairs of impu-

rities. The density of impurities is assumed to be small.

This problem has a long story.[8–15] The following important results have been obtained.

(i) The ground state of the system consists of local singlets.

(ii) Rosso,[8] Thomas and Rosso,[13] and Andres *et al.*[11] used different self-consistent approaches to get the distribution of the excitation energies of the singlet-triplet transitions.

(iii) Bhatt and Lee[12,10] worked out a computational scaling approach which is exact at small density of impurities. They have also mentioned a drastic difference between the Heisenberg and Ising models.

(iv) As far as we know, all previous authors used simplified versions for the function $J(R)$.

Our paper pursues the following goals.

(i) We analyze the existing methods to find the distribution of excitation energies and propose a new modification for the one-, two- and three-dimensional cases. Our approach is exact at low densities and it allows us to get an approximate analytical expression for this distribution.

(ii) To get an estimate for the energy of spin ordering, one needs a reliable calculation of the coefficients J_{ik}, which are defined here as $\frac{1}{2}$ of the singlet-triplet splitting for the two states corresponding to the impurities i and k. We have performed these calculations for a pair of the Coulomb centers at a distance R_{ik}. The result of the computations is a function $J(R)$ which is reliable at all distances from zero to infinity.

The paper is organized as follows. In Sec. II we consider Hamiltonian Eq. (1) in the case of small impurity density. We show that the ground state mostly consists of independent singlets. We show that the problem of finding these singlets can be reduced to a nontrivial geometric problem. We solve it in a mean-field approximation and by computer modeling. The solution of this problem gives the distribution

function $F(E)$ for the energies of the singlet-triplet transitions for a given function $J(R)$.

In Sec. III we calculate $J(R)$ and its inverse function $R(J)$. For the 3D case we present interpolated formulas which are based upon the results of well-known calculations for two hydrogen atoms. These calculations include analytical results for large distances,[18] numerical calculations at intermediate distances, and known results for the singlet-triplet splitting of the He atom. Similar interpolated formulas are presented for the 2D case. They are based upon our original calculations given in the Appendixes. We present an analytical expression for $J(R)$ at large distances, a numerical result for $J(a_B)$, and variational calculations for a ''two-dimensional He atom.''

In the Conclusion we discuss the distribution function of singlet-triplet splittings $F(\ln \varepsilon)$, where $\varepsilon = J/J(0)$, and the density of free spins $\rho(T)$ at finite temperature T. These two functions are the final results of our paper.

II. GROUND STATE AND EXCITED STATES OF THE HEISENBERG HAMILTONIAN IN THE IMPURITY BAND

A. The structure of the ground state

We find the ground state and excited states of the Hamiltonian Eq. (1) using the following properties of J_{ik}.

(i) All $J_{ik} > 0$, which means an antiferromagnetic interaction.

(ii) The density of impurities n is assumed to be small, so that the average distance between them is larger than the characteristic length of the exponential decay of J_{ik}. This means there is a very large dispersion of J_{ik}. In fact, we shall assume that if $J_{ik} > J_{lm}$, then $J_{ik} \gg J_{lm}$. Thus, we ignore the cases when the distance R_{ik} is very close to the distance R_{lm}, assuming that these two pairs are not very far from each other.

To understand the physics of the problem it is very helpful to consider the Hamiltonian (1) with four impurities only [Fig. 1(a)]. From a general principle one can conclude[16] that the energy spectrum consists of six levels, one level with spin $S=2$, three levels with $S=1$, and two levels with $S=0$. Let us assume that J_{12} is much larger than all other J_{ik} in this problem. Then the ground-state wave function describes two singlets at sites (1,2) and (3,4). It is easy to write the energy of the ground state and the first excited state assuming

$$J' = {\sum}' \, J_{ik} \ll J_{12}, \qquad (2)$$

where the sum includes all J_{ik} except J_{12} and J_{34}. The ground-state energy E_0 and the energy of the first excited state E_1 are given by the equations

$$E_0 = -J_{12} - J_{34} + J'/2; \quad E_1 = -J_{12} + J_{34} + J'/2. \qquad (3)$$

The physical meaning of Eq. (3) is simple. Two singlets (1,2) and (3,4) do not interact with each other if condition (2) is fulfilled. The $J'/2$ terms come from the first term in the Hamiltonian (1).

In this approximation the excitation energy is $E = 2J_{34}$. The ground state has a total spin $S=0$ while the first excited state has $S=1$.
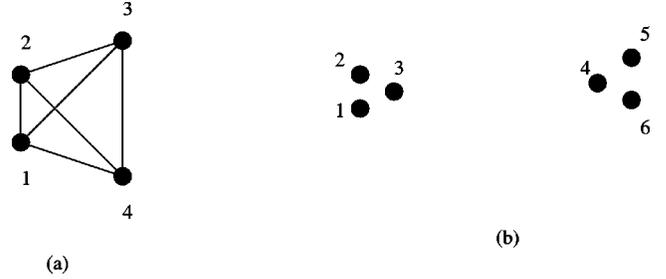
FIG. 1. Different configurations of four (a) and six (b) spins.

Bhatt and Lee[12,10] take into account the next approximation for the excitation energy,

$$E = 2J_{34} + (J_{13} - J_{23})(J_{24} - J_{14})/J_{12}. \qquad (4)$$

Since J_{12} is the largest term, the second term should be small. It looks like it can change the ground state from singlet to triplet if J_{34} is unusually small. However, such configurations are extremely rare. It happens because in the case of small J_{34} one should consider Fig. 1(b) with six spins rather than Fig. 1(a). Indeed, very small J_{34} means a long distance between impurities 3 and 4. It is more likely that in this situation some other strong singlet (5,6) is the nearest neighbor of the impurity 4 rather than the singlet (1,2).

In this six-spin system we have two strongly connected groups of spins, namely 1,2,3 and 4,5,6. Assume that J_{12} and J_{56} provide the strongest bonds in each group. Suppose there is no interaction between the groups. Then, the ground state in each of them is a degenerate doublet. Altogether the system is fourfold degenerate. If one takes into account J_{34}, the degeneracy of the ground state will be lifted. One gets a singlet and a triplet with the energy splitting $2J_{34}$. On the other hand, the general six-spin problem can be solved assuming that both J_{12} and J_{56} are infinite. In this approximation one gets the same result: the ground state is a singlet and the excitation energy $E = 2J_{34}$. It follows that the other bonds connecting the two groups, like J_{35}, may contribute to the excitation energy only in the second order of perturbation theory. This contribution will contain a small dimensionless coefficient like J_{35}/J_{12} and it may be neglected. Thus, it is not necessary to take into account the renormalization of the weak bonds due to their strong neighbors in the limit of small density. Bhatt and Lee also mention[10] that their computations show the triplet ground state in very rare cases.

Thus, we assume that the ground-state energy of any even number of impurities has $S=0$ and the system can be split into localized singlets. To find the pairs of impurities which form the singlet in the ground state, we propose the following geometric problem.

(i) For every impurity in the system, find its nearest neighbor.

(ii) Take the pair with the smallest distance. Generally, the nearest neighbor of a site A does not have site A as its nearest neighbor. But for the closest pair this is the case.

(iii) This closest pair forms a singlet with the largest binding energy. To find all other singlets remove both sites of the first pair. Go to point 1 and continue until all the singlets will be found.

The same geometric problem has been proposed by Thomas and Rosso[13] for the three-dimensional case.

