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HYPERFINE INTERACTION AND SPIN-ELECTRON RESONANCE IN POLARONS AND EXCITONS

M. F. DEIGEN and S. I. PEKAR

Institute of Physics, Academy of Sciences, Ukrainian S.S.R.

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It is shown that in polarons and excitons the energy correction due to the hyperfine interaction is zero in first approximation. Consequently, the hyperfine-interaction part of the width of the spin-electron resonance in polarons and excitons is equal to zero.

The experimentally observed narrowness of the spin-electron resonance bands in metal-ammonia solutions provides additional evidence that the current carriers in these systems are polarons.

It is shown that with intense illumination of a crystal the stationary concentration of excitons can be so large that experimental detection of paramagnetic absorption in excitons may be possible. In virtue of the optical selection rules, excitons that have absorbed a radio-frequency quantum have a very long lifetime against radiative deexcitation.

THE energy operator of the hyperfine interaction between an electron and the magnetic moments of the nuclei of a crystal is

$$\hat{U} = \sum_l \hat{U}_l; \quad \hat{U}_l = \frac{\mu\mu_l}{SI_l} \sum_{\mathbf{n}} \left(\mathbf{S}, \operatorname{curl}\operatorname{curl} \frac{\mathbf{I}_{l\mathbf{n}}}{\rho_{l\mathbf{n}}}\right). \quad (1)$$

Here the index l distinguishes the types of nuclei, U_l is the energy operator for the hyperfine interaction of the electron with the magnetic moments of nuclei of type l, $\mathbf{n}$ is the label of a point of the l-th sublattice; $\mathbf{S}$ and S are the spin of the electron and its absolute value, $\mathbf{I}_{l\mathbf{n}}$ and I_l are the spin of the $(l\mathbf{n})$-th nucleus and its absolute value, μ is the Bohr magneton, μ_l is the magnetic moment of the nucleus, and $\rho_{l\mathbf{n}}$ is the distance from the $(l\mathbf{n})$-th nucleus to the electron. In Eq. (1) the curl operation applies to the coordinates of the electron.

We assume that in zeroth approximation the Hamiltonian of the crystal does not involve the spins of the nuclei. Then the wave function of the crystal can be written as the product of the wave function χ of the nuclear spins and a function $\psi(r, R)$ of the coordinates (r) of all the electrons and the coordinates (R) of the translational motion of the nuclei.

Let χ be an eigenfunction of all the $I_{l\mathbf{n}z}$. Then the first-order energy correction due to the hyperfine interaction is

$$U = \sum_l U_l;$$

$$U_l = \frac{\mu\mu_l}{SI_l} \sum_{\mathbf{n}} I_{l\mathbf{n}z} \int \Big(\psi^*(r, R)\,\mathbf{S}\psi(r, R), \operatorname{curl}\operatorname{curl}\frac{\mathbf{i}}{\rho_{l\mathbf{n}}}\Big)(dr)\,(dR); \quad (2)$$

$$\rho_{l\mathbf{n}} = \mathbf{r} - \mathbf{n} - \mathbf{R}_{l\mathbf{n}}, \quad (3)$$

where $\mathbf{i}$ is a unit vector in the z direction and $I_{l\mathbf{n}z}$ are the eigenvalues of the z components of the nuclear spins.

It can easily be shown that the integral

$$Q_{l\mathbf{n}} = \int\Big(\psi^*(r, R)\,\mathbf{S}\psi(r, R), \operatorname{curl}\operatorname{curl}\frac{\mathbf{i}}{\rho_{l\mathbf{n}}}\Big)(dr)\,(dR) \quad (4)$$

does not depend on $\mathbf{n}$ if $\psi(\mathbf{r}, \mathbf{R})$ is an eigenfunction of the translation operator $T_{\mathbf{m}}$. By the operation $T_{\mathbf{m}}$ we mean a change of the coordinate system such that the electron is displaced by an integer lattice vector $\mathbf{m}$ $(\mathbf{r} \to \mathbf{r} + \mathbf{m})$ and all the deformations of the lattice are also displaced by the vector $\mathbf{m}$ $(\mathbf{R}_{l\mathbf{n}} \to \mathbf{R}_{l,\mathbf{n}-\mathbf{m}})$.

