Letters to the Editor

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On the Interaction of Conduction Electrons with Lattice Vibrations

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BARDEEN[1-4] and Fröhlich[5,6] have recently proposed theories of superconductivity based on interactions between conduction electrons and the zero-point vibrations of the lattice. In his development, Bardeen views this interaction as giving rise to Brillouin zone boundaries with small energy gaps ($\sim kT_c$) at the Fermi surface of the electron distribution. Electrons with energies near the Fermi surface have small effective mass in consequence of the high curvature in their energy *versus* wave number relation at a zone boundary. Bardeen suggests that these are the superconducting electrons and indicates that it is possible to give a consistent interpretation for properties of superconductors in terms of the large diamagnetism exhibited by a gas of noninteracting electrons with small effective mass.

In this note we study the effective mass of conduction electrons which interact with the zero-point lattice vibrations. Fröhlich has calculated, with second-order perturbation theory, the self-energy of an electron interacting with the lattice normal modes of vibration (the phonon field). The energy denominators vanish and this perturbation procedure becomes invalid for virtual intermediate states which conserve energy.[7] Bardeen has avoided this difficulty with a variational treatment that leads to band structure in the energy *versus* wave number curve for the electrons. However, this result is obtained only after a questionable approximation for the mean energy of the virtual intermediate electron plus phonon states. We have calculated the energy of electrons interacting with the lattice vibrations by means of a Bloch-Nordsieck-type canonical transformation.[8] The B-N treatment is particularly suited to this type of problem, in which the energies associated with the crystal normal modes that are excited at low temperatures are very small compared with the electron energies. In this case neglect of electron recoil upon scattering with phonons introduces but a small error. Perturbation theory is avoided and, along with it, the vanishing energy denominators. We interpret our result as arguing against the conclusion that electrons have small effective mass in consequence of their interactions with the lattice normal modes.

The hamiltonian for electrons moving in a periodic lattice potential and interacting with normal modes of the crystal may be written as in reference 1. Neglect of the electrons' recoil upon scattering with the phonon field gives a hamiltonian that is linear in the electron momentum operators $-i\hbar\,\mathbf{grad}_j$. The Schrödinger equation with this hamiltonian is exactly soluble by means of a canonical transformation of the type introduced originally by Bloch and Nordsieck[8] in their study of the "infrared catastrophe," and used more recently in attempts at nonperturbation solutions for meson problems.[9] The eigensolutions correspond to a product of Bloch functions for individual electrons moving in a periodic lattice potential, multiplied by hermite functions for displaced zero-point oscillations of the phonon field, and multiplied by a factor expressing the interactions between the different electrons in consequence of their coupling with the lattice vibrations. The energy eigenvalues differ from those of the band theory for electrons moving in the periodic potential of the static lattice in the following way. In the periodic potential of a static lattice with period **a**, there occur forbidden energy bands for electrons with momenta in the neighborhood of $mv_i=\pi\hbar(n_i/a_i)$, where the n_i are integers. Electrons with these momenta suffer Bragg reflection. The lattice vibrations have the period **L**, the crystal dimensions, and they superimpose, on the above bands, forbidden energy bands for electrons which satisfy an analogous Bragg condition with the lattice vibrations,

$$\omega_f^2=[\mathbf{v}\cdot(\mathbf{\Lambda}_f-\mathbf{k}_n)]^2. \tag{1}$$

Here ω_f, the angular frequency of the lattice vibrations with wave vector $\mathbf{\Lambda}_f=2\pi(f_1/L_1, f_2/L_2, f_3/L_3)$, is given by $\omega_f=s\Lambda_f$; s is the velocity of sound in the crystal, the f_i are integers, and $\mathbf{k}_n=2\pi(n_1/a_1, n_2/a_2, n_3/a_3)$ is a reciprocal lattice vector.[10] The width of these forbidden bands is

$$\sim(\text{amplitude of the lattice potential})/(\text{number of unit cells in the crystal})^{\frac{1}{2}}.$$

It is thus very small. These narrow forbidden bands occur throughout the electron distribution at momentum values that satisfy the condition in Eq. (1). They do not critically change the energy levels of the conduction electrons and hence do not critically alter their effective mass. A first-order perturbation treatment of the neglected electron recoil yields a small correction ($\sim s/v$) to these results.

In summary, our calculations do not indicate a small effective mass for electrons in consequence of their interactions with lattice vibrations. The energy shell distribution as proposed by Fröhlich does not appear to be energetically preferred. When other important factors such as the interelectron coulomb repulsion are considered, one may hope to find an adequate theory of superconductivity developed along lines of these very attractive physical proposals of Bardeen and Fröhlich. A manuscript discussing the details of this calculation is in preparation. Valuable discussions with Professor L. I. Schiff are gratefully acknowledged.