Assuming that all neighboring J_{ik} are very different, one can write the total energy of the lowest state in the form

$$E_0 = -\sum_s J_{ik} + \frac{1}{2} \sum_{other} J_{ik}, \qquad (5)$$

where the first sum includes all pairs which form singlets and the second one includes all other pairs.

One can prove that the distribution of singlets, obtained as a solution of the problem above, gives the minimum of total energy. Suppose, for example, that the solution prescribes the configuration of singlets (1,2), (3,4), and (5,6), for impurities with numbers from 1 to 6. One can show that any other location of singlets at the same impurities, like (1,3), (2,5), and (4,6), has larger energy.

We mention first that the contribution to the energy from all other impurities like 7,8 . . . is the same at all configurations of singlets of six chosen impurities. Suppose now that $J_{12} \gg J_{34}, J_{56}$. Then all other J_{ik} connecting the six impurities are also less than J_{12}. Indeed, if one of them were larger, it would be used to form a singlet instead of J_{12}. Thus, any rearrangement of the pairs within six impurities that destroys singlet (1,2) increases the total energy. In the same way one can show that rearrangement of singlets in the system of four impurities 3,4,5,6 also increases the total energy. The same consideration can be done for any even number of impurities. Thus, the solution of the above geometric problem gives the ground state of the system.

B. Solution of geometric problem and distribution function of excitation energies

We start with the simplest mean-field approximation. Suppose we are at the stage where all pairs with distance less than R are removed and we want to find the residual impurity density $n(R)$. The crucial point of the mean-field approximation is that we neglect correlations in the positions of the remaining impurities except that they cannot be closer to one another than R.

We start with the two-dimensional case. Let us draw a circle around each impurity with the radius R. There will be no other impurities inside the circles. Now increase the radii from R to $R+dR$ and calculate how many impurities occur in the rings between R and $R+dR$. The total number of these impurities gives the decrease of $N(R)$, where $N(R) = Sn(R)$ and S is the total area of the system. Thus, one gets the equation

$$dN(R) = -N(R)2\pi R\tilde{n}(R)dR. \qquad (6)$$

Here $\tilde{n}(R)$ is the density of the impurities outside the circles. It is slightly larger than $n(R)$ (see below), but in the simplest mean-field approximation we ignore this difference.

It is convenient to introduce the dimensionless coordinate $X = \sqrt{\pi n_0}R$ and the normalized number of particles (or density) $\rho(X) = n/n_0 \equiv N/N_0$. Here $n_0 = n(0)$ is the initial concentration of particles. The differential equation for $\rho(X)$ at $\tilde{n} = n$ has the form

$$d\rho = -2X\rho^2 dX. \qquad (7)$$

The solution of this equation with the condition $\rho(0) = 1$ is

$$\rho_2(X) = \frac{1}{1+X^2}, \qquad (8)$$

where $\rho_2(X)$ is the two-dimensional density. Similar calculations for the three- and one-dimensional cases give

$$\rho_d(X) = \frac{1}{1+X^d}. \qquad (9)$$

Here $X = (4\pi/3n_0)^{1/3}R$ at $d=3$ and $X = 2n_0R$ at $d=1$. This distribution has been obtained by Rosso[8] for $d=3$. One can show that at small X the above results are exact, including X^d corrections. Bhatt[9] has pointed out that it is not exact at large X. We believe that the exact distribution has the following form at large X:

$$\rho_d(X) = \frac{1}{b_d X^d}, \qquad (10)$$

where the coefficient $b_d \neq 1$ and it depends on the dimensionality of space d. It follows from Eq. (10) that the average density $n(R)$ is independent of n_0 at large values of R and it is of the order of R^{-d}. This is because the average distance between impurities cannot be smaller than R by definition, and there are no reasons for it to be substantially larger than R. That is why we believe that Eq. (10) is exact at large X. Our computer modeling confirms this point and it gives us the values b_d.

We propose an improved mean-field approach which takes into account the fact that the density $\tilde{n}$ outside the circles is slightly larger than the average density $n(R)$, because there are no impurities inside the circles. For example, at $d=2$, one gets

$$\tilde{n} = \frac{N}{S - N\pi R^2 \alpha}, \qquad (11)$$

where $N\pi R^2 \alpha$ is the excluded area inside N circles. We have introduced a free parameter $\alpha < 1$, which takes into account the overlap of the circles. Its value can be extracted from comparison with numerical computations.

Equation (11) can be generalized for any d to get a differential equation in ρ_d,

$$\frac{d\rho_d}{dX^d} = -\frac{\rho_d^2}{1 - \alpha_d \rho_d X^d}. \qquad (12)$$

The solution is given by the following transcendental equation:

$$X^d = \frac{1 - \rho_d^{b_d}}{b_d \rho_d} \qquad (13)$$

with $b_d = \alpha_d + 1$. It is worth mentioning that if we would neglect the ''circles'' overlapping ($b_d \equiv 2$), then the solution of Eq. (13) is

$$\rho_d(X) = \frac{1}{X^d + \sqrt{1 + X^{2d}}}, \qquad (14)$$
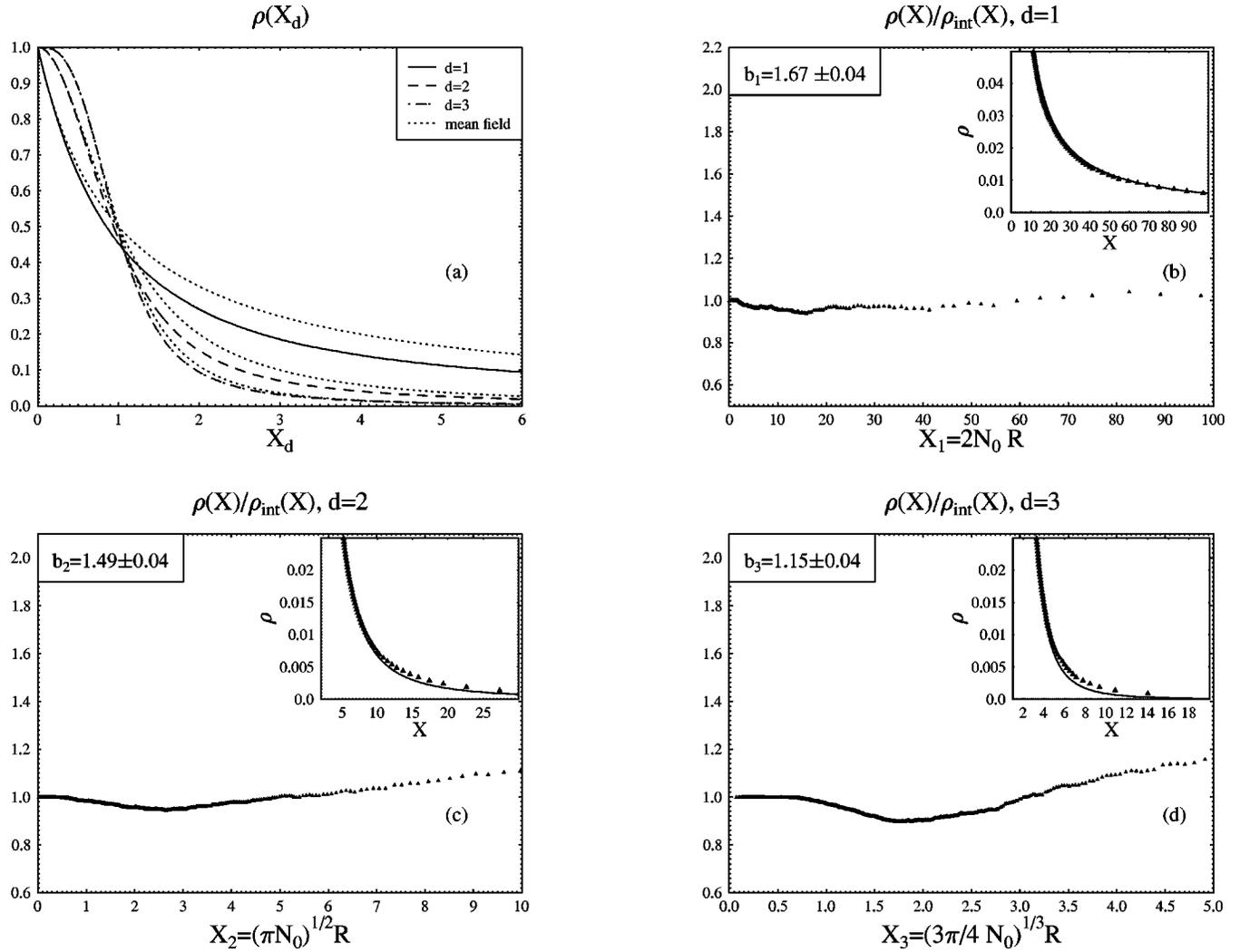
FIG. 2. Residual density of impurities as a function of X. (a) shows the results of numerical computations for $d=1,2,3$ and the result of a simple mean-field approximation Eq. (9). (b)–(d) displays the ratio of ρ_d as obtained by numerical computations to ρ_d found using the interpolated formula Eq. (16) for $d=1-3$. The insets show the asymptotic behavior of the numerical data (triangles) and the interpolated formula (solid line).

