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WAKE STATES OF FAST PROTONS MOVING IN AN ELECTRON GAS

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Capture and loss from and to wake bound states into the electron gas are evaluated, using a self-energy formalism, for a swift proton moving at speed $v (v \gg v_0$ (Bohr velocity)) in an electron gas.

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Introduction. Since the pioneering work by Neufeld and Ritchie [1], Ritchie, and Ritchie and co-workers [2], much theoretical and experimental work has been directed to understand the wake of density fluctuations trailing swift ions moving in condensed matter. When swift ions penetrate gaseous or solid targets, they emerge with free electrons travelling in the same direction and with the same velocity as the ion. They are the so-called convoy electrons [3]. For gaseous targets, this phenomenon was first explained as charge transfer to the continuum states associated with the Coulomb potential of ions moving in vacuum [4]. It has been suggested [5] that part of the convoy electrons from solids might have its origin in electrons bound in the minimum of potential energy of electrons in the wake of electron density fluctuations trailing the swift ion in the solid. This has not been confirmed experimentally, although some investigators [6,7] have measured the energy distribution of convoy electrons using mostly hydrogen and helium projectiles and observed two components in the measured velocity distribution, one of which could be ascribed to wake riding electrons, while the other is well described, in analogy with the gas phase case, in terms of charge transfer to the continuum states of the moving ion. No calculation has yet been performed of the capture and loss to and from wake bound states into the electron gas. In this letter we present the results of such calculation for a proton moving in an electron gas. This is expected to give a good description of a situation in which a proton is moving under channelling conditions in a nearly free electron gas metal such as aluminium.

Outline of the theory. Consider an ion–electron pair interacting with an interacting Fermi gas. It is convenient to work in second quantization [8]. The total hamiltonian $H = H_0 + H_E + H_I$ is divided in three terms: H_0, the hamiltonian of the ion and its associated electron, H_E is the hamiltonian of the interacting electron gas and H_I describes the interaction between the electron gas and the ion–electron system. H_I is given by

$$H_I = \Omega^{-1} \sum_{n,n',\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}} V_q \left[\rho_{n'n}(\boldsymbol{q}) - Z_1 \delta_{n'n}\right] \times C^{+}_{\boldsymbol{k}-\boldsymbol{q}\,n'} C_{\boldsymbol{k}\,n}\, a^{+}_{\boldsymbol{p}+\boldsymbol{q}}\, a_{\boldsymbol{p}}\,, \tag{1}$$

where C^{+}_{kn} and C_{kn} are the creation and annihilation operators of the ion–electron complex, in which k is its centre-of-mass momentum and n specifies its internal motion $E_{kn} = k^2/2(1+M) + \omega_n$. Here a_p is the annihilation operator for an electron with momentum

p and energy $\epsilon_p = \frac{1}{2}p^2$. The normalization volume is Ω and $V_q = 4\pi/q^2$. Z_1 is the ion charge and $\rho_{n'n} = \langle n'|\exp(i\boldsymbol{q}\cdot\boldsymbol{r})|n\rangle$ is the matrix element of the density operator with respect to the state vectors of the internal motion. We use atomic units throughout. To calculate capture and loss rates we estimate the self-energy of the ion–electron in the pair approximation as

$$\Sigma(\omega,k,n) = \frac{i}{\Omega}\sum_{n'}\int\frac{d^3q}{(2\pi)^3}V_q|\rho_{n'n}(q) - Z_1\delta_{n'n}|^2 \times \int\frac{d\omega'}{2\pi}G_{k-q,\omega-\omega',n'}(\epsilon^{-1}_{q,\omega'} - 1), \quad (2)$$

where G is the exact Green function of the ion–electron pair, $G = (\omega - E_{kn} - \Sigma)^{-1}$, and $\epsilon(k,\omega)$ is the dielectric response function of the electron gas. A first order perturbative solution of this equation is found by replacing the Green function G on the right-hand side of eq. (2) for the unperturbed one G^0. The capture and loss rates are then obtained by looking at the terms in which the internal state of the ion–electron pair is changed. We obtain, in the quasiparticle approximation,

$$\gamma_{C(L)} = -2\,\mathrm{Im}\,\Sigma = \frac{2D^{C(L)}}{\Omega}\sum_{P<(>)P_F}\int\frac{dq}{(2\pi)^3}\frac{4\pi}{q^2}|U_0(p)|^2 \times \mathrm{Im}(-1/\epsilon_{q,\pm\omega_A}). \quad (3)$$

