



FIG. 1. Schematic dependence of rotational energy levels on the magnitude S of hindrance to rotation. Full lines represent symmetric states. Broken lines represent antisymmetric states.

pared with the period of rotation, the energy values of the states could not be sharply defined, and would be spread over a range of the same order as the energy itself. Thus, we could not assume, in this case, the existence of a finite gap between the ground and excited states.

Without committing ourselves as to its validity, let us then for the moment accept the alternative assumption; namely that the lifetime is long compared to the period. This means that the orientation of the rotation of a given pair is fixed and we must require that the hindrance to rotation (the magnitude of which we denote by a parameter S) provided by neighboring atoms is constant in time for that particular pair. For example, if we suppose, with Rice, that the average hindrance corresponds roughly to restricting a pair to motion in a plane, we could represent by S the maximum of potential as a function of angle in this plane; the potential being that of the van der Waals repulsive forces due to other atoms. We note that the effective diameter of the rotational orbits is of the same order as the mean distance between atoms, and that the whole system is to represent a *liquid* state. Even at the absolute zero of temperature the fluctuations in the relative positions of neighboring atoms should then result in some pairs having no other atoms within their orbit—these will be nearly free to rotate ($S \rightarrow 0$). Others must find neighboring atoms within their orbit so as completely to restrict their rotation ($S \rightarrow \infty$). We do not require an infinite local density to make S infinite; we merely require a few neighboring atoms (which must be considered fixed, if S is to be constant) sufficiently close to prevent our pair of atoms from exchanging position. We are thus forced to the conclusion that S will assume values ranging from zero to infinity for different pairs in the liquid.

Figure 1 indicates the well-known way in which the rotational energy levels vary with the magnitude of restriction. For large S , each level becomes degenerate, a component arising from what were both odd and even J values (angular momentum) when $S=0$.

Now for J even (or zero), the state is symmetric in the space variables; for odd J , antisymmetric. If the atoms we are considering are Fermi particles with spin $\frac{1}{2}$ (He^3 atoms), the even- J states must be antisymmetric in the spin variables—i.e., the atoms in the pair have opposite spin. For odd J the spins must be parallel. We must consider both odd and even rotational states and the preceding argument shows that the energy difference between the ground and first excited states for different pairs is not the same, but must include values ranging down to zero. If, however, our atoms are Bose particles (He^4) we must include only those rotational states which are symmetric—i.e., those with even J . In this case, the excited and lowest state do not degenerate, and we would expect a finite minimum energy for excitation.

If we can assume that there is no short-range crystalline order in a quantum liquid, our conclusion then is that the pair-rotator model leads to results qualitatively different for atoms of different statistics. Unlike He^4 , He^3 does not possess a finite energy gap. Dr. Rice, in private discussions, has suggested that it may, after all, be a sufficient condition for superfluidity, if some (rather than all) atoms have a nonvanishing minimum excitation energy; thus in liquid He^4 near the λ point, only a small fraction is superfluid. Our argument above can say nothing, of course, about the criterion for superfluidity, but it may be pointed out that this suggested sufficient condition would be satisfied even by an ideal gas of Fermi particles at low enough temperatures.

It may be added that the agreement³ with the observed entropy, susceptibility, etc., that can be achieved by assuming a sharp spectrum would not be greatly altered by the spreading of the levels discussed here, since present experimental results only extend down to temperatures where the effects of such spreading should be small.

† Work supported in part by the National Science Foundation.

¹ O. K. Rice, Phys. Rev. **97**, 558 (1955).

² P. J. Price, Phys. Rev. **97**, 259 (1955); O. K. Rice, Phys. Rev. **97**, 263 (1955).

³ H. N. V. Temperley, Phys. Rev. **97**, 835 (1955).

Interpretation of Donor State Absorption Lines in Silicon*

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IN a recent note,¹ we have reported theoretical results for the positions of excited electronic donor levels in Si. Somewhat similar results were also obtained independently by Kleiner.² In the meantime Burstein,

Picus, and Hennis³ have informed us of results of infrared absorption measurements on arsenic- and phosphorus-doped silicon. We should like to suggest an interpretation of their absorption lines leading to very good agreement with our theoretical results, which have since been supplemented by calculations of the $(3p, m=\pm 1)$ level and of oscillator strengths, as well as by a more refined calculation of the $(2p, m=0)$ level, which in reference 1 had a slightly larger uncertainty.

Theoretical results for the lowest four excited states to which optical transitions take place at all appreciably are listed in Table I. The quoted intensities are for

TABLE I. Optically excited donor states; theory.