which is an underestimate for large distances. In the general case, for $1<b_d<2$, the analytical solution of the transcendental equation (13) can be obtained only for large and small values of X,

$$\rho_d \approx \begin{cases} 1 - X^d + \dfrac{3-b_d}{2}X^{2d} + \cdots, & X \ll 1, \\[2mm] \dfrac{1}{b_d X^d}\left(1 - \left(\dfrac{1}{b_d X^d}\right)^{b_d} + \cdots\right), & X \gg 1. \end{cases} \tag{15}$$

We performed computer simulations of this problem for the one-, two-, and three-dimensional cases. The results are shown in Fig. 2(a) together with the simple mean-field approximation of Eq. (9). We found that fitting our numerical data using Eq. (13) shows excellent agreement if we choose $b_1=1.67$, $b_2=1.49$, $b_3=1.15$. It would be natural to think that the simple mean-field approach with $\alpha=0$ becomes exact for large values of d.

Unfortunately, Eq. (13) does not have an analytical solution for all X and so it is not convenient for our purpose. We found that the simple interpolated formula

$$\rho_d(X) = \frac{1}{X^d + \sqrt{1 + (b_d-1)^2 X^{2d}}}, \tag{16}$$

which resembles Eq. (14), describes the residual density well for the whole range of distances. The comparison of this formula with the results of computer modeling is shown in Figs. 2(b)–2(d) for $d=1,2,3$. Below we use only Eq. (16) with the values of b_d obtained above.

III. CALCULATION OF $J(R)$

A. Three-dimensional case

The spin-spin interaction constant is the splitting energy between the ground states for total spin $S=1$ and $S=0$,

$$2J = E_g^{S=1} - E_g^{S=0} \equiv {}^3\Sigma_u^+ - {}^1\Sigma_g^+,$$

for the hydrogenlike molecule, where nuclei are represented by two impurities. Hereafter, we use effective atomic units (a.u.) which means that all distances are measured in units of the effective Bohr radius $a_B = \hbar^2 \epsilon / m^* e^2$, and energies in

units of $m^*e^4/\hbar^2\epsilon^2$, where m^* is the effective carrier mass and ϵ is the dielectric constant.

We propose a simple interpolated formula for the exchange constant based on the most accurate numerical calculations of the hydrogen molecule[17] and the following asymptotic expression[18] for large R:

$$2J(R) \approx 1.636 R^{5/2} \exp(-2R). \qquad (17)$$

We found $J(0)$ from the data for the singlet-triplet splitting of the helium atom,[21]

$$2J(0) = 0.770 \text{ a.u.}$$

The numerical data[17] show that the behavior of the logarithm of the exchange constant for small R is well described by a second-order polynomial.

To obtain the interpolated formula we match the second derivative of $\ln(J(R))$. In two regions it has the following behavior:

$$\frac{\partial^2 \ln(J)}{\partial R^2} \approx \begin{cases} -2\tilde{A}, & R \lesssim 1 \\ -\dfrac{5}{2R^2}, & R \gtrsim 1, \end{cases} \qquad (18)$$

where $\tilde{A}$ is the matching constant. The simplest formula that satisfies both conditions is

$$\frac{\partial^2 \ln(J)}{\partial R^2} = -\frac{2\tilde{A}}{1 + 4/5\tilde{A}R^2}. \qquad (19)$$

After integrating twice we obtain

$$\ln(J) = \ln(J(0)) - \gamma R - \frac{5}{2}AR \arctan(AR) + \frac{5}{4}\ln(1 + A^2 R^2), \qquad (20)$$

where A and γ are connected by equation

$$A = \sqrt{4\tilde{A}/5} = \frac{4(2-\gamma)}{5\pi}. \qquad (21)$$

This interpolated formula has one fitting parameter γ and the correct asymptotic behavior.

The parameter γ has to be chosen to match small distances in an optimal way. The least-square method gives $\gamma = 0.1$. The final equation is

$$2J_3(R) = 0.770(1 + 0.23R^2)^{5/4}$$
$$\times \exp[-0.1R - 1.210R \arctan(0.484R)]. \qquad (22)$$

For further calculations we need the inverse function $R(J)$ as well. Because of the exponential character of the exchange constant, the inverse function depends on energy logarithmically. Therefore, we performed interpolation for the function $R(x)$, where $x = \ln(J(0)/J)$. The result is

