

Orientation-dependent stopping power of a degenerate electron gas for slow homonuclear dimersI. Nagy^{1,2} and I. Aldazabal^{2,3}¹*Department of Theoretical Physics, Institute of Physics, Technical University of Budapest, H-1521 Budapest, Hungary*²*Donostia International Physics Center DIPC, P. Manuel de Lardizabal 4, E-20018 San Sebastián, Spain*³*Centro de Física de Materiales (CSIC-UPV/EHU) - MPC, P. Manuel de Lardizabal 3, E-20018 San Sebastián, Spain*

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We present a theoretical study on the orientation-dependent retarding force experienced by slow homonuclear dimers moving at arbitrary alignment with the direction of their flight in a three-dimensional degenerate electron gas of metallic densities. The analytical results are derived within the approximate framework of Brueckner for elastic scattering of an electron by a system of two auxiliary potentials of short range. The influence of the screened field of a single constituent of the slowly moving composite projectile on the scattering electron is modeled by an effective phase shift parameter η in the short-range potential in order to characterize the real-constituent system coupling due to displacement. The orientation-dependent closed expressions reveal the dependence of observables on the classical geometry and quantum dynamics. The interplay of wave-interference and multiple scattering in the orientation-dependent friction is analyzed for realistic sets of the input parameters. Comparison with experimental data is made and good agreement is found.

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I. INTRODUCTION

The de Broglie wave nature of massive particles, like an electron, has always been an essential ingredient in the conceptual development [1,2] and applications of quantum mechanics. For instance, the description of the outgoing wave and thus the scattering amplitude in electron scattering off an atomistic field of single or multicenter character is an important theoretical challenge [3] of considerable experimental relevance in the area of heavy-particle penetration in condensed matter [4,5]. The experimentally observable quantities, like the stopping power of the target material, can be related to integrated cross sections derived theoretically by considering the effect of electron-intruder interaction on the scattering of independent electrons of the solid-state environment.

The present paper is motivated by experimental data obtained for a carbon target with slow H_2^+ and C_2^+ projectiles [6–8]. The low-velocity data show convincing evidence of reduced stopping, the possibility of which was pointed out in the perturbative work of Arista for a random situation [9]. Particularly, the intact nature [8] of a carbon dimer in penetration suggests the possible importance of an almost complete alignment with the direction of flight. The experimentally found strong reduction, about 50%, in a carbon dimer stopping at low velocities in self-supported foils would fit to a simple classical picture by using an effective area to represent one carbon atom behind which the second atom travels in the shadow in a precisely aligned manner. Here is, therefore, a real challenge to develop an easily controllable approximation based on wave mechanics. The knowledge achieved in such a way could be useful in other, more complex cases [10,11] with clusters.

The key quantity in such a description of stopping is the quantum mechanical single-particle scattering amplitude, $F(\mathbf{k}, \mathbf{k}')$, which characterizes the matrix element between initial (\mathbf{k}) and final (\mathbf{k}') electron states in an elastic scattering ($k = k'$). In our work we model the condensed matter as a three-dimensional (3D) degenerate gas of free electrons. Therefore, it is the fundamental Pauli exclusion principle

which governs the quantum statistical aspect of the many-body problem and thus prescribes the allowed single-particle excitations responsible for the irreversible [12] slowing down process. For the investigated case of slow ($v < v_F$) intruders, these allowed one-electron states are characterized by the k_F Fermi wave number. Atomic units, $\hbar = m_e = e^2 = 1$, are used in this work. Notice that the collective wake effect [13] becomes important only at high enough ($v > v_F$) projectile velocities.