States	Energy below continuum (in units of 0.01 ev)	Intensity of transition from 1s ground state (arbitrary scale)
$2p, m=0$	-1.09 ± 0.02	4.0
$2p, m=+1$ and -1	-0.59 ± 0.01	10.6
$3p, m=0$	-0.57 ± 0.06	0.4
$3p, m=+1$ and -1	-0.29 ± 0.005	3.1
$4p, f, m=+1$ and -1	No detailed results	No detailed results

arsenic donors and have an uncertainty of perhaps ± 30 percent (phosphorus donors give slightly different values.)

It will be seen that the $(1s)-(3p, m=0)$ transition is quite likely to escape detection in view of its small intensity and the proximity of the latter level to the $(2p, m=\pm 1)$ level (see Table I). The lowest three observed transitions I, II, III should then be associated with the $(2p, m=0)$, $(2p, m=\pm 1)$ and $(3p, m=\pm 1)$ levels. The fourth observed transition, IV, is very likely to be associated with the $(4p, f, m=\pm 1)$ level but no detailed theoretical results are available.

Table II contains the experimental results with the suggested interpretation and Table III compares the

TABLE II. Observed infrared absorption lines.^a

Observed line	Energy above the ground state (in units of 0.01 ev)	
	As-donors	P-donors
I: $(1s) \rightarrow (2p, m=0)$	4.23	3.44
II: $(1s) \rightarrow (2p, m=\pm 1)$	4.72 ^b	3.97
III: $(1s) \rightarrow (3p, m=\pm 1)$	5.06	
IV: $(1s) \rightarrow (4p, f, m=\pm 1)$	5.21	

^a These were kindly communicated to us by Dr. Picus and are more accurate than those mentioned in reference 2.

^b E. Burstein *et al.*, find consistently a small secondary peak on this line which may be associated with the $3p, m=0$ level (see Table I).

spacings between the observed lines with the corresponding theoretical spacings. The agreement between theory and experiment is very satisfactory.⁴

By combining the experimental energy differences between the excited states and the ground state with the theoretical positions of the excited states, relative to the continuum, we obtain the following ionization

TABLE III. Spacings of excited states.

States	Energy difference (in units of 0.01 ev)	
	Theory	Observed
$(2p, m=\pm 1)$ $-(2p, m=0)$	0.50 ± 0.02	0.49 (As) 0.53 (P)
$(3p, m=\pm 1)$ $-(2p, m=\pm 1)$	0.30 ± 0.01	0.34 (As)
$(4p, f, m=\pm 1)$ $-(3p, m=\pm 1)$	No detailed results	0.15 (As)

energies of the ground states. As: 0.0533 ± 0.0003 ev; P: 0.0455 ± 0.0003 ev.

The agreement between theory and experiment, which has been described, constitutes a verification of the consistency of the effective mass formalism: The same effective masses which govern cyclotron resonances also determine quite accurately the positions of the impurity states of "p"-symmetry, as had been theoretically anticipated.⁵

A detailed report is in preparation.

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¹ W. Kohn and J. M. Luttinger, Phys. Rev. **97**, 1721 (1955); see also Phys. Rev. **98**, 1561(A) (1955).

² W. H. Kleiner, Phys. Rev. **97**, 1722 (1955). I am indebted to Dr. Kleiner for sending me a copy of his paper before publication.

³ I am grateful to these authors for acquainting me with their results, obtained with Bell Telephone Laboratories specimens, which will shortly be published.

⁴ W. H. Kleiner, reference 2, has associated the lowest four transitions with the $(2p, m=0)$, $(2p, m=\pm 1)$, $(3p, m=0)$, and $(3p, m=\pm 1)$ levels. By not omitting the $(3p, m=0)$ level he finds poor agreement between theory and experiment.

⁵ W. Kohn and J. M. Luttinger, Phys. Rev. **98**, 915 (1955). The position of the ground state is not well described by the theory (which predicts -0.029 ev for all donors) because it penetrates into the imperfectly understood region near the donor nucleus.

New Method in X-Ray Crystal Structure Determination Involving the Use of Anomalous Dispersion

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WHEN incident x-rays strike a crystal, and the wavelength of the x-rays is just shorter than a resonance level of a particular atom in the crystal, the radiation is scattered with abnormal phase and amplitude. In such a case, Friedel's rule does not hold, and $|F_{hkl}| \neq |F_{\bar{h}\bar{k}\bar{l}}|$. Excellent use of this phenomenon has been made in determinations of absolute configurations of structures which may exist in enantiomorphous arrangements.¹ The technique employed heretofore has involved determination of the structure except for choice between enantiomorphous forms, without anoma-