Decay of weakly bound impurity states in parallel fields

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The application of a weak magnetic field parallel to the electric field substantially changes the lifetime, density, etc., of weakly bound impurity states of negative ions.

Weakly bound impurity states of neutral-atom carriers play an important role in the kinetics of low-temperature processes in semiconductors and insulators[1] and also in the properties of disordered systems.[2] The behavior of these states in external fields (the fields of other impurities,[2] electric fields,[3] and magnetic fields[4]) has recently been the subject of active research. In this letter we show that the probability for the decay of a negative ion decreases in an anomalous way in parallel static electric and magnetic fields (even if very weak), because of a change in the spectrum of the weakly bound state. This decrease in the probability for the decay of impurity states should evidently lead to substantial changes in the kinetic properties (the lifetime, density, etc.) of systems of negative ions at low temperatures.

Let us consider a weakly bound state of an electron (of energy $E \simeq -\kappa_0^2/2$) in the potential of a neutral of radius $r_c \ll \kappa_0^{-1}$ in an electric field ϵ and a parallel magnetic field H ($\epsilon \| \mathbf{H} \| 0z$, where ϵ and H are the field strengths). According to the theory of Ref. 5, the energy of an $l = m = 0$ ground state (l and m are the orbital angular momentum and its projection) is given by

$$-\frac{1}{a_0} = \sqrt{2\eta} + \left(\frac{\omega^2 i}{2\pi}\right)^{1/2} \int_0^\infty \frac{dt}{t^{3/2}} \exp(-i\eta t) \left[\frac{\exp\left(-i\frac{\epsilon^2 t^3}{24}\right)}{1-\exp(-i\omega t)} - \frac{1}{i\omega t}\right], \tag{1}$$

where a_0 is the scattering length, $\eta = -E + \omega/2$, and ω is the cyclotron frequency. External fields cause an energy shift $E - \kappa_0^2/2 = \Delta(\epsilon,\omega,E)$ and give rise to an ionization width $\Gamma_{00}(\omega,\epsilon,E)$. We will find the dependence of Γ_{00} on H in weak fields ($\epsilon a_0^3 \ll 1, \omega \ll \kappa_0^2, a_0 > 0$), and then use $E \simeq -\kappa_0^2/2 = -a_0^{-2}/2$.

In (1) we calculate Γ_{00} by the method of steepest descent, where the saddle point $t_0 \sim \kappa_0/\epsilon$ is on the negative imaginary semiaxis. From (1) we find

$$\Gamma_{00} = \beta(\omega, \kappa_0, \epsilon)\Gamma_{00}^{\epsilon}(\epsilon, \eta); \qquad \beta = \frac{\omega t_0}{1 - \exp(-\omega t_0)},$$

where $\Gamma_{00}^{\epsilon}(\epsilon,\kappa_0) = \Gamma_{00}(\omega = 0)$. The $\beta(\omega) \gtrsim 1$ describes the effect of a magnetic field on the decay. In the limiting cases of a weak magnetic field ($\omega t_0 \ll 1$) and a "strong" magnetic field ($\omega t_0 \gg 1, \omega \lesssim \kappa_0^2$) we have

$$\Gamma_{00} = \Gamma_{00}^{\epsilon}(1 + \omega t_0/2)\exp(-\omega t_0/2); \quad (\omega t_0 \ll 1), \tag{2}$$

$$\Gamma_{00} \doteq \Gamma_{00}^{\epsilon}\, \omega t_0 \exp(-\omega t_0/2); \quad (\omega t_0 \gg 1,\ \omega \ll \kappa_0^2). \tag{3}$$

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The functional dependence of the width $\Gamma_{00}(H)$ in (2) and (3) is determined by two mechanisms. The first mechanism is the raising of the boundary of the continuous spectrum by $+\omega/2$ in a magnetic field, which causes an exponential decay $\Gamma_{00} \propto e^{-\omega t_0/2}$. The linear dependence $\Gamma(H)$, on the other hand, is caused by a "compression" of the electron wave function by the magnetic field in the plane transverse to ϵ. For example, for P donors ($E = 1.7$ meV) in Si at $H = 0.2$T, with $\epsilon = 5\times 10^{-4}$ V/m, $K = \omega t_0 = 8$, and at $T = 1$ K, the probability for the thermal activation of an ion in a magnetic field is low in comparison with the ionization probability.

