phonon line at 0.528 eV. We note that in the O^0 emission there are also two local-mode replicas of the weak no-phonon line. In the O^- situation, we have predicted a local mode due to oxygen alone at 13.1 meV. This is close to the 11-meV difference between the 0.517-eV line and the weak 0.528-eV line. We do not have a complete explanation of either the 28.4-meV O^0 or 8-meV O^- lines but we feel that they are probably related to modes in the unperturbed phonon spectrum to which are weakly coupled the closely adjacent oxygen vibrations (24.7 or 13.1 meV) in the two cases.

The question of the metastable lifetime is a difficult one. If the only motion to go from the metastable to the rebonded configuration were that of oxygen, one would expect the lifetime to be rather short. If substantial rearrangement of the surrounding gallium atoms is also required, it could be much longer. We feel that we have made a strong case that the metastable transition has been observed. This argues for a substantial gallium distortion, such as would be expected for a rebonded configuration as suggested by Henry and Kukimoto.

Clearly, work designed to understand the mechanism of the newly observed luminescence may shed light on the role of the proposed metastable O^- in the GaP:O system.

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Charge States for Protons Moving in an Electron Gas

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In this work, by using many-body techniques we propose a new method for calculating equilibrium charges for ions moving in a uniform electron gas, within any range of velocities. Our procedure has been applied to protons, and our calculations show good agreement with the experimental evidence.

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The problem of ions moving in a solid has been the subject of a long interest. The energy loss processes have been discussed by different authors in different ranges of energies.[1-7] Recently, Brandt and co-workers[8-9] have given an effective-charge theory to explain stopping powers for

intermediate velocities (around 25 keV/u), a region for which there is a lack of fundamental understanding. This approach is related to those experiments measuring the charge states of ions emerging from solids.[10-11] Here, the number of ions of a given charge leaving the solid are determined as a function of the energy of the ions fired at the target.

The purpose of this work is to propose a method for calculating equilibrium charges for ions moving in a uniform electron gas in any range of velocities. Our results are relevant for intermediate and low velocities for which shell corrections can be neglected. We only consider protons in our discussion, although an extension to heavier atoms can be easily done.

In our analysis we assume that the proton has a bound-electron state for the whole range of velocities. Although this assumption will be sustantiated by our final results, note that Cross[12] has shown that, for high velocities, an analysis of the charge states of the proton can be done in terms of the processes of capture into, and loss from, the electron level bound to the proton. On the other hand, recent theoretical calculations[13-15] have shown that a proton at rest inside an electron gas can bind two electrons in a stable orbit.

TABLE I. Values of a and E_A (in a.u.) as a function of v for $r_s = 2$.

v	a	E_A	v	a	E_A
0	0.90[a]	−0.106	0.8	0.72[a]	−0.027
	0.78[b]	−0.046		0.52[b]	0.008
0.2	0.88[a]	−0.096	1.0	0.74[a]	−0.027
	0.72[b]	−0.036		0.58[b]	0.008
0.4	0.86[a]	−0.075	1.2	0.82[a]	−0.041
	0.66[b]	−0.012		0.70[b]	0.011
0.6	0.80[a]	−0.048	1.4	0.86[a]	−0.063
	0.54[b]	0.004		0.74[b]	0.011

[a] $N_A = 0$. [b] $N_A = 1$.

We work with the reference frame of the ion, moving with a constant velocity, v. The key quantity is the self-energy associated to the bound electron defined as[16]

$$\Sigma_A(\omega) = \int d^3r\, d^3r' \langle s, \vec{r}| \Sigma(\vec{r}, \vec{r}', \omega) |s, \vec{r}'\rangle, \qquad (1)$$

where $|s, \vec{r}\rangle$ is the spherically symmetric bound-electron wave function approximated by $(a^3/\pi)e^{-ar}$. $\Sigma(\vec{r}, \vec{r}', \omega)$, the random-phase approximation (RPA) self-energy,[16] is calculated by using the following approximation to the causal Green function:

