

FIG. 1. Comparison of the observed and calculated intensity-dependent sound velocity. The experimental points are taken from Mash <u>et al</u>. (Ref. 2).

the incident beam before focusing. If breakdown occurs the intensity does not increase with decreasing f. The deviation of sound velocity should be independent of f.

In Fig. 1 we compare the observed values of intensity-dependent sound velocity with the values calculated using Eq. (7) (solid curve). The adiabatic sound velocity in N₂ at 125 atm is taken to be 397 m/sec (see Madigosky, Monkewicz, and Litovitz, Ref. 2), and c is taken to be 5×10^2 m⁴/sec². The broken curve shows the case that breakdown occurs. The corresponding breakdown

intensity calculated from the observed maximum change of sound velocity and Eq. (6) is $|e_l|^2 = 9.4 \times 10^{11} \text{ esu/cm}^2$ ($\rho_0 \partial \epsilon / \partial \rho \cong \epsilon - 1 = 7.5 \times 10^{-2}$, $\rho_0 = 0.156 \text{ g/cm}^3$ for N₂ at 125 atm). This value is also in good agreement with the breakdown intensity $|e_l|^2 = 3 \times 10^{11} \text{ esu/cm}^2$ observed by Krasyuk, Pashinin, and Prokhorov.⁵

For liquids and solids the velocity of sound is much larger and the threshold intensities for breakdown and SBS are lower, thus the intensitydependent effect becomes negligible.

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POLARIZATION OF CHANNELED DEUTERONS*

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We advance a possible explanation of the recent experiments by Kaminsky on the polarization of deuterons passed through a magnetized Ni single crystal. The large polarization is attributed to a strong preference for ionization of the deuterium atoms which have an electron spin opposite to the direction of the magnetic field.

Kaminsky¹ has recently reported the production of a beam of polarized deuterons, using channeling through a Ni crystal. The technique involves passing the beam along the [110] direction of a thin-film (~1- μ m) single crystal of Ni magnetized to saturation in a [111] direction in the plane of the film. That portion of the emergent beam which consists of well-channeled neutral D atoms, i.e., those which are traveling still along the [110] direction and have suffered a reduced energy loss, is selected out and passes through a weak magnetic field. The polarization of the deuterons from this component is measured by the reaction T(d, n)He⁴. The quoted result is a tensor polarization $P_{zz} = -0.32 \pm 0.01$, which corresponds to a fractional population of the deuteron $m_I = 0$ state $N_0 = 0.440 \pm 0.003$.

The polarization presumably arises from the

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preferential attachment of electrons of one sign of spin. Thus, when the neutral deuterium atom emerges from the foil, the strong-field (Paschen-Back) states are selectively populated. If the transition to the weak field is adiabatic, this leads to a selective population of the hyperfine states, and thus to a polarization of the deuteron. In other words, the electron polarization is transferred to the deuteron by the hyperfine interaction.

That such a process should occur is completely reasonable. What is difficult to understand is the magnitude of the nuclear polarization so achieved. In fact, if n_+ represents the fraction of channeled deuteron atoms emerging from the foil with spins along the magnetic field, then the three hyperfine states with $F = \frac{3}{2}$, $M_F = \frac{3}{2}$, $\pm \frac{1}{2}$ have fractional populations $\frac{1}{3}n_+$, and the states $F = \frac{3}{2}$, $M_F = -\frac{3}{2}$, and $F = \frac{1}{2}$, $M_F = \pm \frac{1}{2}$ have populations $\frac{1}{3}(1-n_{+})$. This assumes no polarization of the deuterons at this stage, which is reasonable since the transit time through the foil (~5×10⁻¹² sec) is short compared with hyperfine periods. This implies, however, that the fractional population of the $m_I = 0$ state, N_0 , is given by $N_0 = (\frac{2}{9})$ $\times (1 + n_{+})$. The observed value thus would require $n_{\pm} = 0.98 \pm 0.01$. This seems surprisingly high, especially since the effective magneton number of Ni is about 0.6; i.e., 9.4 of the possible ten 3d states in Ni are occupied. Since the 4s-p band is so broad, it is reasonable to consider it to be unpolarized.²

The purpose of this note is to point out a mechanism which can give rise to very large electron polarizations. Indeed, crude calculations indicate the possibility of n_+ values greater than 0.9, and, in view of the approximations involved, values approaching those implied by Kaminsky's measurements may not be unreasonable.