[1] J. Bardeen, Phys. Rev. **80**, 567 (1950).
[2] J. Bardeen, Phys. Rev. **81**, 469 (1951).
[3] J. Bardeen, Phys. Rev. **81**, 829 (1951).
[4] J. Bardeen, Phys. Rev. **81**, 1070 (1951).
[5] H. Fröhlich, Phys. Rev. **79**, 845 (1950).
[6] H. Fröhlich, Proc. Phys. Soc. (London) **A64**, 129 (1951).
[7] Fröhlich takes principal values in the integration over intermediate states.
[8] F. Bloch and A. Nordsieck, Phys. Rev. **52**, 54 (1937).
[9] Lewis, Oppenheimer, and Wouthuysen, Phys. Rev. **73**, 127 (1948); S. D. Drell, Phys. Rev. **83**, 555 (1951).
[10] These bands do not appear in Fröhlich's work because he takes principal values for his integrals over the intermediate states.

Anomalous Intensity Distribution of Rotation Lines in Fundamental Vibration Bands in Triatomic Molecules*

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A MECHANISM will be discussed here to account for the anomalous intensity distribution of the rotation lines in certain fundamental bands in the infrared spectra of triatomic molecules, notably in the 3.8-μ band in the H_2S spectrum. The theory assumes that it is necessary to take into account the mixing of the wave functions for a given rotation state in a vibration level with the wave functions of rotation states in other vibration levels in order to calculate the intensities with accuracy. The mixing must be between wave functions of the first excited states of the three vibration frequencies to give a first-order effect. Such a mixing may come about through the coupling of the vibrations through the Coriolis operator $p_z P_z/I_{zz}$, the z axis having been chosen as the axis of spin of the molecule. The mixed wave function

for the first excited state of the unsymmetrical vibration ν_3 takes the form

$$\psi(0,0,1,J,K,M)=\{\psi^0(0,0,1)-iKC\sum_{s=1}^{2}[\zeta_{3s}/(\omega_3-\omega_s)]\times[(\omega_3+\omega_s)/(\omega_3\omega_s)^{\frac{1}{2}}]\psi^0(V_s=1,V_{s'}=0)\}\Theta(\theta,\psi)e^{iK\xi},$$

C being $h/8\pi^2I_{zz}c$ and ζ_{3s} the Coriolis coupling factors which depend upon the nature of the normal coordinates. Similar wave functions are obtained for the first excited states of ν_1 and ν_2.

Assuming the dipole moment induced by vibration to be

$$E=\sum_{s=1}^{3}a_sq_s,$$

where a_s is a constant and q_s are the normal coordinates the intensities of the lines in ν_s ($s=1$, 2 or 3) are proportional to the squares of the matrix elements $(0,0,0,K|I|V_s=1,V_{s'}=0,K\mp1)$, which are the following

$$(0,0,0,K|I|V_s=1,V_{s'}=0,K\mp1)=\{a_s\pm\Sigma'_{s'}a_{s'}(K\zeta_{3s'}C/\Delta_{s'})[(\omega_s+\omega_{s'})/(\omega_s\omega_{s'})^{\frac{1}{2}}]\},$$

$\Delta_{s'}$ being $\omega_s-\omega_{s'}$.

It is, of course, well known that in molecules like H_2O and H_2S the band ν_2 is intense compared with the band ν_3, which is intense compared with ν_1, i.e., $a_2\gg a_3\gg a_1$. Taking ω_1, ω_2, and ω_3 to be 2610 cm^{-1}, 1290 cm^{-1}, and 2684 cm^{-1} for H_2S and letting $C=h/8\pi^2I_{zz}c$ be approximately 5 cm^{-1} and finally assuming the values of $\zeta_{31}=4.5\times10^{-3}$ and $\zeta_{32}=-1.0$ calculated by Darling and Dennison[1] for water vapor to be valid for H_2S as well, it may be shown that the term in I containing a_1K may be neglected. Moreover, the factor I will decrease to zero as the term containing a_2K approaches 1.4×10^2a_3 for transitions of the type $K\rightarrow K-1$. I will, for the same value of K, have assumed double its original value for transitions of the type $K\rightarrow K+1$. Since $a_2\gg a_3$, the above may happen for small values of K (i.e., $K\approx10$). The general effect upon the intensities is to enhance the transitions $K\rightarrow K+1$ at the expense of the transitions $K\rightarrow K-1$. By choosing the ratio of a_2 to a_3 in the proper manner the transitions $K\rightarrow K-1$ can almost entirely be suppressed so that, as in the case of H_2S, only about one-half of the band may be observed.

The effect of the perturbation on the band ν_2 is small and would probably not be observable. The effect of the perturbation on ν_1 is less readily estimated, but would probably not be observable as long as $a_3\gg a_1$.

* This work was assisted by the ONR.