$$R_3 = \frac{x}{2} + \frac{3.5x}{1 + \dfrac{3.5x}{1.69 + 0.68\ln(1+x)}}. \qquad (23)$$
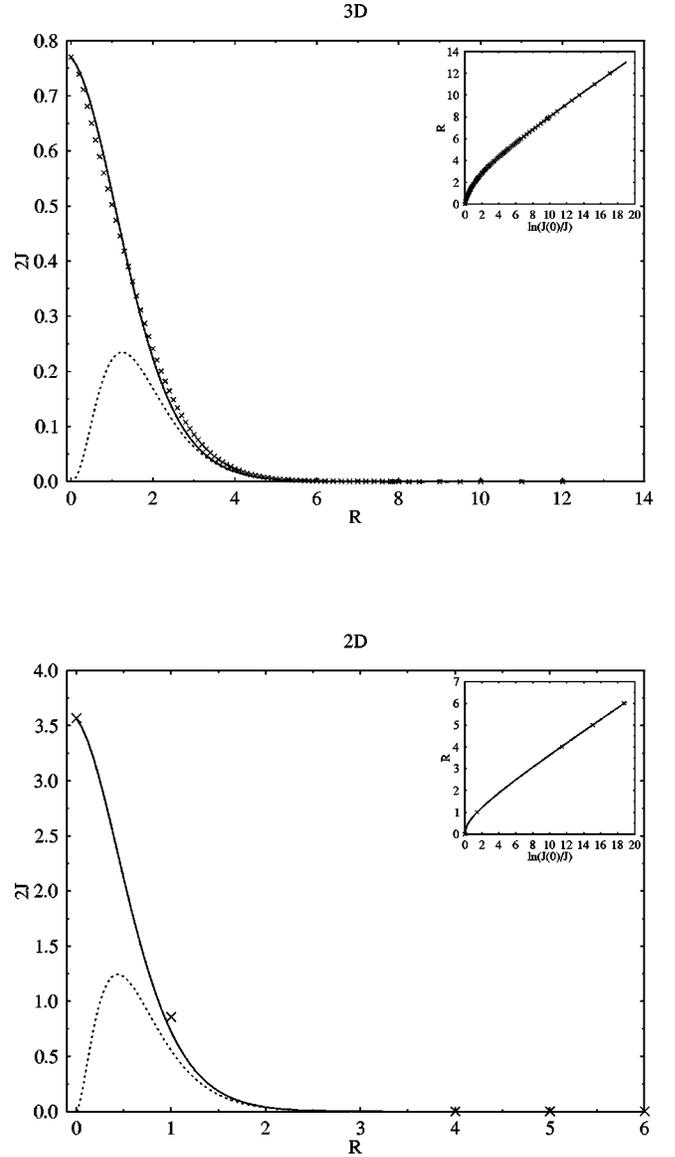
FIG. 3. Interpolated formulas (solid lines) for $J(R)$ in the three- and two-dimensional cases as given by Eqs. (22) and (27). For the 3D case the crosses show numerical results of Ref. 17. For the 2D case the crosses show our numerical results at $R=1$ and $R=0$. Dashed lines show the corresponding asymptotic formulas which are valid at large R. The solid lines in the insets show the behavior of the inverse function R vs $\ln(J(0)/J)$ as given by interpolated formulas (23) and (28). The crosses in the insets have the same meaning as in the main figures.

The interpolated curves and all available data are shown in Fig. 3(a).

B. Two-dimensional case with in-plane impurities

We are unaware of any calculations of $J(R)$ for the two-dimensional case. We have considered a general problem when the motion of the electrons is confined to a plane, but the Coulomb impurities are at distances h_1 and h_2 outside the plane. However, in this paper only the calculations for in-plane impurities ($h_1 = h_2 = 0$) are presented. The results for the general case will be published elsewhere.[22]

The case of the in-plane impurities corresponds to a 2D hydrogenlike molecule with the Hamiltonian

$$\hat{H} = -\frac{\Delta_1}{2} - \frac{\Delta_2}{2} - \sum_{j,i=1}^{2} \frac{1}{\sqrt{(x_i \pm a)^2 + y_i^2}}$$

$$+ \frac{1}{\sqrt{(x_1-x_2)^2 + (y_1-y_2)^2}} + \frac{1}{R}. \quad (24)$$

When $R \gg 1$, the singlet-triplet splitting constant is calculated by making use of the semiclassical approach[18–20] (see Appendix A). We obtained the following result:

$$2J(R) = 30.413 \, R^{7/4} \exp(-4R). \quad (25)$$

To provide the point $R=0$ we performed variational calculations for the two-dimensional helium atom. We found that (see Appendix B)

$$E(^1S) = -11.635 \ \text{a.u.},$$

$$E(^3S) = -8.193 \ \text{a.u.}, \quad (26)$$

$$2J(0) = 3.567 \, (\pm 1\%) \ \text{a.u.}$$

Finally, we performed numerical calculations based on the method described in Ref. 20 for the point $R=1$. Using the same method as in the 3D case, we get the following interpolated formulas for $J(R)$ and $R(\ln(J_0/J))$:

$$2J_2(R) = 3.567(1 + 1.81R^2)^{7/8}$$

$$\times \exp[-0.3R - 2.355R \arctan(1.346R)], \quad (27)$$

$$R_2 = \frac{x}{4} + \frac{3x}{1 + \dfrac{3x}{0.50 + 0.28\ln(1+x)}}, \quad (28)$$

$$x = \ln(J(0)/J)).$$

These results are shown in Fig. 3(b).

IV. CONCLUSION

We obtained an analytical expression (16) for the dimensionless density of impurities which form singlet pairs with a distance larger than R. We have also calculated the strength of the spin-spin interaction J and obtained analytical expressions for the function $R(J)$ for the three-dimensional (23) and the two-dimensional (28) cases. Combining Eq. (16) with Eqs. (23) or (28) one can calculate an analytical expression for the density of singlet pairs $n(E)/2$ that has a singlet-triplet energy splitting smaller than $E=2J$. At finite temperature T the pairs with $E<T$ are destroyed by a thermal motion. Therefore, at a given temperature the function $n(E)$ at $E=T$ gives the density of free spins in the system which contribute to the Curie susceptibility. Thus, we obtain an analytical expression for the density of free spins $n(T)$.

We have also calculated the distribution function of excitation energy in a logarithmic scale. It is defined as follows:

$$F(\ln(\varepsilon)) = \frac{1}{2} \frac{dn}{d\ln(\varepsilon)} \equiv \frac{n_0}{2} \frac{d\rho}{dR} \frac{dR}{d\ln(\varepsilon)}, \quad (29)$$

where $\varepsilon = E/(2J(0)) \equiv J/J(0)$.

The analytical expression for $F(\ln(\varepsilon))$ based on Eqs. (16), (23), and (28) is quite cumbersome. In the two limits of large and small energies (or small and large distances) the behavior of F in the leading order is

$$\frac{F_{2D}}{n_0} \approx \begin{cases} 10.56\pi n_0 a_B^2 \ln(1/\varepsilon), & \varepsilon \to 1 \\[2mm] \dfrac{16}{1.49\pi n_0 a_B^2} [\ln(1/\varepsilon)]^{-3}, & \varepsilon \to 0; \end{cases} \quad (30)$$

$$\frac{F_{3D}}{n_0} \approx \begin{cases} 128\pi n_0 a_B^3 [\ln(1/\varepsilon)]^2, & \varepsilon \to 1 \\[2mm] \dfrac{9}{1.15\pi n_0 a_B^3} [\ln(1/\varepsilon)]^{-4}, & \varepsilon \to 0. \end{cases} \quad (31)$$

Our results for $\rho(T) = n(T)/n_0$ are shown by the full lines in Figs. 4(a) and 4(b) for the two-dimensional and the three-dimensional cases. We choose two different dimensionless densities n_0 for each case. They are $\pi n_0 a_B^2 = 0.1$ and 0.025 for 2D and $4\pi n_0 a_B^3/3 = 0.004$ and 0.016 for 3D.

The dependence of the dimensionless distribution function F/n_0 for the two-dimensional and the three-dimensional cases for the same two donor densities n_0 is presented in Figs. 4(c) and 4(d) by the full lines.

