An Example of Correlation Between Space and Spin Coordinates

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Abstract   An elementary, exactly solvable, quantum rnechanical model in which space and spin coordinates are correlated is fully developed.   It clearly illustrates aspects which are seldom treated in elementary courses. Furthermore, it provides simple examples for the concepts of bonding, antiboding, Franck-Condon effect and effective spin-spin interaction.

1. INTRODUCTION

The examples discussed in basic courses on Quantum Mechanics seldom deal with cases in which spin and spare coordinates are correlated. Here we present an exactly solvable model which displays this characteristic and also other interesting features which make it appropriate to illustrate some common concepts such as bonding, Franck-Condon effect and effective spin-spin interaction through electrons.

2. MODEL

Let us consider an electron coupled through local isotropic exchange interaction to two free spins at sites a and –a, (fi . .   The model is one-dimensional in the electron space coordinate.   The spins, however, will be three dimensional vectors with the z-direction taken as quantization axis. The Hamiltonian is

$$H = \frac{P^2}{2m^\star} + J\vec{s}.\left[\vec{S}_1\delta(x+a) + \vec{S}_2\delta(x-a)\right].\tag{1}$$

The first term represents the kinetic energy of the electron with mass $m^\star$. J is the coupling constant of the exchange interaction between the spin $\vec{s}$ of the electron and the localized spins $\vec{S}_1$ and $\vec{S}_2$ at –a and a, respectively. $\delta(x)$ is Dirac's delta function.

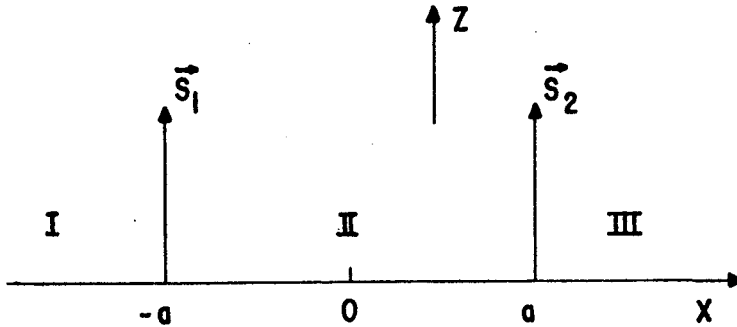An electron in an attractive δ-like potential in one   dimension

Fig.1 - Model potential. The electron interacts through a local exchange coupling with spins $\vec{S}_1$ and $\vec{S}_2$ at -a and a.

has only one bound state which, in the absence of magnetic interactions, is doubly degenerate in the spin coordinate. We will limit ourselves to consider only the bound states of H. We are thus in principle confronted with a system of $2 \times 2 \times \left[(2S_1 + 1) + (2S_2 + 1) \right]$ states. One factor of 2 stands for the spatial bound states of the δ-potentials, another factor of 2 stands for the electron spin states, and the localized spin i has $2S_i + 1$ spin states. For simplicity we will wnsider spins of the same magnitude: $S_1 = S_2 = S$. We develop the solution of the problem as far as we can without specifying S; however, later on, to get manageable closed results, we deal in detail only with the case $S = 1/2$.

3. SOLUTION OF SCHRÖDINGER'S EQUATION

We note that H is ihvariant under a transformation Q which changes x into $-x$ and simultaneously interchanges the spin subindices 1 and 2. Thus, H commutes with Q:

$$\left[H, \vec{Q} \right] = 0 . \tag{2}$$

Since $Q^2 = 1$, the eigenvalues of Q are q = ±1. This allows us to classify the eigenfunctions of H as even $(q = 1)$ or odd $(q = -1)$.[1] Furthermore, since interactions of the form $\vec{s} \cdot \vec{S}_i$ conserve the z-component of the total spin, H commutes also with the z-component 6^z of the total spin $\vec{6} = \vec{s} + \vec{S}_1 + \vec{S}_2$:

$$\left[H, \delta^z \right] = 0 . \tag{3}$$

Therefore, the eigenfunctions of H must also be eigenfunctions of s^z and we will label them with the eigenvalues of 6^z. Accordingly, we propose wavefunctions of the form

$$\psi_{M,q}(x) = \sum_m \left[A_m U_m + B_m V_m \right] e^{-kx} \qquad \text{for} \quad x > a$$