Our treatment rests on the model of two short-range potentials, and a so-called effective spherical-wave approximation to derive a complex scattering amplitude [14–16] in terms of a real, *effective* phase shift $\eta(k)$. The value of this parameter will be fixed by considering the effect of the potential gradient (force) representing an embedded-atom displacement [17–20] in an electron gas. Thus in our treatment via auxiliary short-range potentials, the phase shifts (δ_l) of the conventional partial-wave expansion of electron scattering off a regular static potential field appear in pairs, i.e., we use the $\eta \equiv (\delta_0 - \delta_1)$ *ansatz* in the present case. Remarkably, such an *sp*-based prescription for an effective (*s*-like) phase shift is in a complete agreement with an earlier result [21] based on muffin-tin potentials in multiple scattering. By our *ansatz* we model the effective coupling of constituents of a slowly moving homonuclear dimer to electrons at the Fermi level beyond the conventional assignment, $\delta_0 \rightarrow \eta$, applied routinely to fix the strength of a static short-range potential.

The rest of the calculation is performed without any further assumption, for arbitrary alignment of a homonuclear dimer. In such a way we derived closed analytical expressions for the friction components which contain the effect and interplay of interference and multiple scattering. These expressions show that the modulating influence of multiple scattering on the outgoing wave of the scattering electron becomes negligible only asymptotically when $(k_F d) \gg 1$, where d is the internuclear distance between dimer constituents.

Notice, in passing, that the underlying two-body scattering kinematics and the classical two-center geometry of our

treatment is in complete harmony with earlier [22,23] numerical works, where an overlapping range (small d) was carefully treated to model the $F(\mathbf{k}, \mathbf{k}')$ key quantity. Unfortunately, these two-center approximations, applied for H_2^+ , cannot reproduce [22] the separated-atom limit of the underlying methods. Namely, this limit must correspond to two screened H^- in a local density-functional theory, while the two-center approximation gives two localized electrons in the field of two (well-separated and screened) protons. Such a theory cannot describe accurately the dissociation of even the simplest molecules as was emphasized recently in an insightful work [24] on the proper physics.

The range is a delicate question. We know from molecular physics that in H_2 and C_2 molecules (m) in vacuum the bond lengths are about $d_m = 1.40$ and $d_m = 2.35$, respectively. The internuclear distances in vacuum are about $d_i = 2.06$ and $d_i = 2.46$, respectively, for singly-ionized (i) molecules. Consequently, in a penetration phenomenon with slow diclusters small d values are in the nature of a mathematical construct; indeed the $(k_F d)$ products are not small, but we are still not in an asymptotic limit. The average charge state [25] of constituents of a singly-ionized dicluster intruder should be around zero in a screening environment. Since the chemical radius (R_0 , beyond which there is one electron) is of the order of unity [26] or less ($\propto Z^{-1/3}$), with neutral constituents in a dimer one gets a conservative ($2R_0 < d$) estimation. Our modeling is, therefore, quite realistic.

Section II is devoted to the theoretical details of our calculation and the obtained results. These are compared with motivating data. In Sec. III, we give a predictive summary.

II. THEORY AND RESULTS

The basic expression [22,23] for the magnitude of the energy loss per unit path (denoted here by S for simplicity) of a slow ($v < v_F$) dicluster has the following decomposition in terms of the parallel (\parallel) and perpendicular (\perp) transport cross sections:

$$S(\alpha) = n_0 k_F v [\cos^2(\alpha) \sigma_{\text{tr}}^{\parallel}(k_F) + \sin^2(\alpha) \sigma_{\text{tr}}^{\perp}(k_F)], \quad (1)$$

where $n_0 = k_F^3 / (3\pi^2)$ is the density of the electron gas in 3D. In Eq. (1) α is the polar angle between the dimer orientation and its velocity direction. Notice, that these vectors define a plane in which two coordinate axes can be introduced. In the random situation we have for the angle averages: $\langle \cos^2(\alpha) \rangle = (1/3)$ and $\langle \sin^2(\alpha) \rangle = (2/3)$, in 3D.