$$G(\vec{r}, \vec{r}'; \omega) = \sum \frac{|\vec{k}, \vec{r}\rangle\langle\vec{k}, \vec{r}'|}{\omega - k^2/2 + i\eta_k} + |s, \vec{r}\rangle\langle\vec{r}', s| \left(\frac{N_A}{\omega - E_A - i\eta} + \frac{1 - N_A}{\omega - E_A + i\eta}\right), \qquad (2)$$

where $|\vec{k}, \vec{r}\rangle$ are free-electron states orthogonalized to the atomic level, N_A is the number occupation of the level, E_A is its mean energy, and η_k is a positive infinitesimal for unoccupied states, namely, for $|\vec{k} + \vec{v}| > k_F$. The causal screened interaction is given by

$$W(\vec{r}, \vec{r}', \omega) = \frac{1}{\pi}\int_0^\infty d\omega' \int \frac{d^3q}{(2\pi)^3} \mathrm{Im}[\epsilon_{\mathrm{RPA}}^{-1}(q, \omega)] \frac{4\pi}{q^2} \times \exp[-i\vec{q}\cdot(\vec{r} - \vec{r}')]\left(\frac{1}{\omega + i\eta + \vec{q}\cdot\vec{v} - \omega'} - \frac{1}{\omega - i\eta + \vec{q}\cdot\vec{v} + \omega'}\right). \qquad (3)$$

The self-energy, $\Sigma_A(\omega)$, can be split into four terms:

$$\Sigma_A^{r,c}(\omega)\ [\text{or } \Sigma_A^{r,1}(\omega)] = \int_0^\infty d\omega'' \int_{-\infty}^\infty \frac{d^3q}{(2\pi)^3} \sum_{|\vec{k}+\vec{v}_0| \lesssim k_F} \frac{4\pi}{q^2} \times \mathrm{Im}[\epsilon_{\mathrm{RPA}}^{-1}(q, \omega'')] \frac{\langle s, \vec{r}|e^{i\vec{q}\cdot\vec{r}}|\vec{k}, \vec{r}\rangle\langle\vec{k}, \vec{r}'|e^{-i\vec{q}\cdot\vec{r}'}|s, \vec{r}'\rangle}{\omega \pm \omega'' - k^2/2 - \vec{q}\cdot\vec{v} \mp i\eta} \qquad (4a)$$

and

$$\Sigma_A^{nr,h}(\omega)\ [\text{or } \Sigma_A^{nr,e}(\omega)] = \int_0^\infty d\omega'' \int_{-\infty}^\infty \frac{d^3q}{(2\pi)^3} \frac{4\pi}{q^2} \mathrm{Im}[\epsilon_{\mathrm{RPA}}^{-1}(q, \omega'')] \frac{\rho_q^2}{\omega \pm \omega'' - \vec{q}\cdot\vec{v} - E_A \mp i\eta} N_A\ [\text{or } (1 - N_A)], \qquad (4b)$$

where ρ_q^2 is the Fourier transform of the bound-electron charge density. E_A and a, the energy level and the exponent of the bound electron, are calculated by adapting to the present dynamical case the new method proposed by Guinea and Flores[17] for the case of impurities at rest in the electron gas.

Table I shows E_A and a as a function of the ion velocity.

In Eqs. (4a) and (4b), $\mathrm{Im}\Sigma_A^{r,c}(\omega)$ [or $\mathrm{Im}\Sigma_A^{r,1}(\omega)$] gives the probability per unit time for an electron transition jump from [to] the conduction band to [from] a hole [electron] created in the proton at an ω level; in these processes, an electron-hole pair—or a plasmon—is excited at the same time in the electron gas. On the other hand, $\Sigma_A^{nr,h}(\omega)$ and $\Sigma_A^{nr,e}(\omega)$, the nonrecoil terms, are related to the probability of exciting an electron-hole pair or a plasmon in the electron gas when a hole or an electron is suddenly created in the atom.