Let us apply the operation $T_{\mathbf{m}}$ to the integrand of Eq. (4); this must not change the value of the integral, since it is equivalent to a change of variables. Since ψ is an eigenfunction of the operator $T_{\mathbf{m}}$, we have

$$T_{\mathbf{m}}\psi(r, R) = e^{i\mathbf{k}\mathbf{m}}\psi(r, R).$$

Furthermore it follows from Eq. (3) that

$$T_{\mathbf{m}}\rho_{l\mathbf{n}} = \rho_{l,\mathbf{n}-\mathbf{m}}.$$

Therefore the expression (4) goes over into

$$Q_{l\mathbf{n}} = \int T_{\mathbf{m}} \Big(\psi^* (r,\ R)\, S\psi (r,\ R),$$

$$\text{curl curl}\ \frac{\mathbf{i}}{\rho_{l\mathbf{n}}}\Big) (dr)\,(dR) = \int (\psi^* (r,\ R)\, S\psi (r,\ R),$$

$$\text{curl curl}\ \frac{\mathbf{i}}{\rho_{l,\mathbf{n}-\mathbf{m}}}\Big) (dr)\,(dR) = Q_{l,\ \mathbf{n}-\mathbf{m}}. \tag{5}$$

Thus $Q_{\ell\mathbf{n}}$ indeed does not depend on **n**, and is hereafter denoted by Q_ℓ. Therefore Eq. (2) can be rewritten as follows:

$$U_l = \frac{\mu\mu_l}{SI_l} Q_l P_l;\ P_l = \sum_{\mathbf{n}} I_{l\mathbf{n}z}. \tag{6}$$

Here P_ℓ is the z component of the total spin angular momentum of all the type ℓ nuclei in the crystal. On the average P_ℓ is zero, but actually it fluctuates slightly because the components of the nuclear spins take random values.

Since for $\mathbf{n} \neq \mathbf{n}'$

$$\overline{I_{l\mathbf{n}z} I_{l\mathbf{n}'z}} = \overline{I}_{l\mathbf{n}z} \overline{I}_{l\mathbf{n}'z} = 0,$$

the mean-square value of P_ℓ is given by

$$\overline{P_l^2} = N_l \overline{I_{l\mathbf{n}z}^2}, \tag{7}$$

where N_ℓ is the number of type ℓ nuclei in the crystal. Thus $(\overline{P_\ell^2})^{1/2}$ is proportional to $V^{1/2}$, where V is the volume of the fundamental region of the crystal.

For the polaron and exciton ψ is an eigenfunction of $T_{\mathbf{m}}$, so that results (6) and (7) are valid. Furthermore, in these cases ψ has a normalization coefficient proportional to $V^{-1/2}$. Therefore Q_ℓ is proportional to 1/V.

The remarks made above, and also Eqs. (6) and (7), show that as V is increased U_ℓ, and consequently also U, go to zero as $V^{-1/2}$ (it can be shown that the integral Q_ℓ converges). Consequently, the hyperfine interaction, which in the case of local electron centers was the dominant factor determining the width of the spin-resonance absorption, gives no broadening at all in the case of polarons and excitons.

This fact makes is possible to distinguish experimentally between polarons and local electron centers.

In papers by Deigen[1] it has been shown that in metal-ammonia solutions the alkali metal atoms dissociate and the liberated electrons form polarons. These latter cause the electric conductivity and optical properties of these solutions. On the basis of these ideas, quantitative explanations of many experimental facts have been obtained.

Experimental studies of the spin-electron resonance at color centers in metal-ammonia solutions[2] have shown that the width of the spin-resonance absorption region is of the order of hundredths of a gauss, i.e., 10^4 times smaller than for local electron centers (for example, F centers). This shows clearly that the color centers in question are not local electron centers. Moreover, it serves as a new proof that they are polarons.

The fact that for polarons the hyperfine interaction must be absent and the corresponding width of the spin-electron resonance must vanish was pointed out by Pekar at the All-Union Conference on the Theory of Semiconductors in February, 1955 (cf. Ref. 3). He has also emphasized that the experimentally observed extreme narrowness of the spin-electron resonance region for color centers in metal-ammonia solutions means that they are polarons.

Another view of the explanation of the small width of the spin-electron resonance in metal-ammonia solutions has been given by Kaplan and Kittel.[4] They used the model of color centers proposed by Ogg[5] (a spherical vacuum cavity in the dielectric, in which the electron is localized). The lack of physical foundation for this model has been shown in Ref. 1.