Here $U_0(\boldsymbol{p})$ is the Fourier transform of the wake bound electron wavefunction, $\omega_A = \boldsymbol{q}\cdot\boldsymbol{v} + E_b + \frac{1}{2}(\boldsymbol{p}-\boldsymbol{v})^2$. The + and − signs in the argument of the dielectric function stand for capture and loss respectively; E_b is the binding energy of the wake, bound state; $D^L = 1$ and $D^C = 2$ to account for the spin degeneracy in the capture process.

Results. We use the plasmon pole approximation [9] to $\epsilon(k,\omega)$. In this approximation we calculate the wake bound state wavefunction $U_0(\boldsymbol{r})$ by fitting the potential energy of an electron near its minimum by a harmonic-type well and calculating binding energies and wavefunctions in the standard manner [10]. The function $|U_0(\boldsymbol{p})|^2$ is so strongly peaked about the point $\boldsymbol{P} = 0$ that we may approximate it by $(2\pi)^3$ times a δ-function of its argument. With this approximation capture cannot occur for high velocities and is zero for the whole range of velocities at which wake-bound states may occur. This restriction is smoothed up if we do not approximate $|U_0(\boldsymbol{p})|^2$ by a δ-function and just evaluate the capture rate numerically, using eq. (3) and the wavefunction parameters given in table 1. Then one obtains for $r_s = 2$ and $v = 2$ a value of $\gamma_c \approx 1.4\times10^{-4}$ leading to a mean free path for capture of $\lambda_c \sim 7500$ Å. These numbers are to be compared to the ones obtained for direct capture [11,12] into the hydrogenic bound state of the proton, for this case $\gamma_c \approx 2\times10^{-2}$. Table 2 shows the results of a calculation of γ_L for an electron gas at a density corresponding to the conduction band of aluminium ($r_s = 2$). The

Table 1
Wake bound state wavefunction parameters ($u_0 \propto \exp(-\alpha^2 b^2/2)\exp[-\beta^2(z-z_0)^2/2]$ and binding energies for protons moving with velocity v in an electron gas at a density corresponding to the conduction band in an aluminium metal ($r_s = 2$). The cylindrical coordinates $b = (x^2+y^2)^{1/2}$ and $\tilde{z} = z - vt$ are defined relative to the position of the charge Z_1, $(0,0,vt)$ at the time t for the field point $\boldsymbol{r} = (x,y,z)$. Here z_0 is the position of the minimum of the first trough of the electron potential energy.

v	α^2	β^2	E_b
2	0.12	0.19	0.13
3	0.11	0.13	0.18
4	0.1	0.09	0.195
5	0.09	0.07	0.194
6	0.08	0.05	0.187
7	0.074	0.046	0.18
8	0.07	0.039	0.17
9	0.065	0.033	0.164
10	0.062	0.03	0.157

Table 2
Loss rate γ_L; associated mean free path λ_L and the approximation to it of Ritchie et al. [13] ($\lambda_L \approx v r_s^{1.5}$) in an electron gas ($r_s = 2$) as a function of the proton velocity.

v	γ_L	λ_L (Å)	$v r_s^{1.5}$ (Å)
2	0.30	3.5	5.65
3	0.29	5.5	8.46
4	0.26	8.1	11.28
5	0.24	11	14.1
6	0.22	14.4	16.92
7	0.20	18.5	19.74
8	0.19	22.3	22.56
9	0.17	28	25.4
10	0.16	33	28.3

mean free path for loss is also shown $\lambda_L = v\gamma_L^{-1}$, together with the approximation of Ritchie et al. [12] $\lambda_L = vr_s^{3/2}$.

In conclusion, in an electron gas model the wake capture cross section is negligible for velocities at which wakes and indeed wake bound states develop. This might explain, especially under channelling conditions, the unclear appearance of wake bound electrons in the spectrum of electrons emerging from solids after the passage of swift ions. In real solids, however, besides the Auger mechanism studied here, another process, coming from scattering processes with the ion cores, for capture is available. These mechanisms, such as resonant and shell capture [13,14] will be more efficient outside channelling conditions. In all cases, the Auger type loss of mechanism described here has to be taken into account.

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