The density of states associated to the bound state is defined as

$$N(\omega)=\frac{1}{\pi}\,\mathrm{Im}[\omega-E_{\mathrm{H}}-\bar{\Sigma}_A^{r,c}(\omega)-\bar{\Sigma}_A^{nr,h}(\omega)-\Sigma_A^{r,1}(\omega)-\Sigma_A^{nr,e}(\omega)]^{-1}, \tag{5}$$

where E_{H} is the Hartree energy and $\bar{\Sigma}$ is the complex conjugate of Σ; the complex conjugates are due to the fact that $\Sigma_A^{r,c}(\omega)$ and $\Sigma_A^{nr,h}(\omega)$ are related to the creation of a hole in the atom. Then, we define the following distribution function:

$$n(\omega)=\frac{\mathrm{Im}[\bar{\Sigma}_A^{r,c}(\omega)+\bar{\Sigma}_A^{nr,h}(\omega)]}{\mathrm{Im}[\bar{\Sigma}_A^{r,c}(\omega)+\bar{\Sigma}_A^{nr,h}(\omega)+\Sigma_A^{r,1}(\omega)+\Sigma_A^{nr,e}(\omega)]}, \tag{6}$$

in such a way that N_A is given by

$$N_A=\int_{-\infty}^{\infty}n(\omega)N(\omega)d\omega. \tag{7}$$

Note that $n(\omega)$ is a function of N_A, and that Eq. (7) must be solved self-consistently for the occupation number, N_A.

A good approximation to Eq. (7) is given by

$$N_A=\frac{\mathrm{Im}[\bar{\Sigma}_A^{r,c}(E_0)]}{\mathrm{Im}[\bar{\Sigma}_A^{r,1}(E_0)+\bar{\Sigma}_A^{r,c}(E_0)]}, \tag{8}$$

where E_0 is given by $E_0=E_{\mathrm{H}}+\mathrm{Re}\Sigma(E_0)$, the zero of the real part of the denominator of Eq. (5) (in our calculation, E_0 practically coincides with E_A).

Equation (8) gives the intuitive result that the occupation number depends on the ratio between the capture and loss cross sections for the atomic level. In Fig. 1, we have drawn, for $v=1$ and $r_s=2$, the following function:

$$n^r(\omega)=\frac{\mathrm{Im}[\bar{\Sigma}_A^{r,c}(\omega)]}{\mathrm{Im}[\bar{\Sigma}_A^{r,c}(\omega)+\Sigma_A^{r,1}(\omega)]} \tag{9}$$

which according to Eq. (8) plays the role of a distribution function for the atomic level. For $v=0$, $n^r(\omega)$ has a step behavior with a well-defined Fermi level; however, as far as v increases, $n^r(\omega)$ becomes smoother with a general pattern similar to the one given in Fig. 1. Let us define as the Fermi level, E_{F}, for a given velocity, v, the value of the energy for which $n^r(E_{\mathrm{F}})=0.5$.

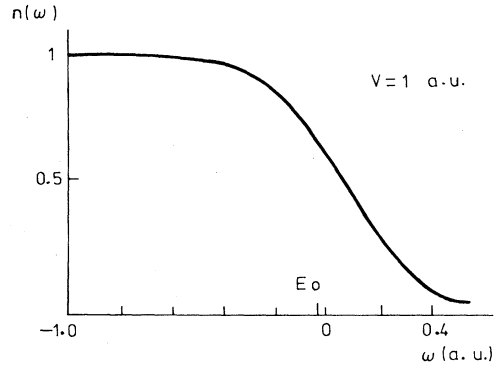

FIG. 1. $n^r(\omega)$ [Eq. 9] is shown as a function of ω for $v=1$ and $r_s=2$. $\omega=0$ is the band bottom, E_{F} is the Fermi level as defined in the text and E_0 is the atomic level.