We begin by observing that for incident particle velocities of the order of $v_0 = \alpha c$, the velocity of the electron in the first Bohr orbit of hydrogen, the cross sections σ_c and σ_l for electron capture and loss in atomic collisions are of the order of πa_0^2 . Thus the deuteron undergoes a number of electron-capture and -loss collisions in its passage through the film. It is easy to see that under these circumstances, the fraction of deuterium atoms emerging with electron spin up relative to those with spin down is given by

$$n_{+}/n_{-} = (\sigma_{c}^{(+)}/\sigma_{c}^{(-)})(\sigma_{l}^{(-)}/\sigma_{l}^{(+)}).$$
(1)

Here $\sigma_c^{(\pm)}$ and $\sigma_l^{(\pm)}$ denote the cross section for spin-up (+) and spin-down (-) electron capture

and loss. If we assume that capture occurs primarily from the 3d states then it is reasonable to take $\sigma_c^{(+)}/\sigma_c^{(-)} \approx 5/(4.4)$. The situation is somewhat different for electron-loss processes, however. We may separate the electron-loss cross section into partial cross sections representing loss to the 3d and loss to the 4s-p (and all other unfilled) bands. Thus we may say $\sigma_{r}^{(\pm)}$ $=\sigma_1^{(\pm)}(3d) + \sigma_1^{(\pm)}(4s)$, but since the spin-up 3dband states are all filled, we must have $\sigma_1^{(+)}(3d)$ =0. Then if the a priori probability for electron loss to a 3d state is much greater than that for loss to a 4s-p or higher state, it is possible to produce a large value for $\sigma_i^{(-)}/\sigma_i^{(+)}$ and a correspondingly large ratio n_+/n_- . In other words, we envision a pumping of electrons from spindown to spin-up deuterium states. Once the electron has spin up, its chances for loss are materially reduced.

The big question is, of course, whether there exists such a preference for loss to 3d over loss to 4s-p or other states. We wish to argue that such a preference is to be expected, at least for the channeled particles selected in the experiment. The collimation system used on the neutrals emerging from the film indicates that they have at most $\sim 2-3$ eV of transverse energy. If the Fermi-Thomas potential suggested by Lindhard³ is used to describe the interaction between the deuteron or deuterium and the Ni atoms, it may be concluded that these particles have not approached closer than about $2a_0$ to a string of Ni atoms. The center of the [110] channel is $2.35a_0$ from one pair of strings, and $3.33a_0$ from the other pair. Thus ionization must come from collisions of the deuterium electron with the electrons and nuclei of the crystal, collisions which must be reasonably close to permit the energy transfer necessary for ionization. Basically, then, the ionization comes principally from that component of the deuterium wave function which extends out to regions where the Ni charge density is appreciable. However, the outermost part of the Ni charge density is provided chiefly by the 3d electrons. It follows therefore that it is in just this region that the amplitude of the 3d wave function for Ni is much greater than that for the 4s, so we may expect ionization to the 3d band to be considerably more likely than to the 4s-pband. Further enhancement is provided by the circumstance that close to the Ninucleus, both the 4s and 4p wave functions oscillate rapidly compared with the rate of change of atomic potential. The matrix element for transfer to the 4s-p

band thus experiences a considerable cancelation.

