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# **Stopping of Slow Hydrogen Dicluster by Different Solid Materials**

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### Abstract

In this theoretical work, the subject of stopping power is investigated for slow hydrogen dicluster by using random phase approximation. The projectile is stopped by variance solids of different Wigner Seitz radiuses. The considered stopping power is related to the interaction between a low velocity dicluster of zero damping interacts with (Au, C, Al, and Cs) targets mediums based on an electron gas model. The subject of an ionic dicluster stopping power has been calculated by using Random Phase Approximation (RPA) at low velocity for the first and second approximation order, where the influence of damping has been ignored. The obtained results of this study show detailed behavior of the ionic dicluster of its duality interaction with several electron density targets mediums of long range collision belongs to aggregation effect, their affected parameters as internuclear distance of dicluster, and its velocity are studied. The results have been achieved by using programs of Fortran-90 language which performed for the numerical calculation.

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#### 1. Introduction

Beams of molecule and cluster ions covering a wide range of energies have become available recently. Such beams are useful tools in fundamental research on the interaction of particles with matter, expanding the number of available degrees of freedom and thus the range of observable phenomena. Moreover, there are promising applications in science and technology. Cluster beams with energies per atom in the KeV or MeV range allow deposition of energy in matter at densities for above that can be achieved with beams of atomic ions [1,2]. This has implications on ion-beam-induced adsorption [3, 4], track formation [5], and inertial confinement fusion [6]. Conversely, clusters with energies per atom in the eV regime are of potential use for depositing material because of the highly achievable particle currents that combined with low damage rates [7, 8].

The present study concerns with the deposition of electronic energy by slow molecular clusters in matter (less than Fermi velocity  $(\mathbf{v}_F)$ .

A central quality characterizing the interaction of cluster projectiles with matter is the mean energy loss per traveled the path length, or stopping power. This quality is approximated by the sum of the stopping powers for the constituent atomic ions of cluster [9],

	$\int dE$	$\sim \sum_{cluster} \left($	$\Sigma \left( -\right)$	$\underline{dE}$	(1)
(	dX		luster	dX) <sub>atom</sub>	

#### 2. Declutter Interaction

Consider a pair of ions  $Z_1$ ,  $Z_2$  in correlated motion a structure that may be obtained by the incidence of diatomic molecules with velocity (v) in a dense medium of valence electrons of solid.

The main electron gas parameters to be used here are the following: Fermi velocity ( $\mathbf{v}_F$ ), plasma frequency ( $\omega_P$ ), and Wigner-Seitz radius of the average volume occupied by each electron in units of Bohr radius  $a_{\circ} = \hbar^2 / me^2 = 0.529 A^{\circ}$ . Values are typically  $r_s \approx 2a.u$ . but they range from  $r_s \approx 1.5a.u$ . to  $r_s \approx 2.8a.u$ . (with relations:  $\vec{v}_F = 1.919/r_s$ ,  $\omega_p = \sqrt{3/r_s^3}$  in atomic units). It has been shown, both

theoretically and experimentally, that the energy lost per particle and per traveled the path length for a cluster of ions moving in a solid target shows important differences usually called vicinage effects- with respect to the energy loss of the separated ions [10]. The origin of this effect is the interference in the electronic excitations of the target due to the correlated motion of the penetrating ions. In this study low dicluster velocity is considered to investigate the vicinage effect on cluster energy loss, where the main contribution to the vicinage effect is Plasmon excitation [11], in this case the wave number (k) of the projectile is less than the critical wave number (KC). A domain of distant or collective interactions. With typical distances where r is the internuclear distance of dicluster, the resonant or plasmon excitation is the relevant process. The induced polarization induced by the charged projectiles produces an electric field, which reacts by generating a stopping force on the projectile. There are two different contributions to this force: one coming from the interaction of each proton with its own induced polarization and

the other due to the interaction of each proton with the electrons exerted on the two moving projectiles [12].

### 3. Dielectric Formalism for the Energy Loss

Consider a cluster of N charges *Zie*, moving with non-relativistic velocity (v) in a material medium of longitudinal dielectric constant (k, $\omega$ ). Neglecting small deviations of the individual velocities with respect to the average velocity v, the corresponding charge density can be written as

Where  $\vec{r_i}$  is the positions of the corresponding charges at time t=zero.