It is interesting to examine whether by illuminating a crystal it is possible to produce such a high concentration of excitons that the spin-electron absorption of radio waves by the excitons could be detected experimentally. If the deexcitation of the excitons occurred only by emission of radiation and the mean lifetime τ of the exciton were of the order of 10^{-8} sec, the stationary concentration of excitons would be given by the formula

$$n = \tau s \varkappa / \hbar\omega, \tag{8}$$

where s is the flux of radiant energy per $\text{cm}^2 \times$ sec, κ is the coefficient of exciton absorption of light in the crystal, and ω is the frequency of the absorbed light. If $\hbar\omega \sim 1$ ev, $\kappa \sim 10^5\ \text{cm}^{-1}$, and $s \sim 1\text{W/cm}^2$, we get $n \sim 10^{16}\ \text{cm}^{-3}$. With such a concentration of excitons it is quite possible that the spin-resonance absorption of radio waves by them can be experimentally observed.

It is desirable to reduce the nonradiative deexcitation of the excitons to a minimum by using ideal crystals free from impurities and working at low temperatures.

It must be emphasized that the total spin of the electrons in a dielectric in its ground state is always zero. In virtue of the spin selection rules for optical transitions, the total spin remains zero when light is absorbed and an exciton is formed.

But when a radio-frequency quantum is absorbed by the exciton the total spin of the electrons becomes ± 1, so that the inverse optical transition from the exciton state to the ground state is forbidden. Thus excitons that have absorbed radio-frequency quanta have considerably longer lifetimes against radiative deexcitation than ordinary excitons.

In an entirely analogous way the lifetime in the excited state is also lengthened for local electron centers that have absorbed radio-frequency quanta.

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PLANE PROBLEMS IN MAGNETOHYDRODYNAMICS

G. S. GOLITSYN

Moscow State University

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The conditions for potential motion in magnetohydrodynamics are deduced and such motions are investigated. The investigations reduce to the usual hydrodynamical problems. The Prandtl-Mayer problem for a conducting gas in a magnetic field and its generalizations and applications are studied in detail.

It is of interest to ascertain what problems of magnetohydrodynamics can be solved by classical methods. In this paper only potential motions are studied.

We write the set of equations of magnetohydrodynamics for the case of an ideally conducting medium in the form

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\nabla)\mathbf{v} + \frac{1}{\rho}(\nabla p + [\mathbf{h}\times\operatorname{curl}\mathbf{h}]) = 0,$$

$$\frac{\partial \ln\rho}{\partial t} + \mathbf{v}\nabla\ln\rho + \operatorname{div}\mathbf{v} = 0, \qquad \frac{\partial \mathbf{h}}{\partial t} = \operatorname{curl}[\mathbf{v}\times\mathbf{h}],$$

$$\frac{\partial}{\partial t}\left(\frac{p}{\rho^{\gamma}}\right) + \mathbf{v}\nabla\left(\frac{p}{\rho^{\gamma}}\right) = 0. \tag{1}$$

Here we use the notation $\mathbf{H} = \sqrt{4\pi}\,\mathbf{h}$. The remaining notation is standard. We limit ourselves here to adiabatic processes only.

We seek the conditions of potential flow. For this, employing a well known vector identity, we write the Euler equation in the form

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla\frac{v^2}{2} - [\mathbf{v}\times\operatorname{curl}\mathbf{v}] + \frac{1}{\rho}(\nabla p + [\mathbf{h}\times\operatorname{curl}\mathbf{h}]) = 0$$

and apply the curl operator:

$$\frac{\partial}{\partial t}\operatorname{curl}\mathbf{v} = \operatorname{curl}\,[\mathbf{v}\times\operatorname{curl}\mathbf{v}] - \operatorname{curl}\left\{\frac{\nabla p}{\rho} + \frac{1}{\rho}[\mathbf{h}\times\operatorname{curl}\mathbf{h}]\right\} \tag{2}$$

[$\operatorname{curl}(\nabla p/\rho) = \operatorname{curl}\nabla i = 0$, where i is the specific enthalpy]. Equation (2) is satisfied identically for $\operatorname{curl}\mathbf{v} = 0$ if only

$$\operatorname{curl}\left\{\frac{1}{\rho}[\mathbf{h}\times\operatorname{curl}\mathbf{h}]\right\} = \frac{1}{\rho}\operatorname{curl}\,[\mathbf{h}\times\operatorname{curl}\mathbf{h}] + \left[\nabla\left(\frac{1}{\rho}\right)\times[\mathbf{h}\times\operatorname{curl}\mathbf{h}]\right] = 0.$$

This equation is valid in two cases: first, where $\mathbf{h}\parallel\operatorname{curl}\mathbf{h}$, i.e., for the so-called force-free fields;[1] second, when