$$\psi_{M,q}(x) = \sum_m \{ \left[C_m e^{-kx} + q C_{M-m} e^{kx} \right] U_m + \left[D_m e^{-kx} + q D_{M+1-m} e^{kx} \right] V_m \}$$

$$\text{for} \quad |x| < a$$

$$\psi_{M,q}(x) = q \sum_m \left[A_{M-m} U_m + B_{M+1-m} V_m \right] e^{kx} \qquad \text{for} \quad x < -a$$

$$(4)$$

where

$$U_m = \alpha |m\rangle_1 \; |M-m\rangle_2 \tag{5}$$

and

$$V_m = \beta |m\rangle_1 \; |M+1-m\rangle_2 \quad . \tag{6}$$

Here α and β are the up and down electron states, respectively, ($\hbar = 1$)

$$s^z \alpha = \frac{1}{2} \alpha \quad , \quad s^z \beta = -\frac{1}{2} \beta \tag{7}$$

$|m\rangle_i$ are the eipenstates of S_i^z:

$$S_i^z |m\rangle_i = m |m\rangle_i \qquad i = 1,2 \quad . \tag{8}$$

In the sums, m runs over the values $-S, -S+1, \ldots, S$, with the condition that the spin states exist, namely, $|M-m| \leqslant S$ or $|M+1-m| \leqslant S$, whichever applies. We can verify that

$$Q\psi_{M,q}(x) = q\psi_{M,q}(x) \quad . \tag{9}$$

and

$$s^z \psi_{M,q}(x) = (M+1/2)\psi_{M,q}(x) \quad . \tag{10}$$

To demonstrate eq. (9) we use the relations

$$QU_m = U_{M-m}$$

$$QV_m = V_{M+1-m} \tag{11}$$

which follow from the definition of Q and eqs. (5) and (6). Eq. (10) follows from the relations

$$s^z U_m = (M+1/2) \, U_m$$

$$s^z V_m = (M+1/2) \, V_m \tag{12}$$

which are a consequence of eqs. (7) and (8). For k positive, $\psi_{M,q}(x)$ has the boundary conditions appropriate to a bound state of energy

$$E = -\hbar^2 k^2 / 2m^* \tag{13}$$

The ansatz (4) contains, besides the energy, $4 \times (2S+1)$ constants to be determined. The continuity of $\psi_{M,q}(x)$ at x=a requires that

$$A_m = C_m + qC_{M-m} \, e^{2ka}$$

$$B_m = D_m + qD_{M+1-m} e^{2ka} \ . \tag{14}$$

The solution of Schrödinger's equation at the singular point x = a requires that[2]

$$\frac{\hbar^2}{2m^*} \left[\left(\frac{d\psi}{dx} \right)_+ - \left(\frac{d\psi}{dx} \right)_- \right]_{x=a} = \vec{J s} . \vec{S}_2 \psi(a) \tag{15}$$

where $(d\psi/dx)_{+(-)}$ stands for the limit of the derivative from the right (left). That is,

$$-A_m + C_m - qC_{M-m}e^{2ka} = \frac{\kappa}{2k} \left[(M-m)A_m + f(M-m)B_m \right]$$

$$-B_m + D_m - qD_{M+1-m}e^{2ka} = \frac{\kappa}{2k} \left[-(M+1-m)B_m + f(M-m)A_m \right] \tag{16}$$

where $\kappa = 2m^*J/\hbar^2$. To derive eq. (16) we write $\vec{s}.\vec{S}_2 = s^z S_2^z + \frac{1}{2}[s^+ S_1^- + s^- S_2^+]$, where $s^{\pm} = s^x \pm i s^y$ and $S_2^{\pm} = S_2^x \pm i S_2^y$ are the raising and lowering operators, and we use the result

$$s^-s^+U_m = f(m)V_m \quad ,$$ (17)

where $f(m) = \left[(S-m)(S+m+1)\right]^{1/2}$,[3] Eqs.(14) and (16) are a system of $4\times(2S+1)$ homogeneous equations. The roots of its secular determinant yield the energy eigenvalues E.

