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NONLINEAR AND DYNAMIC EFFECTS IN THE FRICTION APPROACH TO THE DISSIPATIVE PARTICLE MOTION NEAR A SURFACE

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We investigate the motion and energy dissipation of the adparticle interacting with the solid surface in the classical, nonlinear, exactly soluble model, thus taking into account the important memory effects. The energy loss is governed by the spatially and velocity dependent dissipative force, which encompasses the low velocity »friction« regime and the high velocity regime where the interaction is dynamically suppressed.

In this paper we study the energy accomodation of a heavy particle (atom, molecule) of mass M moving in the vicinity of the solid surface. The dissipation mechanism is described by the spatially dependent force (2) which in our model leads to the particle adsorption on the surface, in the case when the dissipated energy is greater than the normal component $Mv_\perp^2/2$ of the incident kinetic energy, depending on the form and strength of interaction and on the incident energy $E_\perp$ itself. The system is not translationally invariant so we cannot assume a steady-state solution; moreover we shall not use the kinetic theory averaging procedure[1,2] but instead consider a dynamical problem of a particle with the well defined initial energy E. For simplicity we study the one dimensional case, i. e. the particle moving normally towards a flat, homogeneous surface.

The classical equation of motion for the adparticle is

$$Mvv' = F_R(z) + F_D(z, v), \quad v' \equiv \frac{dv}{dz} \tag{1}$$

where $F_R(z)$ and $F_D(z, v)$ is the reactive and the dissipative force, respectively[2,3].

Equation (1) can be solved by linearization, assuming F_D to be linear in v and approximating $Mvv' \to Mv_0v'$. But, as our results will show, the particle velocity near the surface changes rapidly through a wide range of values, so that this approximation becomes unsatisfactory. Secondly, due to the breakdown of translational symmetry near the surface, we cannot obtain a steady-state solution of Eq. (1) for our problem and the memory-effects, contained in the proper solution $v(z)$ are very important. That is another feature which the linearized solution fails to take into account and therefore Eq. (1) should be solved self-consistently. In the general case it can be done by numerical methods but in our model we shall assume the potential $F_D(z, v)$ in the form

$$F_D(z, v) = -M\eta(z)\, v\,(1 + v^2/v_c^2)^{-1} \tag{2}$$

with

$$M\eta(z) = C\,[\operatorname{sgn} F_R(z)]\, F_R(z) \tag{3}$$

C being a constant of proportionallity between F_D and F_R. This choice of F_D allows the exact formal solution of Eq. (1).

Expression (2) is an improved version of the friction force, which is linear in velocity ($F_D(z, v) = -M\eta(z)\, v$), in a low — velocity limit. F_D contains not only the spatial dependence, which we assume to have the same shape as the reactive force $F_R(z)$, but also the dynamical parameter v_c which can take into account the finite response time of the surface excitations which are the microscopic mechanism that creates the dominant contributions to the potentials F_R and F_D[4,5]. For $v \gg v_c$ we expect the dynamically reduced effect of this mechanism as has been shown for the dynamical image potential[6,7].

With the potential (2) one obtains, after separating the variables v and z, the general (implicit) solution of (1)

$$\int_{v_0}^{v(z)} \mathrm{d}v'\, v' \left(1 - \frac{Cv' \operatorname{sgn} F_R(z(v'))}{1 + v'^2/v_c^2}\right)^{-1} = \int_{+\infty}^{z} dz'\, F_R(z')/M. \tag{4}$$

We have plotted the obtained analytic solutions of (4) for the motion of a hydrogen molecule ($M = 3.31 \cdot 10^{-27}$ kg) in a force F_R due to the Morse type potential V_M

$$V_M = \varepsilon_0 \left[\exp\left(\frac{z_0 - z}{a_0}\right) - 1\right]^2; \quad F_R = -\frac{\mathrm{d}V_M}{\mathrm{d}z} \tag{5}$$

with $\varepsilon_0 = 3$ eV, $a_0 = 0.05$ nm and $z_0 = 2a_0$. From now on all quantities will be expressed via ε_0, a_0 and sec, i. e. all velocities will be given in units a_0/sec, the constant C in units sec/a_0, z in units of a_0 etc.

In Fig. 1 we plotted the adparticle velocity and energy for the case of thermalized incident energy $\left(E_0 = \frac{1}{2} k_B \cdot 300\ \mathrm{K}\right)$ as a function of the particle position as it moves through the potential well. We chose $v_c = 6.34 \cdot 10^{13}$ such that the particle

passes from the small — velocity regime ($F_D \sim v$) as it enters the potential well to the large velocity regime ($F_D \sim 1/v$) inside the potential well. This is reasonable since the particle kinetic energy increases more than 100 times in the well and its velocities in this region are equal to or greater than the value above which the dynamical reduction of adparticle-surface interaction occurs, according to relevant theories[6,7]. Although for our range of adparticle velocities, the significant reduction of particle — plasmon interaction[6,7] does not occur, we expect that this reduction occurs in the particle — phonon interaction, due to the much longer phonon response times. This is the physical process we wanted to include in our model, having in mind that the phonons are an important mechanism for the adparticle energy loss.