The most important features of both functions are the long logarithmic tails in the regions of low temperature and low energy. Similar behavior has been obtained by Bhatt and Lee.[10] Note that $\rho(T)$ decreases with increasing density n_0. This is not the case for the distribution function. Larger density corresponds to larger distribution function F at large energies. This is because the derivative $n_0^{-1} dn/dR$ is larger for larger density n_0 at small R. However, the dimensionless distribution function $F(\ln\varepsilon)$ is normalized to 1/2. That is why the functions for different densities cross each other at some energy. Thus, at small energies the larger distribution function corresponds to smaller density.

To clarify the role of the functions $J(R)$, which have been found here, we have calculated the density of free spins $\rho(T)$ and the distribution function $F(\ln(\varepsilon))$ for a simplified function $J_s(R)$ used in Ref. 10,

$$J_s(R) = J(0)\exp(-2R/a_B) \ \text{for} \ 3D,$$

$$J_s(R) = J(0)\exp(-4R/a_B) \ \text{for} \ 2D. \quad (32)$$

In these calculations we used our residual density $\rho(R)$. The results are shown in Fig. 4 by the dashed lines. One can see that the difference is large. The distribution function for our more accurate form of the exchange constant became narrower and the decline in the beginning is steeper. This comes from the different behaviors at small distances.

It is interesting to compare the numerical scaling calculations by Bhatt and Lee[10] with our method of calculation $n(R)$. We have found that at the smallest density used in Ref. 10 both methods give similar results, but for larger densities there is a small deviation. We think that both methods are exact in the limit of small densities, but the method of Bhatt and Lee works in a wider range, because they take into account the renormalization of weak bonds caused by their
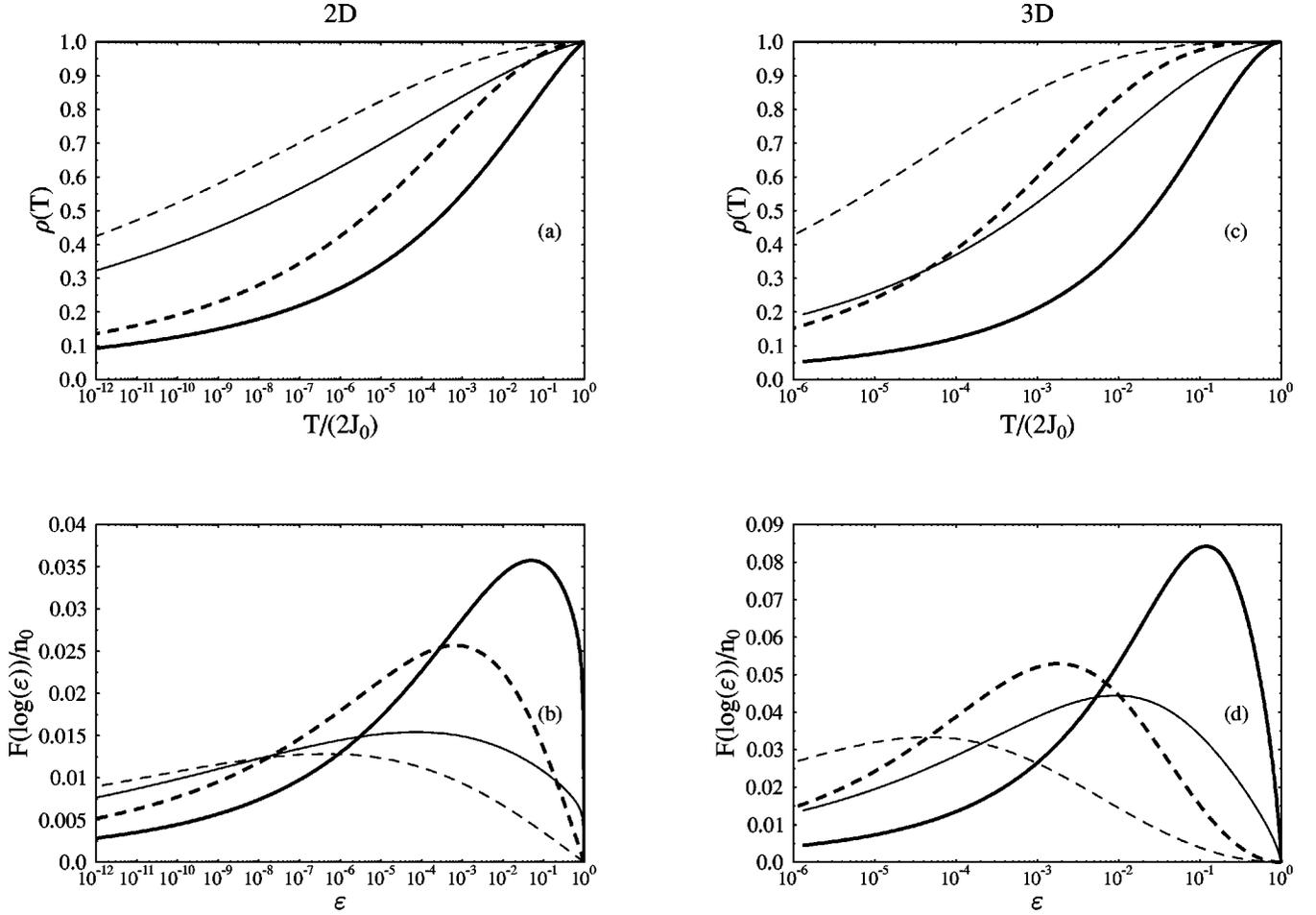
FIG. 4. Dimensionless density of free spins $\rho(T)$ as a function of logarithm of temperature and dimensionless distribution function F/n_0 of the singlet-triplet excitations as a function of logarithm of energy in the two-dimensional case (a),(b) and the three-dimensional case (c),(d). The values of dimensionless density $\pi n_0 a_B^2$ at (a) and (b) are 0.025 and 0.1. The values of dimensionless density $4\pi n_0 a_B^3/3$ at (c) and (d) are 0.004 and 0.016. The solid lines show the final results of our calculations. The dashed lines show the results obtained with the function $J(R)$ as given by Eqs. (32). In all cases larger densities are shown by thicker lines.

strong neighbors. However, the great advantage of our method is that it gives an analytical expression for $n(E)$.

APPENDIX A: EXCHANGE CONSTANT FOR THE 2D HYDROGENLIKE MOLECULE

The exchange constant for the Hamiltonian (24) is determined by

$$2J = (E_g^{S=1} - E_g^{S=0}) \equiv (E_A - E_S), \qquad (A1)$$

where

$$\hat{H}\Psi_S = E_S\Psi_S, \qquad (A2)$$

$$\hat{H}\Psi_A = E_A\Psi_A. \qquad (A3)$$

Because of the Fermi statistics, the two-electron wave function is antisymmetric with respect to permutation. Therefore, the symmetric coordinate wave function corresponds to spin $S=0$ and the antisymmetric one corresponds to $S=1$.

Let us consider the more general Hamiltonian

$$\hat{H} = -\frac{\Delta_1}{2} - \frac{\Delta_2}{2} + V_a(\mathbf{r}_1 + \mathbf{a}) + V_a(\mathbf{r}_2 + \mathbf{a})$$

$$+ V_b(\mathbf{r}_1 - \mathbf{a}) + V_b(\mathbf{r}_2 - \mathbf{a}) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + \frac{1}{R}, \quad (A4)$$

where V_a and V_b are effective potentials of interaction between the electron and the corresponding atomic residue, which is of the Coulomb type far from the atoms: $V_{a,b} \rightarrow -1/r$, $r \rightarrow \infty$. The electron energy

$$E = -\alpha^2/2 - \beta^2/2 - 1/R$$

is accurate up to terms $\sim 1/R^2$. Here $\alpha^2/2$ and $\beta^2/2$ are electron binding energies in the given "atom."