For nonrelativistic velocities, the electric field  $\vec{E}(\vec{r},t)$  generated by the cluster is determined from Poisson's equation, which yields the simple algebraic relation between the space-time Fourier transforms of  $\vec{E}(\vec{r},t)$  and  $\rho(\vec{r},t)$ 

Thus, the following expression for the electric field is obtained by:

In these expressions, the fields due to the external changes and the fields due to the polarization induced in the medium are summed. In particular, the force acting on the jth particle is given by:  $\vec{R} = \vec{R} \cdot \vec{R} \cdot \vec{R}$ 

$$\vec{F}_{j} = Z_{j}e\vec{E}(\vec{r}_{j} + \vec{v}t, t)$$

$$= \frac{Z_{j}e}{(2\pi)^{2}}\sum_{i}Z_{i}e\int d^{3}\vec{k}\frac{2\vec{k}}{k^{2}} \times \left[\operatorname{Im}\left(\frac{1}{\in(\vec{k},\vec{k}.\vec{v})}\right)\cos(\vec{k}.\vec{r}_{ji}) + \operatorname{Re}\left(\frac{1}{\in(\vec{k},\vec{k}.\vec{v})}\right)\sin(\vec{k}.\vec{r}_{ji})\right].....(5)$$
Where here d Berry the investment of a state of  $\vec{k}$  and  $\vec{k} = \vec{k} - \vec{k}$ 

Where Im and Re are the imaginary and real part of  $\frac{1}{\in (\vec{k}.\omega)}$ 

and 
$$\vec{r}_{ji} = \vec{r}_j - \vec{r}_i$$

In Eq. (4), the force has been written explicitly in real form by using the physical requirement that the fields must be of real magnitudes, which imposes the following condition on the dielectric constant:

$$\in (-\vec{k},-\omega) = \in^* (\vec{k},\omega).$$

It is interesting to compare the behavior of the two terms in the integral with respect to a change in the sign of  $\vec{F}_{ji}$ , or what is equivalent, to compare the force that the i charge exerts on the j charge, with the force that the latter exerts on the first. The mutual forces acting through the term in  $\operatorname{Re}\left[\frac{1}{\in(\bar{k})}\right]$  are opposed, and cancel out if the

acting forces overall cluster of charges are summed. The forces acting through the term in  $\text{Im}(1 \in (\bar{k}, \omega))$  are, on the contrary, dissipative (considering the energy of the cluster not of the individual particles).

Thus, the energy loss (per unit time) of the cluster of charges is given by

$$\frac{dW}{dt} = -\sum_{j} \vec{v} \cdot \vec{F}_{j}$$
  
And  
$$\frac{-dE}{dx} = \frac{1}{v} \frac{dW}{dt}$$
  
Then

The terms have separated with i=j, which give the energy loss of totally independent charges, and the terms with  $i \neq j$ , which represent interference effects on the energy loss due to the simultaneous perturbation of the medium by the charges in correlated motion.

Eq. (6) is a general formula for the stopping power of the diclusters of charges  $(z_1e)$  and  $(z_2e)$  then

$$\left(-\frac{dE}{dx}\right) = \frac{e^2}{2\pi^2 v} \int d^3 \vec{k} \, \frac{\vec{k}.\vec{v}}{k^2} \, \mathrm{Im}\left(\frac{-1}{\in (\vec{k},\vec{k}.\vec{v})}\right) \times \left[\left(z_1^2 + z_2^2\right) + 2z_1 z_2 \cos\left(\vec{k}.\vec{r}_{12}\right)\right] \qquad \dots (7)$$

Where the two charges in correlated motion with velocity  $\vec{v}$  and internuclear separation  $\vec{r}_{12} (\vec{r}_{12} = \vec{r}_1 - \vec{r}_2)$ . In Eq. (7) the stopping power is given as a function of the relative orientations of  $r_{12}$  and v. Consider the orientations  $r_{12}$  are randomly distributed and the mean energy loss  $-\langle dE/dx \rangle$  corresponding to random orientations of  $r_{12}$  may be obtained by using the property of  $\delta$  – function. Eq. (7) becomes,

$$\left\langle -\frac{dE}{dx} \right\rangle = \frac{e^2}{2\pi^2 v} \int d^3 \vec{k} \, \frac{\vec{k}.\vec{v}}{k^2} \operatorname{Im}\left(\frac{-1}{\epsilon \, (\vec{k}, \vec{k}.\vec{v})}\right) \times \left[ \left( z_1^2 + z_2^2 \right) + 2z_1 z_2 \, \frac{\sin\left(\vec{k}.\vec{r}_{12}\right)}{\vec{k}.\vec{r}_{12}} \right] \dots$$
(8)