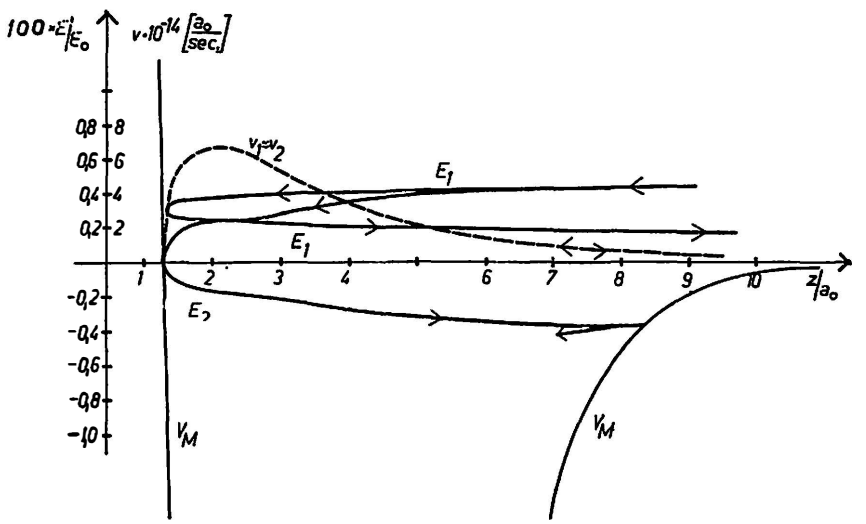

Fig. 1: Adparticle velocity (dotted lines) and energy (solid lines) for the case of a thermalized incident energy ($E_0 = 1/2\, k_B \cdot 300$ K) as a function of the particle position. E_1 and E_2 correspond to $C_1 = 6 \cdot 10^{-17}$ and $C_2 = 2 \cdot 10^{-16}$, respectively.

Fig. 1. shows the two cases: a freely reflected particle (E_{01}, $C_1 = 6 \cdot 10^{-17}$) and a trapped particle (E_{02}, $C_2 = 2 \cdot 10^{-16}$). It is obvious that the particle motion is very little affected by the dissipative forces for so low incident energy and for the other given parameters, due to the high ratio of the potential well depth ε_0 to the dissipated energy in this case. We also notice that the main dissipation is happening in the region of the »hard wall« (due to the proportionality of dissipative and reactive forces in our model).

In Fig. 2 we plotted the adparticle velocity and energy for the higher incident energies ($E_{03} = E_{04} = 0.5$ eV, $E_{05} = 1.2$ eV) also for the cases of a freely reflected (E_3, $C_3 = 3.5 \cdot 10^{-15}$) and a trapped particle (E_4, $C_4 = 5 \cdot 10^{-15}$; E_5, $C_5 = 10^{-14}$)

Due to our classical description of the adparticle, the sticking coefficient s (probability of the particle trapping in the potential well during one round trip) is either 1 or 0. Fig 3 shows the critical coefficient C_{cr}, above which the particle is always