The directions of the scattering electron momenta, \mathbf{k} and \mathbf{k}' , in the center-of-mass system and in 3D, are not necessarily in the above-defined plane. This geometrical fact introduces an azimuthal angle ($\varphi_{\mathbf{k}}$) needed for solid-angle integrations; $d\Omega_{\mathbf{k}} = d\varphi_{\mathbf{k}} \sin \theta_{\mathbf{k}} d\theta_{\mathbf{k}}$ in 3D, where $\varphi_{\mathbf{k}} \in [0, 2\pi]$ and $\theta_{\mathbf{k}} \in [0, \pi]$. The relevant transport cross sections in 3D are [22] as follows:

$$\sigma_{\text{tr}}^{\parallel}(k_F) = \frac{3}{4\pi} \int d\Omega_{\mathbf{k}_F} \int d\Omega_{\mathbf{k}'_F} (\cos \theta_{\mathbf{k}_F} - \cos \theta_{\mathbf{k}'_F}) \times \cos \theta_{\mathbf{k}_F} |F(\mathbf{k}_F, \mathbf{k}'_F)|^2, \quad (2)$$

$$\sigma_{\text{tr}}^{\perp}(k_F) = \frac{3}{4\pi} \int d\Omega_{\mathbf{k}_F} \int d\Omega_{\mathbf{k}'_F} \sin^2 \theta_{\mathbf{k}_F} \cos^2 \varphi_{\mathbf{k}_F} |F(\mathbf{k}_F, \mathbf{k}'_F)|^2. \quad (3)$$

In order to implement the above expressions, we need the complex scattering amplitude which encodes the effect of geometry and field on the scattering of the one-electron wave.

In the spirit of our detailed Introduction on the physics of the problem, we shall use

$$F(\mathbf{k}, \mathbf{k}') = \frac{2b}{a^2 - b^2} \cos \left[(\mathbf{k} - \mathbf{k}') \cdot \frac{\mathbf{d}}{2} \right] - \frac{2a}{a^2 - b^2} \times \cos \left[(\mathbf{k} + \mathbf{k}') \cdot \frac{\mathbf{d}}{2} \right], \quad (4)$$

following earlier works [14–16] in stationary scattering theory in 3D. To this equation we have $a = e^{ikd}/d$ and $b = ik[1 + \cot \eta(k)]$, where $\eta(k)$ is a phase shift parameter [15] introduced to characterize, via short-range potentials, the effect of an individual slowly moving atom on electrons at the Fermi level. Since the geometric factor (a), prescribed by the 3D Green's function with outgoing boundary condition, is not zero in our case because d is finite, the multiple scattering effect on the electron-wave should have an impact on integrated cross sections also. A detailed quantification of this impact is the main goal of our study.

The first step to Eqs. (2) and (3) is to characterize the flux, i.e., to evaluate the $|F(\mathbf{k}, \mathbf{k}')|^2$ quantity, which is an areal quantity in 3D. In this evaluation [$(1/b) \equiv (1/k)e^{i\eta} \sin \eta$] with the form given by Eq. (4), we found it useful to introduce the following abbreviations:

$$A(x, \eta) = \frac{1}{1 + \left(\frac{\sin \eta}{x}\right)^2 - 2\frac{\sin \eta}{x} \cos(x + \eta)}, \quad (5)$$

$$B(x, \eta) = \frac{1}{1 + \left(\frac{\sin \eta}{x}\right)^2 + 2\frac{\sin \eta}{x} \cos(x + \eta)}, \quad (6)$$

$$C(x, \eta) = \frac{1 - \left(\frac{\sin \eta}{x}\right)^2}{\left[1 - \left(\frac{\sin \eta}{x}\right)^2\right]^2 + \left[2\frac{\sin \eta}{x} \sin(x + \eta)\right]^2}, \quad (7)$$

where $x \equiv k_F d$ is a shorthand. The rest of the calculation needs only a long but fairly straightforward algebra. Using $\mathbf{k} \cdot \mathbf{d} = (kd) \cos \theta_{\mathbf{k}}$ also, finally we arrived at