Eqs. (14) yield

$$C_m = \frac{A_m - qA_{M-m}e^{2ka}}{1-e^{4ka}}$$

$$D_m = \frac{B_m - qB_{M+1-m}e^{2ka}}{1-e^{4ka}}$$ (18)

which replaced in eq.(16) give

$$qA_{M-m} - A_m e^{2ka} = \frac{\kappa}{2k} \sinh(2ka)\left[(M-m)A_m + f(M-m)B_m\right]$$ (19)

$$qB_{M+1-m} - B_m e^{2ka} = \frac{\kappa}{2k} \sinh(2ka)\left[-(M+1-m)B_m + f(M-m)A_m\right] \quad .$$

This system of equations cannot be further reduced because coefficients with different subindices m are coupled together.

4. RESULTS FOR S = 1/2

In the following we restrict ourselves to the case $S=1/2$. For convenience, we introduce the dimensionless variables

$$t = \frac{\kappa}{2k} \quad \text{and} \quad d = 2m^*Ja/\hbar^2 \quad ,$$ (20)

and use the subindices + and − for +1/2 and −1/2.

i) Case *M*=1

For M=1, eqs.(19) reduce to

$$A_+\left(q - e^{2ka} - \frac{1}{2}t \sinh(2ka)\right) = 0$$

$$A_- = B_+ = B_- = 0 \quad .$$ (21)

The secular equation can be written in the form

$$R_1 \equiv \frac{t}{4} (1 + qe^{-d/t}) + 1 = 0 \ . \tag{22}$$

Only the roots for which $d/t > 0$ (that is, $k > 0$) are physical. For $d > 0$ ($J > 0$), eq. (22) has no positive root. For $d < 0$ ($J < 0$), there are negative roots; that for $q = 1$ corresponds to the ground state E (bonding) and that for $q = -1$ to the excited state E (antibonding). Fig.2 shows E and E as a function of d, which is a measure of the separation of the 6-like potentials ($d \propto a$). The energy E is given in units of $J^2 m^* \times 10^{-2}/(2\hbar^2)$.[4]
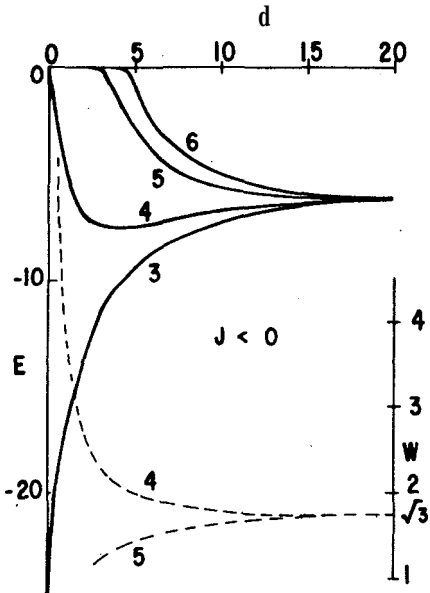

Fig.2 - Energy levels E as a function of the distance between the localized spins d, for $J < 0$. The coefficient w (which is a measure of the singlet amplitude of the localizes spins) is shown on a different scale (to the right). Levels 3 and 6 belong to pure spin states ($s = 3/2$, s^z).

From eqs. (18), (19) and (21)

$$C_+ = \frac{e^{-ka}}{e^{-ka} + qe^{ka}} A_+ \tag{23}$$

$$C_- = D_+ = D_- = 0$$

and the wavefunction takes the form

$$\psi_{1,q}(x) = A_+ |3/2,3/2\rangle \begin{cases} e^{-kx} & \text{for } x > a \\ \dfrac{e^{-kx}_+}{e^{-ku}+qe^{\cdot uu}} \; e^{-ka} & \text{for } |x| < a \\ qe^{kx} & \text{for } x < -a \end{cases}$$

$$(24)$$

Here $|3/2,3/2\rangle \equiv \alpha|1/2\rangle_1 |1/2\rangle_2$ and A_+ becomes a normalization constant. The values of k can be obtained from curves 3 and 6 of fig.2 using $k = \kappa/(2t)$ for $q = 1$ and $q = -1$, respectively.

ii) Case $M=0$.