When $R \gg 1$, the most appropriate method for determination of the energy term splitting due to the spin-spin interaction is the Gor'kov-Pitaevskii method.[18–20]

Since $J(R)$ is exponentially small as $R \to \infty$, Ψ_A and Ψ_S are solutions of the same Schrödinger equation, and therefore, with exponential accuracy their combinations

$$\Psi_{1,2} = \frac{\Psi_S \pm \Psi_a}{\sqrt{2}}$$

are also the solutions of the same Schrödinger equation with the Hamiltonian (A4). They correspond to the states of "distinguishable" particles when, e.g., for $\Psi_1(\mathbf{r_1}, \mathbf{r_2})$, the first electron is principally located near the first ion at $x = -a$ and the second electron near the second ion with $x = a$. Here $R \equiv 2a$ is the distance between "nuclei," which we place at the points $\pm a$ on the x axis. In the main region of the electron distribution, the wave functions $\Psi_{1,2}$ are products of the atomic single-particle wave functions with the asymptotic behavior of the radial atomic wave functions of the electron in the Coulomb field of the atomic residue being determined by the formulas

$$\varphi_a(r) = A_\alpha r^{1/\alpha - 1/2} e^{-\alpha r}, \quad \varphi_b(r) = A_\beta r^{1/\beta - 1/2} e^{-\beta r}.$$
(A5)

Indeed, for large r the potential is $U \sim -1/r$, and the single-particle wave function of the electron obeys the equation

$$-\frac{\Delta}{2} \varphi - \frac{1}{r} \varphi = -\frac{\alpha^2}{2} \varphi.$$

It has the asymptotic solution (A5) up to φ/r^2 accuracy. The coefficients $A_{\alpha,\beta}$ are determined by the behavior of the wave functions of the electron inside the atoms.

It is possible to show[20] that

$$2J = -2 \int \left[\Psi_2 \frac{\partial \Psi_1}{\partial x_1} - \Psi_1 \frac{\partial \Psi_2}{\partial x_1} \right]_{x_1 = x_2} dx_2 \, dy_1 \, dy_2.$$
(A6)

Our main purpose is to find the wave function $\Psi_{1,2}$. Let us suppose that $\Psi_{1,2}$ has the form

$$\Psi_1(\vec{r}_1, \vec{r}_2) = \phi_\alpha(|\vec{r}_1 + \vec{a}|) \phi_\beta(|\vec{r}_2 - \vec{a}|) \chi(\vec{r}_1, \vec{r}_2),$$
(A7)

$$\Psi_2(\vec{r}_1, \vec{r}_2) = \phi_\alpha(|\vec{r}_2 + \vec{a}|) \phi_\beta(|\vec{r}_1 - \vec{a}|) \chi(\vec{r}_2, \vec{r}_1),$$

where $\phi_{\alpha,\beta}$ have the behavior of Eqs. (A5) and χ is a slowly varying function of r_1 and r_2. Substituting Ψ_1 into the wave equation and neglecting the second derivatives of χ, we obtain

$$\alpha \frac{\partial \chi}{\partial x_1} - \beta \frac{\partial \chi}{\partial x_2} + \left[\frac{1}{\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}} \right.$$
$$\left. + \frac{1}{2a} - \frac{1}{a - x_1} - \frac{1}{a + x_2} \right] \chi = 0.$$
(A8)

Equation (A8) is valid under the conditions

$$|x_{1,2}| \leq a, y_{12} \equiv |y_1 - y_2| \ll \sqrt{a},$$
(A9)

$$R\alpha, R\beta \gg 1, \quad R|\alpha - \beta| \ll 1.$$

The general solution of Eq. (A8) is

$$F(C_1(x_1, x_2), C_2(\chi, x_1, x_2, y_{12})) = 0,$$
(A10)

where C_1, C_2 are integrals of the motion of the ordinary differential equations:

$$\frac{dx_1}{\alpha} = -\frac{dx_2}{\beta} = -\frac{d\chi}{\chi} \left[\frac{1}{\sqrt{(x_1 - x_2)^2 + y_{12}^2}} \right.$$
$$\left. + \frac{1}{2a} - \frac{1}{a - x_1} - \frac{1}{a + x_2} \right]^{-1}.$$

Hence

$$\chi(x_1, x_2, y_{12})$$
$$= \frac{\exp\left(-\frac{x_1}{2a\alpha}\right) \left[\sqrt{(x_1 - x_2)^2 + y_{12}^2} - x_1 + x_2 \right]^{1/(\alpha + \beta)}}{[a - x_1]^{1/\alpha} [a + x_2]^{1/\beta}}$$
$$\times f\left(\frac{x_1}{\alpha} + \frac{x_2}{\beta}\right),$$
(A11)

where the unknown function $f(u)$ is determined from the fact that $\chi \to 1$ when $x_1 \to -a$, x_2 is arbitrary, or when $x_2 \to a$ and x_1 is arbitrary. Finally, after expanding $|\vec{r} \pm a| \simeq |a \pm x| + y_{12}^2/2|a \pm x|$ in the exponent, we obtain

$$\Psi_1(\vec{r}_1, \vec{r}_2) = A_\alpha A_\beta (a + x_1)^{(2 - \alpha)/2\alpha} (a - x_2)^{(2 - \beta)/2\beta}$$
$$\times \exp\left[-a(\alpha + \beta) + \beta x_2 - \alpha x_1 - \frac{\alpha y_1^2}{2(a + x_1)} \right.$$
$$\left. - \frac{\beta y_2^2}{2(a - x_2)} \right] \chi(\vec{r}_1, \vec{r}_2),$$
(A12)

$$\chi(x_1, x_2, y_{12}) = \begin{cases} e^{a + x_1/2a\alpha} \left[\dfrac{2a}{a - x_1} \right]^{1/\alpha} \alpha^{-\alpha/(\alpha + \beta)\beta} \left[\dfrac{\beta(a + x_1) + \alpha(a + x_2)}{a + x_2} \right]^{1/\beta} \left[\dfrac{\sqrt{(x_1 - x_2)^2 + y_{12}^2} - x_1 + x_2}{\sqrt{[\beta(a + x_1) + \alpha(a + x_2)]^2 + (\alpha y_{12})^2} + \beta(a + x_1) + \alpha(a + x_2)}} \right]^{1/(\alpha + \beta)} \\[4ex] e^{-a - x_2/2a\beta} \left[\dfrac{2a}{a + x_2} \right]^{1/\beta} \beta^{-\beta/(\alpha + \beta)\alpha} \left[\dfrac{\beta(a - x_1) + \alpha(a - x_2)}{a - x_1} \right]^{1/\alpha} \left[\dfrac{\sqrt{(x_1 - x_2)^2 + y_{12}^2} - x_1 + x_2}{\sqrt{[\beta(a - x_1) + \alpha(a - x_2)]^2 + (\beta y_{12})^2} + \beta(a - x_1) + \alpha(a - x_2)}} \right]^{1/(\alpha + \beta)} . \end{cases}$$
(A13)

Here the upper expression is given for $x_1+x_2 \leq 0$ and the lower expression for $x_1+x_2 \geq 0$.