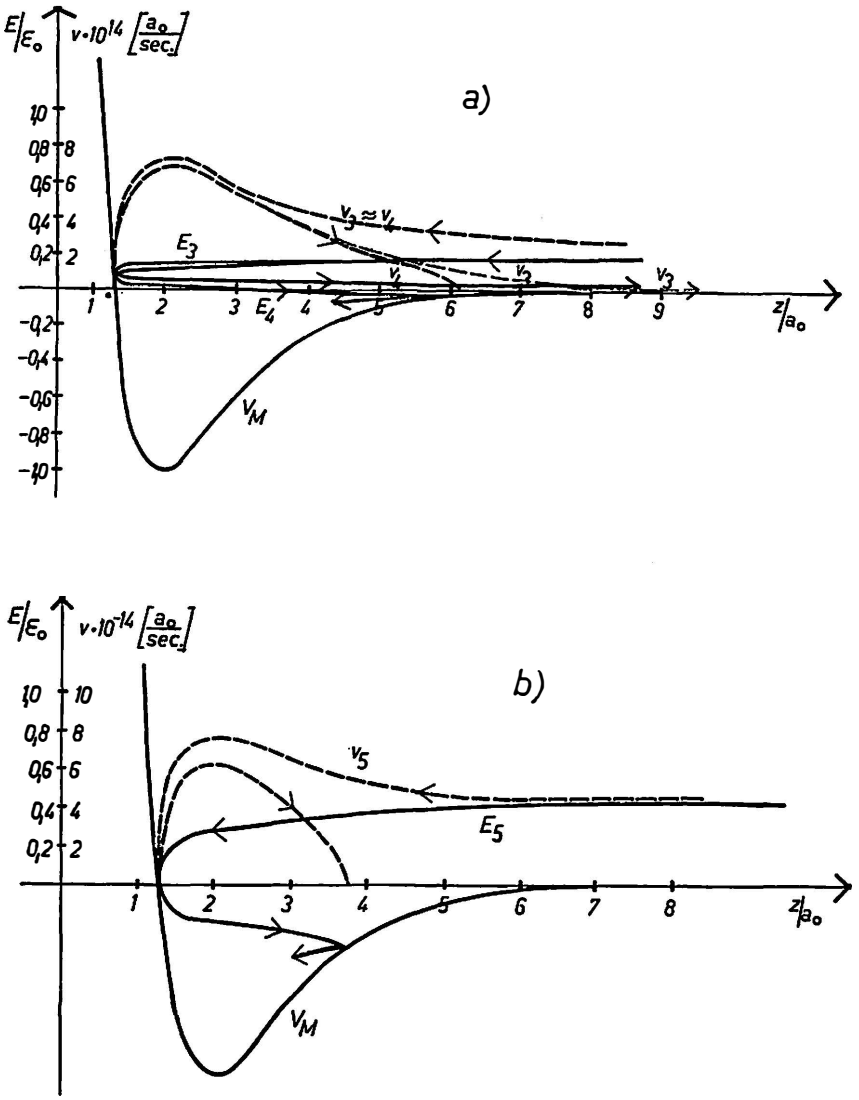

Fig. 2: Adparticle velocity (dotted lines) and energy (solid lines) for a) $E_{03} = E_{04} = 0.5$ eV with corresponding constants $C_3 = 3.5 \cdot 10^{-15}$, $C_4 = 5 \cdot 10^{-13}$, b) $E_{05} = 1.2$eV, $C_5 = 10^{-16}$. Curve E_3 corresponds to reflected particle, other two curves to trapping.

trapped, as a function of the incident energy for $v_c = 10^{12}$ and $v_c = 10^{14}$. For incident energies E_0 smaller than ε_0 an almost linear dependence of C_{cr} on E_0 is obtained, holding better as the incident energy E_0 is lowered. To explain this we should refer to Fig. 2 which indicates, as we already mentioned, that the main dissipation happens in the »hard wall« region. We also see that for the incident energies

lower than ε_0 the motion in this region is governed mainly by the form of the reactive potential and it barely depends on the incident energy. Therefore the net energy loss marginally for such incident energies depends linearly on C.

In conclusion, we have shown that, due to the breakdown of translational invariance in the problem of a particle motion near the surface, one has to take self — consistently into account the variation of the local velocity $v(z)$ and velocity dependent potential $F_D(z, v)$. We have done so in the approximation (2) and (3) solving exactly the equation (1). For the general potentials a numerical solution of an integral equation would be necessary to take into account these »memory effects«[7,8].

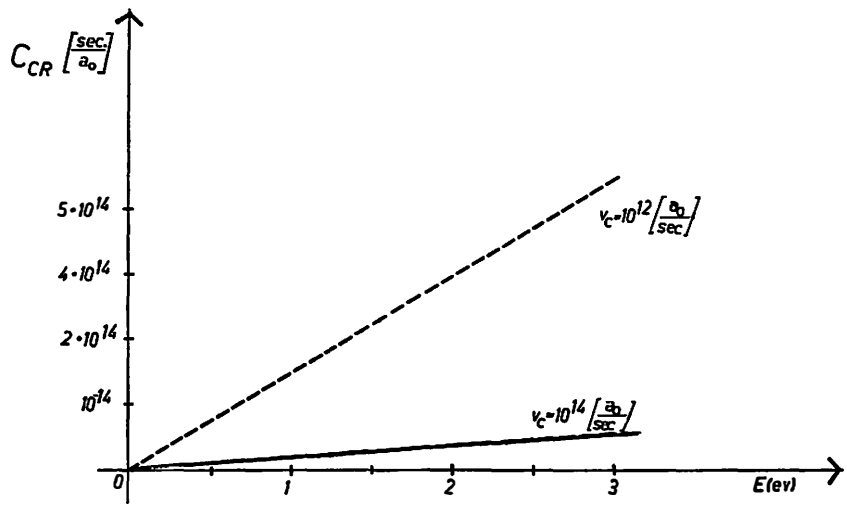

Fig. 3: The critical coefficient C_{cr} above which the particle is trapped as a function of the incident energy E_0 for $v_c = 10^{12}$ (dotted line) and $v_c = 10^{14}$ (solid line).

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NELINEARNI I DINAMIČKI EFEKTI PRI DISIPATIVNOM GIBANJU ČESTICE BLIZU POVRŠINE U MODELU TRENJA

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Ispitano je gibanje i gubitak energije čestice u međudjelovanju s površinom u klasičnom, nelinearnom, egzaktno rješivom modelu, čime su uzeti u obzir važni efekti memorije gibanja. Pokazano je kako na gubitak energije utječe uvedena prostorno i brzinski ovisna disipativna sila koja obuhvaća režim malih brzina (režim trenja) i režim velikih brzina gdje dolazi do dinamičke redukcije međudjelovanja.