For $M=0$, eqs. (16) reduce to

$$(\frac{t}{2} \sinh 2ka - \overset{2ka}{0})A+ + qA_- - t \sinh (2ka)B_+ = 0$$

$$qA_+ - (\frac{t}{2} \sinh 2ka + e^{2ka})A_- = 0 \qquad (25)$$

$$-t \sinh(2ka)A_+ + (q - e^{2ka} + \frac{t}{2} \sinh 2ka)B_+ = 0$$

$$B_- = 0 \; .$$

The secular equation can be written in the forrn

$$R_1 R_2 = 0 \qquad (26)$$

where

$$R_2 = 3 \frac{t^2}{16} (1-e^{-2d/t}) + \frac{t}{2} (1+qe^{-d/t}) - 1 \; , \qquad (27)$$

and R_1 has been defined in eq. (22). The energy eigenvalues coming from the roots of R_1 were already discussed in {i}. For those roots, eqs. (25) yield

$$A+ = A_- = B_+ \quad (\text{for } R_1 = 0) \qquad (28)$$

as it is easily seen by direct substitution. From eqs. (18) and (19) we obtain

$$C_+ = C_- = D_+ = \frac{e^{-ka}}{e^{-ka} + qe^{ka}} \; A_+ \, , \tag{29}$$

and replacing in eq. (4) we get a wavefunction which is like that given by eq. (24) with the spin state $|3/2,3/2\rangle$ replaced by

$$\sqrt{3}\,|3/2,1/2\rangle \equiv \alpha|1/2\rangle_1|-1/2\rangle_2 + \alpha|-1/2\rangle_1|1/2\rangle_2 + \beta\,|1/2\rangle_1|1/2\rangle_2$$

$$\equiv \sqrt{2}\,\alpha|1,0\rangle + \beta\,|1,1\rangle \, . \tag{30}$$

In fact, the energy branches 3 and 6 in fig. 2 are four-fold degenerate, corresponding to the four spin states $|3/2,\delta^z\rangle$ with $\delta^z = 3/2, 1/2, -1/2,$ $-3/2,$ which must have the same energy in virtue of the isotropy of the spin interactions.

We now consider the eigenvalues and eigenfunctions produced by the roots of R_2:

$$R_2 = 0 \tag{31}$$

For $J<0,$ eq. (31) has one positive root (in terms of t) for each value of q. The corresponding energies are plotted in fig. 2 (curve 4 for q = -1 and curve 5 for q = 1). For $J > 0,$ eq. (31) has one negative root for each value of q; the corresponding energies are plotted in fig. 3 (curves 1
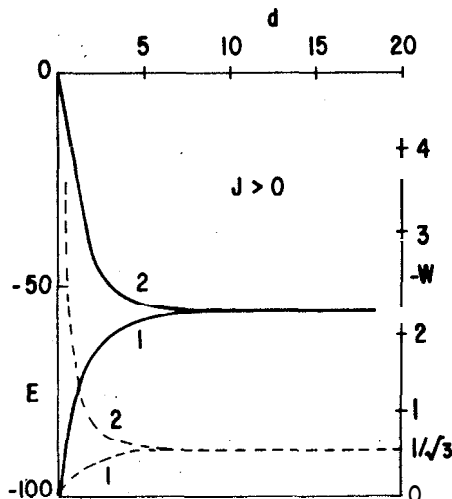

Fig.3 - Energy levels E as a function of the distance between the localized spins d, for $J>0$. The coefficient w (which is a rneasure of the singlet amplitude of the localized spins) is shown on a different scale (to the right). Note that here w is negative.

and 2 for $q = 1$ and -1, respectively). Eqs. (25) now yield

$$A+ + A_- + B_+ = 0 \qquad \text{for } R = 0 \; , \tag{32}$$

and from eqs. (18), (19) and (32)

$$C_+ = \frac{e^{-ka}}{e^{-ka} - qe^{ka}} A_+ + \frac{q}{e^{-2ka} - e^{2ka}} B_+$$

$$C_- = \frac{-e^{-ka}}{e^{-ka} - qe^{ka}} A_+ - \frac{e^{-2ka}}{e^{-2ka} - e^{2ka}} B_+ \tag{33}$$

$$D_+ = \frac{e^{-ka}}{e^{-ka} + qe^{ka}} B_+ \; .$$

At this point it is convenient to introduce the notation used in the algebra of coupling angular momenta[5]. With the localized spin states we can construct the following triplet states

$$|1,1\rangle = |1/2\rangle_1 \; |1/2\rangle_2$$
$$|1,0\rangle = \frac{1}{\sqrt{2}} \left[|1/2\rangle_1 |-1/2\rangle_2 + |-1/2\rangle_1 |1/2\rangle_2 \right] \tag{34}$$

and also the singlet state

$$|0,0\rangle = \frac{1}{\sqrt{2}} \left[|1/2\rangle_1 |-1/2\rangle_2 - |-1/2\rangle_1 |1/2\rangle_2 \right] \; . \tag{35}$$