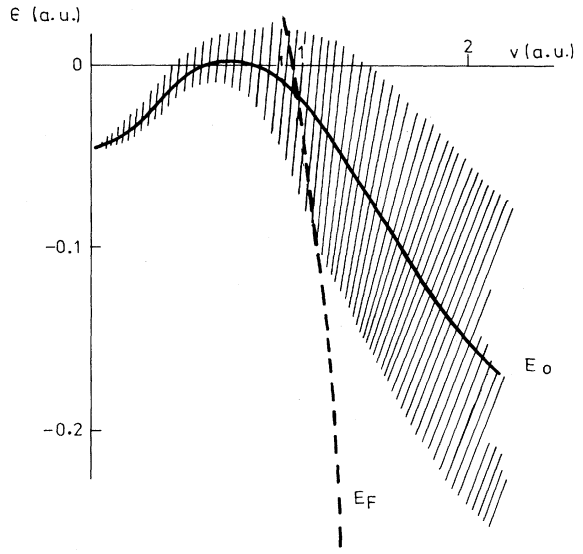

FIG. 2. E_0 and E_F are shown as a function of v. The dashed region around E_0 shows the values of $\Gamma/2$, the broadening of the atomic level.

Then, the occupation number for the atomic level is determined by the relative position between E_F and E_0. In Fig. 2, E_0 and E_F have been drawn as a function of v for $r_s = 2$; for $v = 1.03$ a.u., $E_0 = E_F$, this being the velocity for which $N_A = \frac{1}{2}$. Note that E_F decreases quickly as a function of v, going like $-v^2/2$ with respect to the bottom of the band for large values of v; this is a consequence of the reference framework which moves the proton.

We can also define the level broadening by means of the equation

$$\Gamma/2 = \mathrm{Im}[\bar{\Sigma}^{r,c}(E_0) + \Sigma^{r,1}(E_0) + \bar{\Sigma}^{nr,h}(E_0) + \Sigma^{nr,e}(E_0)]. \quad (10)$$

The different values of $\Gamma/2$ as a function of v, for $r_s = 2$, have been shown in Fig. 2 by means of the shaded region drawn around the level E_0. It is important to note that, except for a small region near $v = 1$, this shaded area does not touch the conduction band; the meaning of this result is that the assumption about the existence of a well-defined atomic level is entirely correct.

The ratio of the fraction of bare protons to the fraction of protons with one electron emerging from the solid is given, in our approximation, by $(1 - N_A)/2N_A$. It is important to point out that this is a consequence of neglecting intra-atomic electron-electron correlation. At low velocities, however, intra-atomic electron correlations are not quite negligible and corrections should be made to obtain a more accurate description, especially when the mean occupation number is close to one. In the case of protons emerging with two electrons, intra-atomic electron correlation is of primary importance, so our method cannot be used to obtain the mean number in that case.

$(1 - N_A)/2N_A$ has been drawn in Fig. 3 as a function of v, for $r_s = 2$. In the same figure, we show the experimental data obtained by Phillips[10] for protons emerging from aluminum. The agreement between our theoretical calculations and these experimental data is rather good, although we have some discrepancies at low velocities. However, note that our calculation gives practically a linear relation between $\ln(v)$ and $\ln[(1 - N_A)/2N_A]$ in agreement with general arguments,[18] while Phillips data show a deviation from this linear relation for $v < 0.8$ a.u. We think that this deviation is partially due to the neglect of intra-atomic correlation noted above. Surface effects could play a significant role since for low velocities the atom has enough time to feel the presence of the surface.

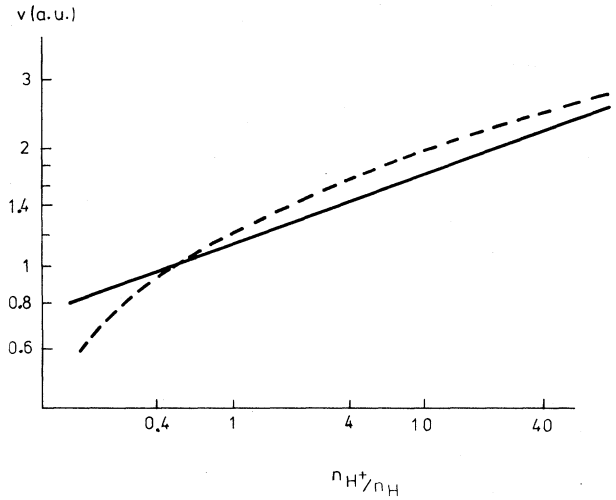

FIG. 3. The ratio of the fraction of bare nuclei to the fraction of nuclei with one electron as a function of the velocity, v. (Dashed line: experimental data; full line, our results.)

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