cannot be used as a criterion for deciding between these two transport models. However, given the signs of the J_{ij}, the signs of Hall mobilities can give information about the magnitude of the J_{ij}, i. e., about the width of the bands. Thus if all mobility components are found to be positive when the narrow band and hopping models predict some to be negative, the bands must be very wide compared with kT. The existence of any anomalous Hall mobility components, on the other hand, implies that at least in some directions the bands are not wide compared to kT. For anthracene some of the bands appear to be appreciably wider than kT,[12] so that theoretical prediction of the sign is only possible on the basis of quantitative calculations. A detailed discussion of the Hall effect in anthracene is given elsewhere.[13]

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†N. R. C. C. postdoctorate fellow 1968–70. Present address: Department of Natural Philosophy, University of Edinburgh, Scotland.

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Theoretical Investigation of the Possibility of Chemical Binding of Neutrons in F Centers*

D. W. Schlitt
Department of Physics, University of Nebraska, Lincoln, Nebraska 68508
(Received 31 December 1969)

A recent paper [Phys. Rev. Letters 23, 741 (1969)] reported experimental evidence that neutrons can be chemically bound to trapped electrons. The spin-independent electron-neutron interaction due to the electromagnetic structure of the neutron is found to be inadequate to produce such a bound state.

In a recent paper[1] Grant and Cobble report experimental evidence that neutrons are retained in LiF at 4 °K for periods greater than 30 sec and that this retention is related to the existence of trapped electrons in the LiF. Although the experiment does not identify the nature of the trapped electrons, both the method of producing the trapped electrons and the method of removing them point to F centers as the most likely candidate. If this interpretation of the experimental data is accepted then it is necessary to find a physical mechanism that will give a weak bond between a neutron and the electrons trapped in LiF. It is the purpose of this paper to investigate one such mechanism.

The model we investigate uses the following basic assumptions: (a) The neutron is bound to the F-center electron. (b) The F center consists of a negative ion vacancy with an electron trapped in it. (c) The interaction between the electron and the neutron is the attractive spin-independent electrostatic interaction determined by the neutron electromagnetic form factor.[2] (d) The interaction between the neutron and electron is sufficiently weak that we can neglect modifications to the F-center electron wave function due to the presence of the neutron.

The simplest "back of an envelope" calculation using the measured strength of the electron-neutron force is not encouraging. However, there are enough examples of the failure of crude estimates because of unexpected details of the physics that it seems worthwhile to investigate this problem in a little more detail. The calculations reported here take into account two distinctive features of the relevant neutron-electron system, the fact that the electron is already bound in the lattice of LiF and

that the electron-neutron force comes from the structure of the neutron.

Proceeding from these basic assumptions we consider the neutron as moving in an external electrostatic potential due to the ions of the crystal and the F-center electron. The binding energy can be determined by a variational calculation using the normalized neutron wave function $\psi(\alpha_i, \vec{x})$ where α_i are the variational parameters.

The expectation value of the energy is

$$\langle W(\alpha_i)\rangle = \langle \text{K. E.}\rangle + \langle \text{P. E.}\rangle, \tag{1}$$

where

$$\langle \text{K. E.}\rangle = (-\hbar^2/2M)\int d^3x \psi^*(\alpha_i, \vec{x})\nabla^2\psi(\alpha_i, \vec{x}). \tag{2}$$

Potential energy of the neutron. The neutron has an intrinsic charge distribution $\rho_{\text{int}}(\vec{x})$ which is determined by the electromagnetic form factors as described below. The probability of finding the neutron at $\vec{x}'$ is $\psi^*(\alpha_i, \vec{x}')\psi(\alpha_i, \vec{x}')$ or the charge density of the neutron at $\vec{x}$ is consequently

$$\int d^3x' \psi^*(\alpha_i, \vec{x}')\rho_{\text{int}}(\vec{x}-\vec{x}')\psi(\alpha_i, \vec{x}').$$

The expectation value of the potential energy of this charge distribution in the external electrostatic potential is

$$\langle \text{P. E.}\rangle = e\int d^3x\, d^3x' \psi^*(\alpha_i, \vec{x}')V(\vec{x})\rho_{\text{int}}(\vec{x}-\vec{x}')\psi(\alpha_i, \vec{x}')$$

$$= \int d^3x' \psi^*(\alpha_i, \vec{x}')V_{\text{eff}}(\vec{x}')\psi(\alpha_i, \vec{x}') \ . \tag{3}$$

For the potential $V(\vec{x})$ we will have

$$V(\vec{x}) = V_F(\vec{x}) + V_{\text{ion}}(\vec{x}), \tag{4}$$

where V_F is due to the F-center electron and V_{ion} is the contribution of the ions in the lattice. In this model we expect that the major part of the binding comes from V_F. The nearest-neighbor ions are positive and contribute a net repulsion. We argue that in order to take advantage of the attractive potential due to the electrons in the ions making up the lattice we must pay a prohibitive price in kinetic energy and, therefore at this stage in the calculation we neglect V_{ion}.