And by coupling the electron spin to the above triplet states we can also construct the states

$$|3/2,1/2\rangle = \sqrt{2/3} \; \alpha |1,0\rangle + \sqrt{1/3} \; \beta |1,1\rangle$$
$$|1/2,1/2\rangle = \sqrt{2/3} \; \beta |1,1\rangle - \sqrt{1/3} \; \alpha |1,0\rangle \; . \tag{36}$$

In the kets, the first number denotes the total spin and the second one its z-component. Using eqs. (32-36) and after a bit of algebra, eq. (4) yields

$$\psi_{0,q} = \sqrt{3/2} \; B_+ \; \{|1/2,1/2> + w\alpha|0,0>\}e^{-kx} \quad \text{for} \quad x > a$$

$$\psi_{0,q} = \sqrt{3/2} \; B_+ \; e^{-ka} \left\{ \frac{e^{-kx}+qe^{kx}}{e^{-ka}+qe^{ka}} \right\} |1/2,1/2> \; +$$

$$+ \; w \; \frac{e^{-kx}-qe^{kx}}{e^{-ka}-qe^{ka}} \; \alpha|0,0>\} \qquad \text{for} \quad |x|<a \tag{37}$$

$$\psi_{0,q} = \sqrt{3/2} \; B_+ q\{|1/2,1/2> \; - \; w\alpha|0,0>\}e^{kx} \qquad \text{for} \quad x < -a$$

where

$$w = \frac{2A_+ + B_+}{\sqrt{3} \; B_+} = -\frac{\sqrt{3}}{4} \; t(1-qe^{-d/t}) \tag{38}$$

and $ka=d/(2t)$. B_+ becomes a normalization constant. For $|x|>a$, w is the ratio of the amplitudes of the singlet and triplet components of the localized spins in the wave function. The valuesof w are ploted in figs. 2 and 3 (dotted lioes labeled in correspondence to the energy branches, scale to the right).

5. DISCUSSION

i) Energy Spectrum

For $\delta=3/2$ (and any δ^z), the only possibility is the parallel coupling of the three spins. Thus, for $J>0$ there is a repulsive force between the electron and the localized spins and bound states cannot exist. On the other hand, for $J<0$, the interaction is attractive and there are bound states (curves 3 and 6 of fig. 2). In the limit $d\rightarrow\infty$ and neglecting spin degeneracy, we have two degenerate bound states, corresponding to those of the individual δ-potentials. As d decreases to the point that the overlaping of the localized wavefunctions becomes appreciable, the levels split into a bonding even ground state (curve 3) and an antibonding odd excited state (curve 6). At a critica1 distance $d = d_c = 4$, the antibonding state merges into the continuum, and for $d < d_c$ only one bound state is left. This is consistent with the fact that for $d = 0$ the problem becomes equivalent to that of a single δ-po-

tential of strength $2J$, and a 6-potential has only one bound state.

When the coupling of the three spins is such that the total spin $\delta=1/2$, an interesting and *frustrating* situation arises for $J < 0$. The electron would like to be parallel to the two localized spins but it cannot, as it is forbidden by the conservation of the total spin $\delta=1/2$. Thus, a complicated spacial-spin correlation develops between the electron and the localized spins aimed to minimize the energy. In the limit $d\to\infty$ there is, in principle, no problem as the electron may be localized at one δ-function with its spin parallel, leaving the other (far away) to have antiparallel spin. This state is twice degenerate because the localization may happen at either 6-site. As d decreases, the electron may profit from the correlation and the delocalization to lower the energy of the bonding state. However, as $d\to 0$ the only possible state is one in which the localized spins are in the singlet state and the exchange energy vanishes (curve 4 of fig.2). Thus, there is a finite distance d_{min} for which the energy is a minimum (d_{min} = 3.661, E_{min} = -7.54). The equilibrium distance in the excited electronic state, $d=d_{min}$, differs from the equilibrium distance, $d=0$, of the ground state (fig.2). This situation is commonplace in molecular systems and leads to the Franck-Condon effect, that is, to a displacement toward lower frequencies of the emission with respect to the absorption bands (Stokes shift)[6]. In an energy diagram like that of fig.2, optical transitions would be represented by vertical lines between energy levels (transitions with fixed coordinates, in this case the coordinate being d). The reason for this effect in molecules is that the electronic transition is too fast to allow the relaxation of the coordinates into the new equilibrium values. Thus; in absorption our system would go from E_3 = -25 to E_4 = 0 at d = 0 ($\hbar\omega_a$ = E - $E_3 \simeq 25$), and in emission from E = -7.54 to E_3 = -10.62 at d = 3.66 ($\hbar\omega_e$ = E_4 - E_3 = 3.08); the Stokes shift is then $E = \hbar(\omega_a - \omega_e)$ = 22.92. The antibonding state merges into the continuum at d = 8/3.

