Neutral impurity scattering in semiconductors

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The drift mobility and ratio of Hall to drift mobility are computed for the scattering of carriers by a hydrogenic neutral impurity. The scattering is treated using the almost exact values of the phase shifts for scattering of electrons by neutral hydrogen scaled for the effective mass and dielectric constant of the semiconductor.

Scattering of carriers by hydrogenlike neutral impurities has been treated by a number of authors.[1–3] All of these calculations have exploited the similarity of this problem to that of elastic scattering of electrons by neutral hydrogen (the neutral-hydrogen approximation). In this approximation the scattering by neutral hydrogen is adapted to the case of scattering by neutral impurities by scaling the Bohr radius a_0 and the ground-state binding energy E_0 to obtain an effective Bohr radius a_s and binding energy E_B:

$$a_S \equiv a_0(\kappa m_e/m^*), \tag{1}$$

$$E_B \equiv E_0(m^*/m_e\kappa^2), \tag{2}$$

where κ and m^* are the dielectric constant and effective mass of the semiconductor, respectively, and m_e is the free-electron mass.

The difference between the various calculations comes in the type of approximation that is made to the problem of electron scattering by neutral hydrogen. Erginsoy[1] fits the approximate results of Massey and Moiseiwitsch[4] to a simple analytic expression for s-wave phase shift δ_0 at an energy E and obtains

$$\sin^2\delta_0 \simeq 20\,ka_S/4\pi, \tag{3}$$

where

$$k = (2m^*E/\hbar^2)^{1/2}. \tag{4}$$

From Eq. (3), he predicts a temperature-independent mobility (in mks units) given by

$$\mu_E = \frac{8\pi\kappa\epsilon_0 E_B}{20N_I\hbar e}, \tag{5}$$

where N_I is the density of neutral impurities.

Anselm[2] and Sclar[3] sought to improve Erginsoy's calculation by improving the approximation to the scattering by neutral hydrogen. In particular, they concentrated on the "resonant" scattering which might be expected at low energies in connection with the existence of a weakly bound negative ion. Sclar used his calculation of the scattering from a three-dimensional square well[5] to estimate the influence of a weakly bound state on the scattering. From his calculation he obtained

$$\mu_S = 0.82\mu_E\left[\frac{2}{3}\left(\frac{k_BT}{E_N}\right)^{1/2} + \frac{1}{3}\left(\frac{E_N}{k_BT}\right)^{1/2}\right], \tag{6}$$

where μ_E is given by Eq. (5), E_N is the scaled binding energy for the negative ion,

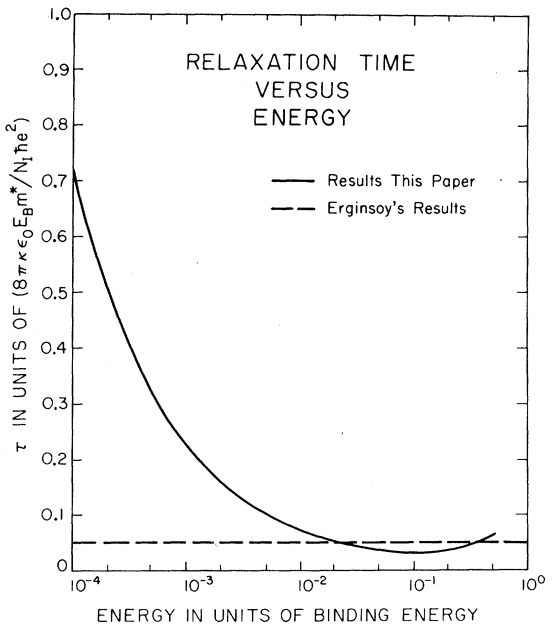

FIG. 1. Relaxation time vs electron energy. The relaxation time is measured in units of $8\pi\kappa\epsilon_0 E_B m^*/N_I\hbar e^2$, where κ and m^* are the dielectric constant effective mass of the semiconductor, respectively, E_B is the binding energy of the impurity, and N_I is the density of neutral impurities. The energy is measured in units of the binding energy. The solid line is the results for this calculation using Eq. (10) for $n \leq 2$. The dashed line is the result of Erginsoy's approximation (Ref. 1).

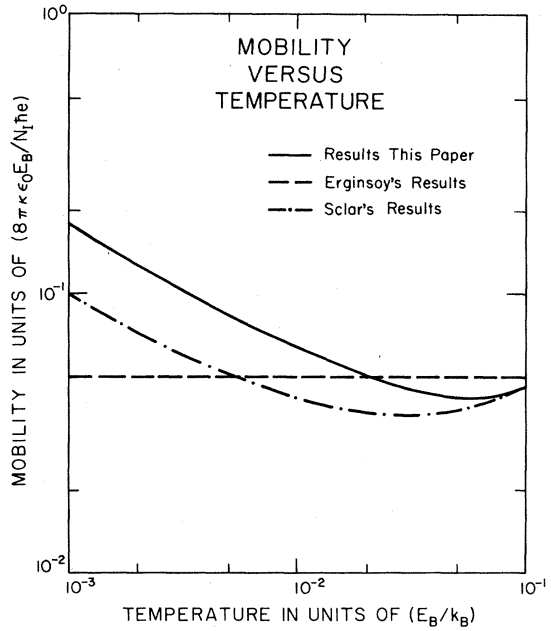

FIG. 2. Drift mobility vs temperature. The mobility is measured in units of $8\pi\kappa\epsilon_0 E_B/N_I\hbar e$, where κ is the dielectric constant of the semiconducotr, E_B is the binding energy of the impurity, and N_I is the density of neutral impurities. The temperature is measured in units of E_B/k_B, where k_B is Boltzmann's constant. The solid line is the result of our calculation using Eqs. (10) and (11) for $n \leq 2$. The dashed and dash-dotted lines are the results obtained by Erginsoy (Ref. 1) and Sclar (Ref. 3), respectively.

$$E_N = 0.71\ \text{eV}(m^*/m_e\kappa^2), \tag{7}$$

and k_B is Boltzmann's constant.