The physical explanation for the linear increase in $\Gamma_{00}(H)$ in a magnetic field is that as a particle moves into the region $z \geqslant z_0$ (where z_0 is determined from the condition $\epsilon z_0 = -\kappa_0^2/2$) it acquires in the electric field an energy greater than the binding energy $E = -\kappa_0^2/2$, so that it goes into the continuum. Consequently, the rate of ionization of the state is determined by the probability for a particle to be in the region $\infty > z \geqslant z_0$, and for Γ_{00} we have $\Gamma_{00}/\kappa_0^2 = \int_{z \geqslant z_0} dV|\Psi|^2$, where Ψ is the wave function. The ionization width is formed at large distances from the center, $z \gg \kappa_0^{-1}$. Consequently, there is an important change in this width even upon a very slight change in the wave function in the region ($z \gtrsim z_0 \gg \kappa_0^{-1}$), and when a magnetic field is imposed, we must follow the ratio of the probability densities for a particle to be in the region $z \gtrsim z_0$: $|\Psi(H \neq 0)|^2/|\Psi(H=0)|^2|_{z=z_0}$. In a weak magnetic field ($L \gg \kappa_0^{-1}$) the wave function of the electron is

$$\Psi = \Psi_0 + \Psi_1 = C\left[\exp(-\kappa_0 r)r^{-1} + \frac{1}{\kappa_0 L^2}\exp\left(-\kappa_0 z - \frac{\rho^2}{4L^2}\right)\right],$$

where $\rho_0^2 = z_0 \kappa_0^{-1} \sim t_0, \omega = L^{-2}$, and L is the magnetic length. The first term is caused by the impurity potential, and the second by the magnetic field. In a very weak magnetic field, $\rho_0^2/L^2 \ll 1$ (or $\omega_0 t_0 \ll 1$), Γ_{00} is dominated by Ψ_0, and Ψ_1 is a small perturbation. In this case we have $\Gamma_{00}^{\epsilon} = \kappa_0^2 \rho_0^2/z_0^2 \exp(-\kappa_0 z_0)$ and $\Gamma_{00} = \Gamma_{00}^{\epsilon}(1 + \rho_0^2/2L^2)$. Aside from the coefficients, Γ_{00} and Γ_{00}^{ϵ} are the same as in (2). In a strong magnetic field, $\rho_0^2 \gg L^2 \gg \kappa_0^{-2}$ (or $t_0^{-1} \ll \omega \ll \kappa_0^{-2}$), the width of the level is determined by Ψ_1. After an integration, we find $\Gamma_{00} = \Gamma_{00}^{\epsilon}\rho_0^2/L^2$, in accordance with (3). The increase $\Gamma_{00} \propto \omega$ is thus caused by a radial compression of the tails of the wave functions by the magnetic field and thus an increase in the probability for the particle to be in the region $z \geqslant z_0$.

For $l \gg 1$ and $l = m$, the concentration of the wave function of the particle in the radial plane causes a stronger dependence of Γ_{00} on H.

We now consider the ionization of a magnetic impurity state[4] $l = m = 0$. For $r_c \ll |a_0| \ll L$, $a_0 < 0$, there is a quasibound magnetic impurity state with an energy $\Delta E = -a_0^2/2L^4$ and a width $\Gamma_{00}^H \sim a_0^3 L^{-5}$ under the bottom of an arbitrary Landau band ($N \geqslant 1$). The width of this state is caused by the possibility of a transition to the continuum of lower bands. The imposition of an electric field changes the width: $\Gamma_{00}^H \Rightarrow \Gamma_{00} + \Gamma_{00}^H$. An equation determining the energy of this state is found by analytically continuing (1) into the region $E > 0$. The solution is

$$\Gamma_{00}^H / \Gamma_{00} \simeq \epsilon L^3 \beta^0 \exp\beta^0 ; \quad \beta^0 \sim a_0^3 (\epsilon L^6)^{-1} . \tag{4}$$

It follows from (4) that, while the width in very weak fields $[(\epsilon L^3) \ll (a_0/L)^3]$ is determined primarily by the transition to states of lower Landau bands, at $[\epsilon \sim \tilde{\epsilon} \lesssim (a_0/L^2)^3]$ the decay is caused by the electric field. The same situation is observed for states $l > 1$. For Li^- and As^- impurities in Si (Ref. 6) we find $\tilde{\epsilon} = 7 \times 10^{-3}$ V/cm at $H = 6$ T.

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