For $\delta=1/2$ and $J>0$ there is a strong antiferromagnetic correlation between the electron and the localized spins in the ground state for small d (curve I of fig.3). The strong binding energy as compared with the case $J < 0$ reflects the fact that for two spins 1/2, the scalar

product $\vec{s}.\vec{S}$ in the singlet state (antiferromagnetic ordering) is $-3/4$ while in the triplet state (ferromagnetic ordering) is $1/4$.

ii) The wavefunctions. Correlations.

In the wave functions belonging to the total spin $s=3/2$, (eqs. (24)), the spin coordinates can be factorized out and therefore the spin and space coordinates are not correlated.

For $s=1/2$ however, the mixture of spin states depends on x. Space and spin coordinates are correlated and we can, for instance, ask questions like: In the state 4 (fig.2), what is the density of probability $P(x)$ of finding the electron with the spin up when spin 1 is up and spin 2 is down? By projecting the wave function given by eq.(37) with $q = -1$ on the state $\alpha|1/2\rangle_1|-1/2\rangle_2$ we obtain

$$
P(x) = \frac{B_+^2}{4} \cdot
\begin{cases}
(\sqrt{3}\, w-1)^2 \; e^{-2kx} & \text{for } x>a \\[2mm]
\left(\dfrac{\sqrt{3}\, w \cosh(kx)}{\cosh(ka)} - \dfrac{\sinh(kx)}{\sinh(ka)} \right)^2 e^{-2ka} & \text{for } |x|<a \quad (39) \\[2mm]
(\sqrt{3}\, w +1)^2 \; e^{2kx} & \text{for } x<-a
\end{cases}
$$

Fig.4 shows $P(x)$ for $d=5$. The state 4 belongs to $J < 0$ and accordingly, the probability of finding the electron with spin up at $-a$ (where the spin 1 is up) is larger than at a (where spin 2 is down).

Since the model has been completely solved we can calculate and interpret all possible cases in a similar way.

iii) Effective spin-spin interaction

The energy branch E_3 belongs to states with $s=3/2$ (for instance (24)), for which the localized spins are parallel, that is $\langle\vec{S}_1.\vec{S}_2\rangle=1/4$ (curves 3,6 in fig. 5). Here $\langle...\rangle$ stands for mean value in the state considered. Along the energy branch E_4, however, there is an admixture of singlet and triplet states (eq.(37)). In fig.5 we have also plotted the mean value of the scalar product $\langle\vec{S}_1.\vec{S}_2\rangle$ in all four states with $s=1/2$ as a function of d. We see that for branch E_4, it is $-3/4 \leqslant \langle\vec{S}_1.\vec{S}_2\rangle \leqslant -1/2$, indicating that the localized spins are mostly an-
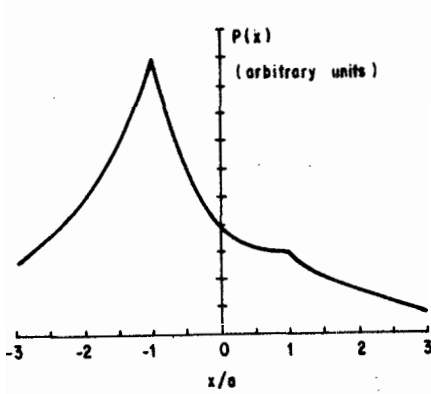
Fig.4 - Density of probability $P(x)$ of finding the electron with spin up when it is in the state 4 (fig. 2), and the spins 1 and 2 are up and down, respectively. The parameters are $d=5$, $w=1.9878$, $ka=0.68$. The distribution is given in arbitrary units (not normalized).
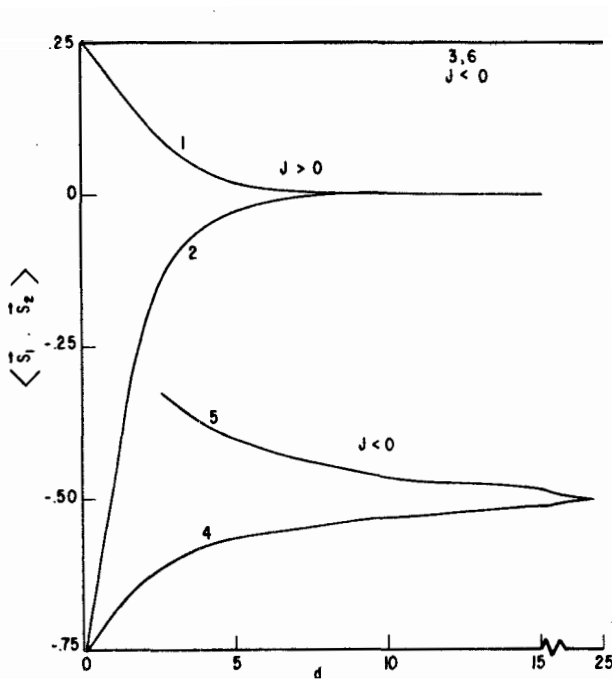