The F-center electron contribution to the potential will be calculated from a "known" electron wave function $\psi_F(\vec{x})$ and is

$$V_F(\vec{x}) = -e\int d^3x' \psi_F^*(\vec{x}')\psi_F(\vec{x}')\,|\,\vec{x}-\vec{x}'\,|^{-1} \ . \tag{5}$$

The intrinsic charge distribution of the neutron. The intrinsic charge density of the neutron $\rho_{\text{int}}(\vec{x})$ is found by taking the nonrelativistic limit of the neutron electromagnetic current. This is[3]

$$\rho_{\text{int}}(\vec{x}) = e(2\pi)^{-3}\int d^3q \exp(i\vec{q}\cdot\vec{x})$$

$$\times[F_1^N(q^2) - (K_N/4)\Lambda_N^2 q^2 F_2^N(q^2)]. \tag{6}$$

In this expression $K_N(=1.91)$ is the neutron anomalous magnetic moment in nuclear magnetons and F_1^N and F_2^N are the usual neutron electromagnetic form factors normalized to $F_1^N(0)=0$; $F_2^N(0)=1$. The nuclear compton wavelength is $\Lambda_N = \hbar/Mc$. This can be simplified by integrating by parts in the second term with the result that

$$\rho_{\text{int}}(\vec{x}) = ef_i(\vec{x}) - (eK_N/4)\Lambda_N^2\nabla_x^2 f_2(\vec{x}) \ , \tag{7}$$

where

$$f_i(\vec{x}) = (2\pi)^{-3}\int d^3q \exp(i\vec{q}\cdot\vec{x})F_i^N(q^2). \tag{8}$$

The experimental evidence[4] is consistent with the assumptions that

$$F_1^N(q^2) = 0 \quad \text{and} \quad F_2^N(q^2) = F_2^P(q^2). \tag{9}$$

We adopt these relations as assumptions.

Integration by parts in Eq. (3) gives

$$\langle \text{P. E.}\rangle = -(e^2K_N/4)\Lambda_N^2\int d^3x\, d^3x' \psi^*(\alpha_i, \vec{x}')$$

$$\times(\nabla_x^2 V(\vec{x}'-\vec{x}))f_2(\vec{x})\psi(\alpha_i, \vec{x}') \tag{10}$$

or

$$V_{\text{eff}}(\vec{x}') = -e^2K_N/4)\Lambda_N^2\int d^3x(\nabla_x^2 V(\vec{x}'-\vec{x}))f_2(\vec{x}) \ . \tag{11}$$

This result for V_{eff} depends only on the assumption that $F_1^N(q^2)=0$.

Binding to the F center. The F-center electron alone gives

$$V_{\text{eff}}(\vec{x}') = -e^2K_N\pi\Lambda_N^2\int d^3x\, \psi_F^*(\vec{x}'-\vec{x})\psi_F(\vec{x}'-\vec{x})f_2(\vec{x}) \ . \tag{12}$$

We will present two checks on the adequacy of this potential to bind a neutron. First, we will use the requirement for a bound state[5]

$$(\hbar^2/M) \lesssim -\int_0^\infty dr V(r)r. \tag{13}$$

Second, we will make a general order-of-magnitude estimate of $\langle \text{P. E.}\rangle$.

For the purposes of the first test we will assume a specific F-center electron wave function. The wave function chosen is like that used in the variational calculations of Smith[6]

$$\psi_F(\vec{x}) = N_F(1+\lambda r)\exp(-\beta r/2) \ . \tag{14}$$

Smith took $\beta = 2\lambda$ and $N_F^2 = \lambda^3/7\pi$. It is also necessary

to have an explicit expression for $f_2(x)$. From Ref. 4 we find a simple choice which fits the experiments is the exponential

$$f_2(\vec{x}) = (\delta^3/8\pi)\exp(-\delta r), \tag{15}$$

with $\delta = 4.32\times10^{13}$ cm^{-1}.