As an approximation to the radial 3d wave function in the crystal we may take the Hartree-Fock wave function⁴ for the isolated atom. We recognize that close to the nucleus the 4s and 4p wave functions should approximate those of the free atom. We have arbitrarily modified these wave functions by extending them as constant from the peak of the last maximum in the free-atom wave function to the boundary of the atomic volume. Such wave functions are probably not too unrealistic and contain both the qualitative features alluded to above.

In order to make these ideas more quantitative, we have calculated by Born approximation the relative probabilities of ionization to the 3d or to the 4s-p band states. In this calculation the motion of the deuteron has been treated classically and assumed to consist of a straight-line trajectory down the center of the channel. Deviations from this are slight and presumably would tend to increase the probability of transfer to the more localized 3d state. The deuterium atom is taken to be in its ground state before ionization; again, a higher state would provide a broader extent to the electronic wave function and thus an enhanced 3d probability.

For simplicity, the calculation has been made only for those final states which correspond to no excitation of the Ni atoms. The argument here is based on energy considerations. Any appreciable excitation of the crystal atoms, i.e., an excitation involving k vectors which extend a significant distance to the boundary of the first Brillouin zone, requires an energy which is comparable with a Rydberg. Since, however, the initial energy is lower than the final one, any additional excitation may be expected to favor the 3d final state over the 4s-p ones, which already are higher in energy. To put it another way, the number of 4s-p states which participate is determined by the total energy available. If the Ni crystal is excited, the number of permitted 4s-p states is correspondingly reduced.

By restricting ourselves to elastic, or almost elastic, ionization processes, we are able to take as the perturbing potential the shielded Coulomb potential experienced by an electron in the field of the Ni atom. This has been chosen to be the modified Hartree-Fock-Slater potential given by Herman.⁵ Presumably it is only the long-range tail of this potential which is significantly modified by the presence of the other atoms in the crystal. Various trials indicate that a modification of this tail seems to have little effect on the relative probability of ionization to the 3d or 4s-p bands.

Experience indicates that the Born approximation is rarely in error by more than a factor of 2, even at these energies. It seems reasonable to expect that it would predict the ratio between transfers to 3d and 4s-p states much better than this.

The result of this calculation is that the probability for transfer to a vacant 3d state is roughly a factor of 100 greater than the probability of transfer to a low-lying 4s-p state. Furthermore, the probability of transfer varies exponentially with the energy of the final state as

 $P(\epsilon) \propto \left[1 + (\epsilon a_0/\hbar v)^2\right]^{-3/2}$

$$\times \exp\{-(2b/a_{0})[1+(\epsilon a_{0}/\hbar v)^{2}]^{1/2}\},$$
(2)

where ϵ is the final state energy, v is the electron velocity, and $b/a_0 = 2.35$ is the impact parameter in atomic units. We note that $[P(0)]^{-1} \times \int_0^{\infty} dP(\epsilon) \approx 0.8$ Ry.

The total density of 4s - p states (of a given sign of electron spin) is approximately⁶ 2 atom⁻¹ Ry⁻¹ at this energy. The density of 3d spin-down states may be represented approximately by $0.6\delta(\epsilon)$ in the narrow-band approximation. Upon integrating this over final-state energies we find that the density-of-states factor favors transitions to the 4s - p states by a factor which is approximately $2 \times 0.8/0.6 \approx 2.7$. Therefore, our estimate for the ratio $\sigma_i^{(-)}(3d)\sigma_i^{(+)}(4s)$ is 100/2.7 ≈ 37 . Thus we find $\sigma_i^{(-)}/\sigma_i^{(+)} \approx 38$, which implies that $n_+ \approx 0.98$.

We do not suggest that this agreement is anything more than fortuitous, or indeed that the probability of transfer to 3d states should be nearly as great as 100 times that of the 4s-ptransfer. It is likely that transfers to the 4s-pband in which the crystal is excited involve matrix elements which may be somewhat larger than those calculated here, since the degree of cancelation of the 4s-p wave functions would be reduced. However, if we were to increase the probability of transfer to the 4s-p band by a factor of 4, keeping the 3d transfer probability the same, we still would achieve an electron polarization $n_+ \approx 0.92$.