Fig.5 - Mean value of the scalar product of the spins $\vec{S}_1$ and $\vec{S}_2$, $<\vec{S}_1.\vec{S}_2>_i$, in state i as a function of the distance d between them. Note the change of scale at $d=15$.

tiparallel. We could imagine that the electron is not there and inter-
pret the energy difference E_4-E_3 as the necessary energy to flip one
localized spin in virtue of the presence of an effective interaction
of the form

$$H_{\text{eff}} = I \ \vec{S}_1 . \vec{S}_2 \quad . \tag{40}$$

Then, by definition, the effective exchange coupling constant I between
the localized spins is

$$I \equiv \frac{E_3 - E_4}{<\vec{S}_1 . \vec{S}_2>_3 - <\vec{S}_1 . \vec{S}_2>_4} \tag{41}$$

I is plotted as a function of d in fig.6. Its asymptotic behavior is

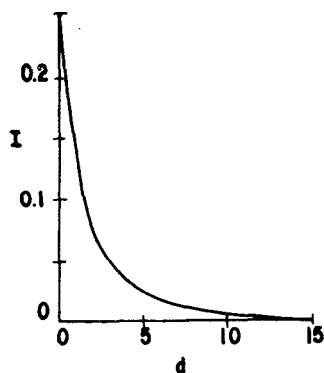$$I \simeq - \frac{3}{64} e^{-d/4} \quad . \tag{42}$$

Fig.6 - Effective exchange couplingconstant
I between the localized spins as a function
of their distance d.

Thus, H_{eff} given by eq. (40) is an effective spin-spin interaction me-
diated by the electron. This mechanisrn is analogous to that responsible
for the magnetism of the rare earth metals and for an interaction be-
tween nuclear spins in rnetals; in those cases, however, the interaction
is mediated by conduction electrons[7].

REFERENCES

1. We caution that the expressions even and odd do not refer to the space only (even or odd in x), but to the transformation properties of the eigenfunctions under Q, which also includes an interchange of the spin labels 1 and 2.   .

2. I. I. Gol 'dman and V.D.Kirvchenkov, *Problems in Quantum Mechanics,* Pergamon Press, London (1961).   c

3. In virtue of the Q symmetry, Schrödinger's equation will be auto-rnatically satisfied at $x=-a$.

4. We are used to think of the exchange energy as being proportional to J. In this model, however, the energy is proportional to J^2. The reason is that in this case the exchange energy is providing the localization of the electron. Usually the localization is due to Coulomb potentials, the exchange being a small correction to it.

5. This convenience is a consequence of the fact that H comutes also with δ^2.

6. R. P. Bauman, *Absorption Spectroscopy,* John Wiley & Sons, N.Y., 1963, p.278.

7. C.Kittel, *Quantum Theory of Solids,* John Wiley & Sons, K.Y., 1963, p. 360.

Resumo

Um modelo quântico elementar no qual coordenadas espaciais e de spin estão correlacionadas, e que admite solução analítica é exatamen-te resolvido. Ilustra aspectos que raramente são tratados em cursos básicos, além do que, exemplifica claramente, os conceitos de ligação e antiligação, efeito Franck-Condon e a interação efetiva entre spins.