$$\frac{\sigma_{\text{tr}}^{\parallel}(k_F)}{(4\pi/k_F^2) \sin^2 \eta} = (A + B)[1 + 3j_0^2 - (6/x)j_0 j_1] + 4(A - B)[j_0 - (3/2x)j_1] - 6Cj_1^2, \quad (8)$$

$$\frac{\sigma_{\text{tr}}^{\perp}(k_F)}{(4\pi/k_F^2) \sin^2 \eta} = (A + B)[1 + (3/x)j_0 j_1] + (A - B)[j_0 + (3/x)j_1], \quad (9)$$

in which the argument of spherical Bessel functions of the first kind is $x = k_F d$. The above closed expressions show the nontrivial interplay of quantum dynamics and geometry in wave-mechanical electron scattering. They allow a detailed and easy analysis of the orientation-dependent stopping power, without uncontrollable steps.

First, we discuss a few limits for the stopping power. With $A = B = C = 1$, i.e., without the multiple scattering effect,

one gets after orientation averaging the simple form of

$$\frac{1}{2} \frac{\langle S \rangle}{(4\pi/k_F^2) \sin^2 \eta} = (n_0 k_F v) [1 + j_0^2(x) - j_1^2(x)], \quad (10)$$

derived [27] earlier by performing an angle average in the Born scattering amplitude (in momentum space) with $a \equiv 0$. In this case, as was emphasized [5,23] earlier, the geometric part of the result is very similar to the one obtained in dielectric theory with point charges. The minimum of the right-hand side is at $x \simeq 2.74$, and thus one has $[1 + j_0^2(x) - j_1^2(x)] \simeq 0.87$.

Notice at this important point that the dielectric (linear-response) theory corresponds to the first-order Born approximation for the (real) scattering amplitude obtained from the Fourier transform of a screened scattering potential [9]. On the other hand, this theory can be formulated as an infinite-order expansion for the scattering amplitude in terms of Born phase shifts. Thus the observed strong similarity of the above right-hand-side form with the final result of a dielectric theory implies that the proximity effect is described very well with few leading Bessel functions. This fact suggests to us that one can use a substitution only in the left-hand-side denominators with

$$\sigma_{\text{tr}}(k_F) = \frac{4\pi}{k_F^2} \sum_{l=0}^{\infty} (l+1) \sin^2[\delta_l(k_F) - \delta_{l+1}(k_F)], \quad (11)$$

the exact transport cross section if the description of the influence of an individual slow atom requires such a representation to the magnitude of the stopping power.

Still with $A = B = C = 1$, the stopping expression for a completely aligned dicluster has a slightly more complicated form

$$\frac{1}{2} \frac{S(\alpha = 0)}{(4\pi/k_F^2) \sin^2 \eta} = (n_0 k_F v) \{1 + 3[j_0^2(x) - j_1^2(x) - (2/x)j_0(x)j_1(x)]\}. \quad (12)$$

In this case the minimum is at $x \simeq 2.32$, and we have $\{\dots\} \simeq 0.40$ for the geometrical factor. This value is very similar to the one obtained earlier [28] in linear response (dielectric) theory for the same geometrical ($\alpha = 0$) situation with point charges. This observation gives a further credit to the statement based on the above averaged form for the proximity effect. The right-hand-side forms are sensitive only to the leading Bessel functions, in practice.

It is easy to show by the careful Taylor expansions of Eqs. (8) and (9) that all of the transport cross sections behave as

$$\sigma_{\text{tr}}(k_F \rightarrow 0) = 2[4(\pi d^2)]. \quad (13)$$

This fact is well known from the pioneering work [14] of Brueckner. The above equation describes, at $k_F \rightarrow 0$ in quantum mechanics, the case of two hard spheres [3]. Remarkably enough, $(4\pi d^2)$ is close (with $d \simeq 2$) to the spin-averaged electron-hydrogen cross section [$\sim 18\pi$ (in a_0^2)] of the static-exchange approximation, at the scattering length (vanishing scattering momentum) limit [29]. We do not consider the $d \rightarrow 0$ case since a so-called united atom limit of two slow charged constituents (nuclei) is in the nature of mathematical construct. The realistic value of d is governed (c.f., the Introduction) by proper physics. It is not

an arbitrarily tunable parameter, especially not to a vanishing value.