Combining (14), (15), and (12) leads to the result

$$V_{\text{eff}}(\vec{x}') = -(e^2K_N/8)\Lambda_N^2N_F^2\delta^3\int d^3x(1+2\lambda|\vec{x}'-\vec{x}| + \lambda^2|\vec{x}'-\vec{x}|^2)\exp(-\beta|\vec{x}'-\vec{x}|)\exp(-\delta r). \tag{16}$$

The integrals can be evaluated by straightforward but tedious methods. The complete result is too involved algebraicly to write in its entirety in this paper, but if we make use of the fact that δ is very large in comparison to λ and β (which are of order 10^8 cm^{-1}) we can extract the dominant terms.

With these approximations Eq. (16) becomes

$$V_{\text{eff}}(\vec{x}') = -e^2K_N\pi\Lambda_N^2N_F^2\delta^6r'^{-1}(\delta^2-\beta^2)^{-5}\{\delta^4r' \times(1+2\lambda r'+\lambda^2r'^2)e^{-\beta r'} + [\delta^2(4+\delta r')(\beta-2\lambda)+8\beta(9\lambda^2+\lambda\beta-\beta^2) + 2\beta\delta r'(12\lambda^2+\lambda\beta-\beta^2)]\exp(-\delta r')\}. \tag{17}$$

The neglected terms are smaller than those retained by factors like 10^{10}. This is sufficient to give the general flavor of the complete result.

Computation of $-\int_0^\infty dr\,V_{\text{eff}}(r)r$ results in a value of

$$e^2K_N\pi\Lambda_N^2N_F^2\beta^4(\beta^2+4\lambda\beta+6\lambda^2)(1+O(\beta^2/\delta^2))\approx(\hbar^2/m)10^{-8}. \tag{18}$$

This is strong evidence against a bound state.

Second, a qualitative argument can be made which will indicate the origin of this small number. From (3) and (12) it follows that

$$\langle\text{P. E.}\rangle \approx (10^{-34}\text{ eV cm}^3)\int d^3x\,d^3x'[\psi^*(\alpha_i,\vec{x}')\psi(\alpha_i,\vec{x}')] \times[\psi_F^*(\vec{x}'-\vec{x})\psi_F(\vec{x}'-\vec{x})]f_2(\vec{x}). \tag{19}$$

Each of the three factors in the integral is localized within a given volume and is normalized. The integral will have a maximum value when they have a maximum overlap and the order of magnitude of the integral will be of order of magnitude of the reciprocal of the largest volume. The order of magnitude of the volume occupied by the F-center electron must be about 10^{-24} cm^3 so the best we should expect to do would be

$$\langle\text{P. E.}\rangle \sim 10^{-34}\times10^{24}\text{ eV} = 10^{-10}\text{ eV}.$$

This final qualitative argument is of wider validity than this F-center model. It is based on Eq. (19) which comes from the analysis of the details of the neutron-electron interaction. Interpreting ψ_F as the wave function of the electron in the bound system we see that the over-all dimensions of the bound neutron-electron system must be much smaller than the dimensions characteristic of the lattice or the atoms in it, otherwise the potential energy is too small. Making the system smaller also increases the kinetic energy.

A variational calculation using $\psi(\alpha,\vec{x}) = N(\alpha)\times\exp(-\alpha r)$ has also been attempted. The only minimum of $\langle W(\alpha)\rangle$ for $\alpha \geq 0$ was at $\alpha = 0$ if it was assumed that $\alpha \ll \delta$ and $\beta \ll \delta$.

The clear conclusion from these calculations is that the neutron is not bound to the F-center electron by the spin-independent electron-neutron interaction. Either a much more complicated model using this interaction is required, or the spin-spin interaction is responsible for the binding.

Spin-spin interaction. No detailed calculations have been done using the spin-dependent interaction, but a crude estimate is not encouraging. The interaction energy should be of the order of magnitude of

$$\mu_e\mu_N\langle r^{-3}\rangle = (e^2/4)\Lambda_e\Lambda_N\langle r^{-3}\rangle \approx (3\times10^{-32}\text{ eV cm}^3)\langle r^{-3}\rangle,$$

where $\Lambda_e = \hbar/m_ec$. It seems reasonable that $\langle r^{-3}\rangle \sim 10^{24}$ cm^{-3} which leads to an energy of 10^{-8} eV. While this compares favorably with the electron-neutron interaction used above, it is not large enough to explain the experimental observations.

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