[1] B. T. Darling and D. M. Dennison, Phys. Rev. 57, 128 (1940).

Magnetic Moments of Even-Odd Nuclei

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THE success of the shell model[1] indicates that it is a good approximation to consider even-odd nuclei as single-particle systems with the odd nucleon moving in a spherically symmetrical potential provided by the even-even core. The model leads thus to the basic classification of nuclear states by the orbital angular momentum $l\hbar$ of the odd nucleon as well as by the spin I and to the expectation that the magnetic moment μ should have one of the two Schmidt values,[2] determined by $l=I\pm\frac{1}{2}$.

Two modifications have been proposed to explain the observed deviations from these values:

A.—l is not a good quantum number, and nuclear states represent actually a mixture of states[3] with $l=I+\frac{1}{2}$ and $l=I-\frac{1}{2}$.

B.—A tidal wave which contributes to μ can be formed in the core by the interaction with the odd nucleon.[4]

It has been pointed out before[4] that either modification has its peculiar serious difficulties: modification A requires a considerable mixing of states which, according to the shell model, are widely separated in energy and which have different parity in the odd nucleon; modification B fails to give deviations from the Schmidt values for nuclei with $I=\frac{1}{2}$, while they occur here actually with comparable magnitude as for other nuclei. Unless they are considered as small corrections, insufficient to explain the observed deviations, both proposals require besides a major departure from essential features of the shell model.

TABLE I. The effective intrinsic moment μ' of the odd nucleon, calculated from the Landé formula for an even-odd nucleus with magnetic moment μ, spin I and for both values of the orbital quantum number $l=I\pm1/2$.

	Odd proton	Odd neutron
l	μ'_P	μ'_N
$I-1/2$	$\mu-I+1/2$	μ
$I+1/2$	$I+(3/2)-(I+1/I)\mu$	$-(I+1/I)\mu$

We propose an alternative interpretation of the empirical results which is compatible with a strict adherence to the shell model.

C.—The intrinsic magnetic moment of the odd nucleon is affected by the binding to the core; depending upon the nucleus, it can differ by an appreciable amount from the magnetic moment of the free nucleon.

Accepting this interpretation, one can use the Landé formula to determine the effective intrinsic moments μ_P' or μ_N' of the odd proton or neutron, respectively, from the observed magnetic moment μ and spin I of an even-odd nucleus. They are given in Table I for either alternative $l=I\pm\frac{1}{2}$ in units of the nuclear magneton.

Using available data for both odd-proton and odd-neutron nuclei, we have plotted in Fig. 1 the corresponding deviations $\Delta\mu_P=\mu_P-\mu_P'$ and $\Delta\mu_N=-(\mu_N-\mu_N')$ of the intrinsic moment from its magnitude $\mu_P=2.79$ and $-\mu_N=1.91$ in the free nucleon against the number n of odd nucleons up to $n=83$. For each nucleus the assignment of l in Table I was made according to the shell model, i.e., according to the Schmidt value which is closer to μ; it leads in our presentation equivalently to the smaller deviation $\Delta\mu$.

Within minor fluctuations and particularly up to $n=40$, the odd neutron points not only follow remarkably well those for the odd protons[5] but the plot reveals also a certain regularity for both: a very coarse general trend, indicated by C_1, exhibits an initial rise to the approximately constant value $\Delta\mu\cong1$ for $n>20$. A pronounced alternating variation is superimposed on this general trend and is indicated by C_2; its periods are evidently related to the shells, closed at $n=2$, 8, 20, 50, 82, insofar as the maxima occur approximately in the middle and the minima towards the end of each shell. Possible secondary variations in the second half of the fourth and fifth shell are indicated by

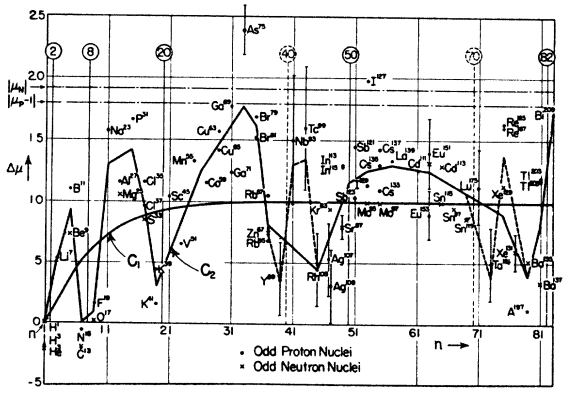

FIG. 1. The defect $\Delta\mu$ of the effective intrinsic moment of the odd nucleon *versus* the number n of odd nucleons in even-odd nuclei. Odd-proton nuclei are indicated by dots, odd-neutron nuclei by crosses. The encircled numbers on top represent the closing of shells; the subshells closed before the filling of the $g_{9/2}$ and $h_{11/2}$ states, are indicated by broken numbers and circles.