Next, we turn our attention to the realistic range. A simple inspection of the denominator structures of Eqs. (5)–(7) heralds that the $(k_F d + \eta)$ argument quantity in the corresponding trigonometric functions can play an important role. In fact, the important $A(x, \eta)$ and $B(x, \eta)$ modulating functions can still be close to unity, at not too small x values and for $(k_F d + \eta) \simeq m(\pi/2)$, with $m = 1, 3, \dots$. The change from unity in the $C(x, \eta)$ function is second order in the inverse of x . Furthermore, it is this $C(x, \eta)$ function with a strong negative character which determines a reduction in $\sigma_{\text{tr}}^{\parallel}(k_F)$. These details suggest that the estimation obtained in Eq. (12) for the minimum value could have a broader validity.

In Fig. 1 we exhibit the illustrative ratios (denoted as \mathcal{R}) of S^{\parallel} (solid), S^{\perp} (dashed), their averages $\langle S \rangle$ (dotted), and the common $2[(4\pi/k_F^2) \sin^2 \eta]$ quantity. The underlying computations rest on the analytical, closed expressions given above. The curves in the three panels are calculated, respectively, with $\eta = (\pi/4)$ (top panel), $\eta = (\pi/2)$ (middle panel),

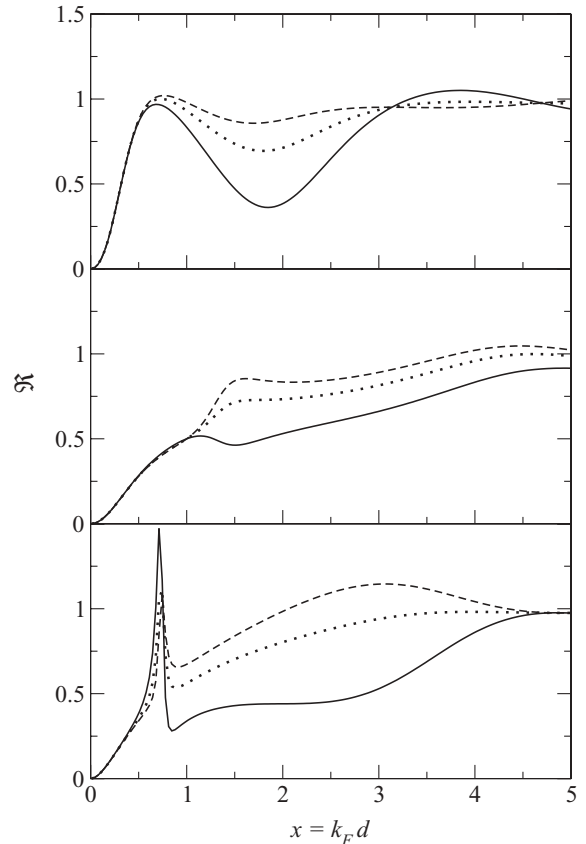


FIG. 1. Illustrative dimensionless ratios, \mathcal{R} , showing the orientation dependence of the renormalized stopping power of a degenerate electron gas for homonuclear diclusters under parallel (\parallel) (solid curves), perpendicular (\perp) (dashed curves), and random (dotted curves) conditions of traversing the target material. The curves are exhibited for the $x \in [0, 5]$ range, where $x = k_F d$. The input effective phase shifts are from the $\eta \in [\pi/4, 3\pi/4]$ interval, in steps of $\Delta(\eta) = \pi/4$.

and $\eta = (3\pi/4)$ (bottom panel) inputs. They are plotted for the mathematical range of $x \in [0,5]$, where $x = k_F d$ is a dimensionless product.