In this paper we report on a calculation of the temperature dependence of the drift mobility and ratio of Hall to drift mobility using phase shifts which have been accurately determined for the scattering of electrons by neutral hydrogen.[6] That is, these calculations are not subject to any of the previous approximations to the scattering and represent an accurate implementation of the neutral-hydrogen approximation.

Throughout this discussion, we will use a normalized energy ϵ and temperature T^* which are defined in terms of the unnormalized energy E and temperature T by

$$\epsilon \equiv E/E_B \tag{8}$$

and

$$T^* \equiv k_B T/E_B. \tag{9}$$

Use of these normalized units makes it possible to apply these results to a number of semiconductor-impurity systems by simple scaling with the binding energy of the impurity.

The calculation proceeds with a standard partial-wave expansion of the scattering amplitude with the relaxation time τ being given by[5]

$$\tau^{-1}(\epsilon) = \left(\frac{N_I\hbar e^2}{8\pi\kappa\epsilon_0 m^* E_B}\right) 4\pi \sum_{n=0}^{\infty} \frac{(n+1)}{4\sqrt{\epsilon}} \{3\sin^2 \times [\delta_n^-(\epsilon) - \delta_{n+1}^-(\epsilon)] + \sin^2[\delta_n^+(\epsilon) - \delta_{n+1}^+(\epsilon)]\}, \tag{10}$$

where δ_n^+ is the nth partial-wave phase shift for the singlet state of the two electrons and δ_n^- is the nth partial-wave phase shift for the triplet state of the two electrons. The appropriate temperature average is defined by

$$\langle\tau\rangle = \frac{4}{3\sqrt{\pi}(T^*)^{5/2}} \int_0^\infty \epsilon^{3/2} e^{-\epsilon/T^*} \tau(\epsilon)\, d\epsilon, \tag{11}$$

where, in keeping with our assumptions, we have taken the energy variation of the density of states to be $\sqrt{\epsilon}$. The ratio of Hall to drift mobility r is defined by[7]

$$r = \langle\tau^2\rangle/(\langle\tau\rangle)^2. \tag{12}$$

The results of this calculation, which include phase shifts for n up to 2, are presented in Figs. 1–3. In Fig. 1 the energy-dependent relaxation time is plotted versus the normalized energy. The solid line is the result of this calculation, while the dashed line indicates the approximation used by Erginsoy.[1] The good agreement between our results and Erginsoy's calculation for energies between 2×10^{-2} and 5×10^{-1} indicates that Erginsoy's approximation is quite good in this range. However, for energies less than 10^{-2} there is a significant deviation between the two results. Our calculations give a much larger value for $\tau(\epsilon)$ than that obtained by Erginsoy.

Our results for the drift mobility as a function of

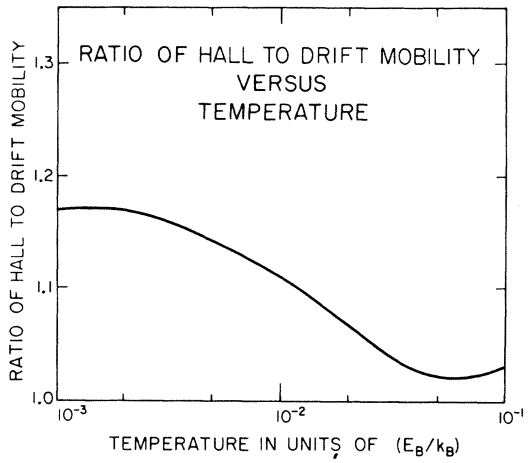

FIG. 3. Ratio of Hall mobility to drift mobility vs temperature. The temperature is measured in units of E_B/k_B, where k_B is Boltzmann's constant.

temperature are given in Fig. 2. The mobility is plotted in units of $8\pi\kappa\epsilon_0 E_B/N_I\hbar e$. This particular choice for the unit of mobility is convenient when applying these results to impurity-semiconductor systems with different binding energies E_B. In fact, this scaling procedure seems to be approximately correct when one applies these results to impurities which have binding energies that deviate from that predicted by the simple hydrogen model.[8]

For comparison, we have also plotted the results of Erginsoy[1] and Sclar's[3] calculations in Fig. 2. From this figure, we can see that Erginsoy's approximation, Sclar's approximation, and our calculations are in approximate agreement for temperatures between 2×10^{-2} and 10^{-1}. At lower temperatures, significant deviations exist between the three calculations. Both our results and Sclar's predict an observable temperature dependence of the mobility.

In Fig. 3 we have plotted the temperature dependence of the ratio of Hall to drift mobility r. The theory predicts a slight variation of r with temperature, ranging between 1.17 at $T^* = 10^{-3}$ and 1.02 at $T^* = 10^{-1}$. The ratio is very near unity over this temperature range because the relaxation time is relatively independent of energy over the range of energies which make the most significant contribution to the averages in Eq. (12).

In summary, these calculations predict that significant deviations from the previously calculated values for the mobility should occur at low temperatures $T^* < 2\times10^{-2}$. This would correspond to T less than 2.3 °K for a binding energy of 0.01 eV or T less than 23 °K for a binding energy of 0.1 eV. Both of these values are well within the potentially observable range of binding energy and temperature. For higher temperatures, $2\times10^{-2} < T^* < 10^{-1}$, all of the results are approximately equal, indicating that a better treatment of the scattering within the neutral-hydrogen approximation produces little change in the results obtained by Erginsoy and Sclar.

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