These calculations are admittedly very crude; more refined analyses are in preparation. Nevertheless, this seems to provide a possibility of understanding these very interesting experimental results. Crucial tests of this hypothesis could be provided by studying the dependence of the final polarization on velocity of the electrons, by varying the angle of acceptance of the final collimating system so as to sample different channeling trajectories, and finally, of course, by replacing the Ni film by a ferromagnetic film in which one component of the d band is not completely filled.

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CLASSICAL GREEN'S FUNCTIONS FOR THE IDEAL GAS*

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We use the equation-of-motion technique to establish a chain of equations for retarded, double-time Green's functions of an ideal gas. Exact termination of this chain allows reproduction of the usual results obtained by other methods.

Bogolyubov and Sadovnikov¹ have introduced double-time retarded and advanced Green's functions into the statistical mechanics of classical systems. This development is of course closely related to the earlier work of Kubo.² In their paper, Bogolyubov and Sadovnikov established a hierarchy of classical Green's functions by varying the single-time distribution functions of the Bogolyubov-Born-Green-Kirkwood-Yvon hierarchy with respect to an infinitesimal external field. For a Coulomb plasma, the simplest decoupling of this system allowed them to obtain the usual Debye form for the correlation function. The method was used by Sadovnikov in a number of papers.³⁻⁵ Herzel⁶ rederived the Bogolyubov-Sadovnikov Green's function hierarchy using the double-time theory of Rostoker.

This Letter investigates the problem of evaluating the Green's function related to the density correlation of an ideal gas. In contradistinction to the Bogolyubov-Sadovnikov approach,¹ we establish a hierarchy by the equation-of-motion technique common to the development of hierarchies for quantum systems.^{7,8} We thereupon introduce a device which allows exact decoupling of the hierarchy.

To begin, we consider the ideal gas, which has a Hamiltonian given by

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m}.$$
 (1)

The number density is given by

$$n(\mathbf{\bar{r}},t) = V^{-1} \sum_{i=1}^{N} \sum_{\mathbf{\bar{k}}} e^{i \mathbf{\bar{k}} \cdot [\mathbf{\bar{d}}_{i}(t) - \mathbf{\bar{r}}]}.$$
(2)

The retarded Green's function we wish to calculate is

$$\langle \langle \boldsymbol{n}(\boldsymbol{x}); \boldsymbol{n}(\boldsymbol{y}) \rangle \rangle = V^{-2} \sum_{\substack{\mathbf{k} \mid \mathbf{i} \\ \mathbf{k} \neq \mathbf{i}}} \sum_{i,j=1}^{N} G_{ij \, \mathbf{k} \uparrow \mathbf{i}}^{-i} (\tau) e^{-i(\vec{\mathbf{k}} \cdot \vec{\mathbf{r}} + \mathbf{i} \cdot \vec{\mathbf{r}}')}$$
(3)

where V is the volume of the system, $x = (\mathbf{\tilde{r}}, t), y = (\mathbf{\tilde{r}'}, t')$, and

$$G_{ij\vec{k}\vec{1}}{}^{0}(\tau) = \theta(\tau) \langle [e^{i\vec{k}\cdot\vec{q}_{i}(\tau)}, e^{i\vec{1}\cdot\vec{q}_{j}(0)}] \rangle \equiv \langle \langle e^{i\vec{k}\cdot\vec{q}_{i}(\tau)}; e^{i\vec{1}\cdot\vec{q}_{j}(0)} \rangle \rangle.$$

$$\tag{4}$$

Here $\theta(\tau)$ is the unit step function, $\langle \cdots \rangle$ indicates a statistical average, and $[\cdots]$ Poisson brackets.