The motivating experimental (expt) data obtained in carbon targets ($v_F = 1.2$) by slow ($v < v_F$) H_2^+ projectiles at a random condition [5,7], and with C_2^+ projectiles [8] at a presumably close-to-parallel (\parallel) situation, are about $\mathcal{R}_{\text{expt}}(\text{H}_2^+) \simeq (0.8\text{--}0.9)$ and $\mathcal{R}_{\text{expt}}(\text{C}_2^+) \simeq (0.46\text{--}0.56)$, respectively. The presumed orientation in traversing reflects the emphasized [8] intactness of carbon dimers. We note furthermore that for a $1 \mu\text{g}/\text{cm}^2$ carbon foil, the experimental $\mathcal{R}_{\text{expt}}(\text{C}_2^+)$ is only about $(0.25\text{--}0.3)$. On the other hand, as was carefully [8] stated, this particular target is not a self-supported one, and some cavities of several μm in diameter were opened through the whole thickness of it.

In order to implement our theory for the above-discussed experimental cases with dimers, we need to specify the *effective* phase shift parameter [$\eta \equiv (\delta_0 - \delta_1)$] and geometrical factor (d) values. These last factors are considered as about $x \simeq 2.5$ for the H_2^+ case, and about $x \simeq 3$ for the C_2^+ case. The practical estimation (c.f., the Introduction) for the η parameters rests on phase shifts values obtained [30] within the Kohn-Sham orbital version of density-functional theory for atom embedding in the electron gas of a carbon target. Thus, we use $(\delta_0 - \delta_1) \simeq 0.70$ for the case of H_2^+ , and $(\delta_0 - \delta_1) \simeq 2.30$ for the case of C_2^+ .

Our results are $\langle \mathcal{R} \rangle \simeq 0.82$ and $\mathcal{R}^{\parallel} \simeq 0.53$ for hydrogen (random) and carbon (parallel) dimers. The agreement of these theoretical values with the before-mentioned [6–8] motivating data is good. More recent data [31,32] obtained by slow H_2^+ under channeling conditions in a gold target also show reduced stopping powers, i.e., a negative vicinage effect. The agreement with different data sets supports our detailed analyses given above in Eqs. (10) and (12) on the determining role of the first few Bessel functions, and of our physically motivated *sp*-based *ansatz* for an effective phase shift parameter introduced to characterize the relevant coupling via auxiliary short-range potentials.

III. SUMMARY

Closed, analytical results are derived for the orientation-dependent stopping power of a degenerate electron gas for slow homonuclear diclusters. We characterized the slowly moving scattering object by two short-range (auxiliary) potentials, and considered the effect of multiple scattering at an effective spherical wave level. Using realistic parameters, a good agreement with two different experimental data sets, obtained by slow H_2^+ and C_2^+ intruders in a carbon target, is established. The analytical expressions derived in this work could be useful for other (for instance, for N_2^+ or O_2^+ intruders) homonuclear-dimer–metallic-target cases, in a computer simulation [31] with slow dimers, and for orientation-dependent [33] friction coefficients of molecules on surfaces.

Notice, finally, that the box-like character of our \mathcal{R}^{\parallel} in the bottom panel is quite intact. Namely, a very similar shape for the \mathcal{R}^{\parallel} quantity appears, in the given range of $x = k_F d$, for about $(\delta_0 - \delta_1) \equiv \eta \in [2,3]$ with small alterations. This character, similarly to the well-known [14] peaked structure at smaller x , is the result of a nontrivial interplay between classical geometry and quantum mechanical interference. We can call the box-like behavior a robust one since the important $\eta(k_F)$ parameter is in the above range for embedded carbon and heavier atoms, at the practically important metallic densities, i.e., for the range of $0.6 < k_F < 1.3$. Thus, using detailed phase-shift Tables [30] and Eqs. (5)–(9), one could easily obtain realistic estimations for orientation-dependent vicinage effects in cases of other dimer-intruder–metallic-target combinations.

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