Substituting Eq. (A12) in Eq. (A6), and differentiating only the exponential, we obtain

$$2J = +2(\alpha+\beta) \int_{-a}^{a} [\Psi_1\Psi_2]_{x_1=x_2=x} \, dx \, dy_1 dy_2. \tag{A14}$$

Introducing the notations $\mu = \alpha+\beta$ and $\nu = \beta-\alpha$ and taking into consideration the fact that at the approximation (A9)

$$\sqrt{[(\beta+\alpha)(a-x)]^2+(\beta y_{12})^2}+(\beta+\alpha)(a-x)$$
$$\approx 2(\beta+\alpha)(a-x),$$

the formula (A14) transforms to

$$2J(\alpha,\beta,R) = R^{2/\alpha+2/\beta-1/\mu} e^{-\mu R}[D(\alpha,\beta,R)+D(\beta,\alpha,R)], \tag{A15}$$

where $D(\alpha,\beta,R)$ is the following function:

$$D(\alpha,\beta,R) = 4\sqrt{\pi} A_\alpha^2 A_\beta^2 \left(\frac{\mu}{2}\right)^{-1/\mu} \Gamma\left(\frac{2+\mu}{2\mu}\right) \left(2^{-\mu/\alpha}\frac{\mu}{\alpha}\right)^{2\alpha/\mu\beta}$$
$$\times \int_0^1 \frac{\exp[-(1-x)/\alpha-\nu Rx](1+x)^{2/\beta-2/\alpha+1/\mu}(1-x)^{2/\alpha-1/\mu}}{(1-x\nu/\mu)^{1+1/\mu}} dx. \tag{A16}$$

In the case $\alpha=\beta$ it is independent of R:

$$D_0(\alpha) \equiv 2D(\alpha,\alpha,R)$$

$$= 8\sqrt{\pi} A_\alpha^4 \left(\frac{1}{4\alpha}\right)^{1/2\alpha} \Gamma\left(\frac{\alpha+1}{2\alpha}\right)$$

$$\times \int_0^1 \exp(-t/\alpha)(2-t)^{1/2\alpha} t^{3/2\alpha} dx, \tag{A17}$$

and

$$2J(\alpha,\alpha,R) = D_0(\alpha) R^{7/2\alpha} \exp(-2\alpha R). \tag{A18}$$

For the two-dimensional hydrogen molecule ($\alpha=2$, $A_\alpha = 4/\sqrt{2\pi}$) it gives

$$J(2,2,R) = 30.413 \, R^{7/4} \exp(-4R). \tag{A19}$$

APPENDIX B: TWO-DIMENSIONAL HELIUM ATOM

1. Variational method

To find $J(0)$ one should consider the singlet-triplet splitting of two impurities which are at a distance much smaller than the Bohr radius of one impurity state. The motion of electrons is restricted by the plain, so this is as a ''two-dimensional helium atom.'' In this case the variational approach is the most appropriate. The Hamiltonian is

$$\hat{H} = -\frac{\Delta_1}{2} - \frac{\Delta_2}{2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \tag{B1}$$

and Schrödinger's variational principle is

$$E = \min \frac{\int \Psi\hat{H}\Psi \, d\tau}{N}, \tag{B2}$$

where

$$N = \int \Psi^2 \, d\tau.$$

The most important thing is the correct choice of the coordinate system. Namely, it is better to choose as independent variables those that the potential energy depends on. These are the three sides of the triangle r_1, r_2, r_{12} between the nucleus and two electrons.[25] The Hamiltonian and, as we expect, the wave functions for S terms do not depend on the orientation of the triangle in the space:

$$\Psi(\vec{r}_1,\vec{r}_2) = \Psi(r_1,r_2,\theta) = \Psi(r_1,r_2,-\theta), \tag{B3}$$

$$r_{12}^2 = r_1^2 + r_2^2 - 2r_1 r_2 \cos(\theta). \tag{B4}$$

Therefore, the volume element $d\tau$ is

$$d\tau = r_1 r_2 \, dr_1 \, dr_2 \, d\phi \, d\theta = 8\pi \frac{r_1 r_2 r_{12} \, dr_1 \, dr_2 \, dr_{12}}{\sqrt{4r_1^2 r_2^2 - (r_1^2 + r_2^2 - r_{12}^2)^2}}.$$

Finally, we introduce the ''elliptic'' coordinates

$$s = r_1 + r_2,$$
$$t = r_1 - r_2, \tag{B5}$$
$$u = r_{12},$$

which reflect the symmetry of two-particle eigenfunction: the wave function has to be an even function of t for total spin $S=0$, and an odd function of t for $S=1$. Thus,

$$d\tau = \frac{\pi(s^2-t^2)u}{\sqrt{(s^2-u^2)(u^2-t^2)}} \, ds \, dt \, du. \tag{B6}$$

The factor π can be omitted, and if we take into consideration the fact that

$$\Psi^2(s,t,u) = \Psi^2(s,-t,u), \quad \Psi\hat{H}\Psi(s,t,u) = \Psi\hat{H}\Psi(s,-t,u),$$

we can restrict the integration region by the inequalities:

$$0 \leq t \leq u \leq s \leq \infty, \tag{B7}$$

$$(\text{or } t \leq u \leq s, \ 0 \leq t \leq s \leq \infty). \tag{B8}$$

The potential energy in the new coordinates is

$$\left\langle \Psi \left| -\frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \right| \Psi \right\rangle = \left\langle \Psi \left| -\frac{4Zs}{s^2 - t^2} \right| \Psi \right\rangle$$

$$+ \left\langle \Psi \left| \frac{1}{u} \right| \Psi \right\rangle = V_1 + V_2 \tag{B9}$$

and the mean value of the kinetic energy is

$$K = \left\langle \Psi \left| -\frac{\Delta_1}{2} - \frac{\Delta_2}{2} \right| \Psi \right\rangle$$

$$= \frac{1}{2} \int \ [(\nabla_1 \Psi)^2 + (\nabla_2 \Psi)^2] \, d\tau$$

$$= \int_0^\infty ds \int_0^s du \int_0^u \left(\frac{u(s^2 - t^2)}{\sqrt{(s^2 - u^2)(u^2 - t^2)}} \right.$$

$$\times \left[\left(\frac{\partial \Psi}{\partial s} \right)^2 + \left(\frac{\partial \Psi}{\partial t} \right)^2 + \left(\frac{\partial \Psi}{\partial u} \right)^2 \right]$$

$$\left. + 2 \frac{\partial \Psi}{\partial u} \left[s \sqrt{\frac{u^2 - t^2}{s^2 - u^2}} \frac{\partial \Psi}{\partial s} + t \sqrt{\frac{s^2 - u^2}{u^2 - t^2}} \frac{\partial \Psi}{\partial t} \right] \right) dt. \tag{B10}$$

2. Ground state of He

For the ground state we use the trial wave function in a form

$$\Psi = \frac{1}{2} (e^{-(\alpha_1 r_1 + \alpha_2 r_2)} + e^{-(\alpha_2 r_1 + \alpha_1 r_2)}) = e^{-\alpha s} \cosh(\beta t),$$

$$\alpha = (\alpha_1 + \alpha_2)/2, \tag{B11}$$

$$\beta = (\alpha_1 - \alpha_2)/2,$$

and we also introduce the parameter $\gamma = (\beta/\alpha)^2$.

After calculating all necessary integrals, we obtain

$$N^{-1} = \frac{(2\alpha)^4}{\pi} \frac{(1 - \gamma)^2}{1 + (1 - \gamma)^2},$$

$$K/N = \alpha^2 \frac{1 + \gamma + (1 - \gamma)^3}{1 + (1 - \gamma)^2}, \tag{B12}$$

$$V_1/N = -4\alpha Z,$$

$$V_2/N = \frac{\alpha}{2} \frac{(1 - \gamma)^2}{1 + (1 - \gamma)^2} \left(\frac{3\pi}{4} + F(\gamma) \right),$$

$$F(\gamma) = \int_0^1 \frac{2 - u^2 + \gamma u^2 (1 - 2u^2)}{\sqrt{1 - u^2} (1 - \gamma u^2)^{5/2}} du, \tag{B13}$$

where $N, V_1, V_2,$ and K are defined by Eqs. (B2), (B9), and (B10) correspondingly. Here, in order to find V_2 we used the values of the following integrals:

$$\int_0^1 \cosh(bt)[1 - t^2]^{\mp 1/2} dt$$

$$= \frac{\pi}{2} \begin{cases} I_0(b) & (\text{see Ref. 23, 3.534.2}) \\ I_1(b)/b, \end{cases}$$

$$\int_0^\infty x^{n-1} e^{-x} \frac{I_\nu(cx)}{c^\nu} dx = (-1)^{n-1} \frac{\partial^{n-1}}{\partial p^{n-1}}$$

$$\times \left[\frac{(p + \sqrt{p^2 - c^2})^{-\nu}}{\sqrt{p^2 - c^2}} \right]_{p=1}$$

$$(\text{see Ref. 24, 2.15.3}).$$

Thus, the energy is

$$E(\alpha, \gamma) = \alpha^2 \frac{1 + \gamma + (1 - \gamma)^3}{1 + (1 - \gamma)^2}$$

$$- \alpha \left[4Z - \frac{1}{2} \frac{(1 - \gamma)^2}{1 + (1 - \gamma)^2} \left(\frac{3\pi}{4} + F(\gamma) \right) \right]. \tag{B14}$$

We can also rewrite it in the form

$$E(\alpha, \gamma) = \alpha^2 f(\gamma) - \alpha g(\gamma). \tag{B15}$$

The minimum value of the energy is realized for values of α and γ, which satisfy the equations

$$\frac{\partial E}{\partial \alpha} = 0, \ \frac{\partial E}{\partial \gamma} = 0,$$

or

$$2\alpha f(\gamma) - g(\gamma) = 0, \quad \alpha f'(\gamma) - g'(\gamma) = 0.$$

Eliminating α, we get the equation in γ,

$$\frac{f'(\gamma)}{f(\gamma)} - 2 \frac{g'(\gamma)}{g(\gamma)} = 0. \tag{B16}$$

It has the solution $\gamma = 0.11436$.

Then,

$$\alpha = 3.4059,$$

$$E_S = -11.760. \tag{B17}$$

The corresponding values of α_1 and α_2 are

$$\alpha_1 = \alpha(1 + \sqrt{\gamma}) = 4.5576,$$

$$\alpha_2 = \alpha(1 - \sqrt{\gamma}) = 2.2541. \tag{B18}$$

For comparison we also represent the results for the one-parameter wave function $\Psi = e^{-\alpha_1(r_1 + r_2)} = e^{-\alpha s}$:

$$E(\alpha) = \alpha^2 - \alpha\left(8 - \frac{3\pi}{8}\right), \tag{B19}$$

$$\frac{\partial E}{\partial \alpha} = 0 \Rightarrow \alpha = 4 - \frac{3\pi}{16} = 3.4109, \tag{B20}$$

$$E = -11.635.$$

Thus, the difference between these two ground state energies (B17) and (B19) is 1%.

3. Term ^3S of He

Taking into consideration the screening effect of the electrons, we construct our trial wave function from an antisymmetric combination of the $1s$ electron in a field of the charge $Z_1 \equiv \alpha_1/2$ and the orthogonal $2s$ electron state in a field of the charge $Z_2 \equiv 3\alpha_2/2$:

$$\varphi_{10}(r) = \exp(-\alpha_1 r), \tag{B21}$$

$$\varphi_{20}(r) = \exp(-\alpha_2 r)\left(1 - \frac{\alpha_1 + \alpha_2}{2} r\right),$$

$$\Psi(r_1, r_2) = \varphi_{10}(r_1)\varphi_{20}(r_2) - \varphi_{10}(r_2)\varphi_{20}(r_1). \tag{B22}$$

Or rewriting in s, t variables,

$$\Psi(s,t) = e^{-\alpha s}[\alpha t \cosh(\beta t) + (\alpha s - 2)\sinh(\beta t)], \tag{B23}$$

$$\alpha = \frac{\alpha_1 + \alpha_2}{2}, \tag{B24}$$

$$\beta = \frac{\alpha_1 - \alpha_2}{2}.$$

Performing a procedure similar to, though more tedious than, the ^1S case, we obtain the following results ($\lambda = \beta/\alpha$):

$$E(\alpha, \lambda) = \alpha^2 \frac{K}{N} - \alpha \frac{V_1 + V_2}{N},$$

$$N = \frac{2\pi}{(2\alpha)^4} \frac{2\lambda^2 + 1}{(1-\lambda)^4(1+\lambda)^2}, \tag{B25}$$

$$K/N = 2\frac{\lambda^4 - \lambda^3 + 4\lambda^2 - 2\lambda + 1}{2\lambda^2 + 1},$$

$$V_1/N = 8\frac{3\lambda^2 - \lambda + 1}{2\lambda^2 + 1},$$

$$V_2/N = -\frac{1}{16} \frac{(1-\lambda)^4(1+\lambda)^2[F(\lambda) - 171\pi/16]}{2\lambda^2 + 1}. \tag{B26}$$

Here

$$F(\lambda) = \int_0^1 \frac{\phi(u,\lambda)}{(1-\lambda^2 u^2)^{9/2}\sqrt{1-u^2}} du, \tag{B27}$$

$$\begin{aligned}\varphi(u,\lambda) = {}&16 u^6(1 - 2 u^2)\lambda^6 + 24 u^6(1 - 2 u^2)\lambda^5 \\&+ (45 u^4 - 24 u^8)\lambda^4 + (162 u^4 - 144 u^6)\lambda^3 \\&+ 12 u^2(1 + 3 u^2 - 6 u^4)\lambda^2 \\&+ 6 u^2(4 - 3 u^2)\lambda + 32 - 4 u^2 - 9 u^4.\end{aligned}$$

From minimizing $E(\alpha, \lambda)$ we find

$$\lambda = 0.742\,17, \quad \alpha = 2.309\,98, \tag{B28}$$

which correspond to the effective charges $Z_1 = 2.0122$ and $Z_2 = 0.8934$. For these values of λ and α we get the energy

$$E_A = -8.193\,45. \tag{B29}$$

It is worthwhile to note that for the wave function with $Z_1 = 2$ and $Z_2 = 1$ the energy $E = -8.190\,62$ is only higher by 0.03%.

Thus the exchange constant for the 2D helium atom is

$$J = E_A - E_S = 3.567 \; (\pm 1\%) \; \text{a.e.} \tag{B30}$$

*Electronic address: ilya@newt.phys.unsw.edu.au

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