Or  

$$\left\langle -\frac{dE}{dx}\right\rangle = \frac{2e^2}{\pi v^2} \left[ f_s(\vec{k},\omega) + f_c(\vec{k},\omega) \right]$$
....(9)

Where

 $f_s(\vec{k},\omega) \& f_c(\vec{k},\omega)$  are the functions for single charge interaction and correlated term. And  $\operatorname{Im}\left[\frac{-1}{\in (\vec{k},\vec{k},\vec{v})}\right]$  is solved in section 3.

4. Low Dicluster Velocity (LV.)  $\vec{v} < \vec{v_F}$  with no damping  $\gamma \to 0$ 4.1 Imaginary Part of the Dielectric Function:

The well-known Lindhard function [13] gives in a self-consistent way an exact description of the dielectric function for a non-relativistic free electron gas of high density at zero temperature. In the low frequency limit, within this Random Phase Approximation (RPA) for the dielectric function, the loss function can be written as:

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Multiplying and dividing Eq. (10) by its conjugate, yields:

therefore the imaginary part of  $\frac{-1}{\in(\vec{k},\omega)}$  can be written as:

$$\operatorname{Im}\left(\frac{-1}{\in(\bar{k},\omega)}\right) = \frac{\in_2(\bar{k},\omega)}{\in_1^2(\bar{k}) + \in_2^2(\bar{k},v)}$$
(12)

From Echenique et al. [14] we have that:

$$\epsilon_1(\vec{k}) = C(\vec{k})f_1(\vec{k}) + 1 \text{ for arbitrary } \vec{k}$$

$$\epsilon_2(\vec{k}, \omega) = C(\vec{k}) \frac{\pi\omega}{1-\omega} \text{ for } \vec{k} < 2\vec{k}_2$$

$$(14)$$

$$C(\vec{k}) = \frac{4k_F}{\pi k^2} \qquad .....(15)$$

$$f_1(\vec{k}) = \frac{1}{2} \left[ 1 + \frac{4k_F^2 - k^2}{\sqrt{1-k_F}} \ell n \left| \frac{\vec{k} + 2\vec{k}_F}{\sqrt{1-k_F}} \right| \right] \qquad .....(16)$$

Substituting Eq.(13)-(16) into Eq. (12), yields:

$$\operatorname{Im}\left(\frac{-1}{\in(\vec{k},\omega)}\right) =$$

$$\frac{4\vec{k}_F}{\pi k^2} \times \frac{\pi\omega}{2\vec{k}.\vec{k}_F}}{\frac{4\vec{k}_F}{\pi k^2}} \left[\frac{1}{2}\left(1 + \frac{4k_F^2 - k^2}{4\vec{k}.\vec{k}_F} \ell n \left|\frac{\vec{k} + 2\vec{k}_F}{\vec{k} - 2\vec{k}_F}\right|\right)\right] + 1\right\}^2 + \left[\frac{4\vec{k}_F}{\pi k^2} \times \frac{\pi\omega}{2\vec{k}.\vec{k}_F}\right]^2 \dots (17)$$

**4.1.1 Derivations of Approximate Formula for the Dicluster Stopping Power** Substitute Eq. (17) into Eq. (8) one can get

Eq. (18) and (19) are the exact value equations for calculating average stopping power of single ions and correlated ions  $\langle -\frac{dW_s}{dx} \rangle \& \langle -\frac{dW_c}{dx} \rangle$  respectively (with no damping). These equations can be solved numerically. Therefore, we seek forms of  $\in (\vec{k}, \omega)$  and  $f_1(\vec{k})$  that permit analysis without exclusive resource to numerical methods. First for  $\in (\vec{k}, \omega)$  an approximation is made to Eq. (12), if  $\in_1 (\vec{k}) \gg \in_2 (\vec{k}, \omega)$ ; therefore,

Different approximations to the function  $f_1(\vec{k})$  ead to different expressions for the stopping power, for the charges  $z_1$  and  $z_2$ .

In the present work, we shall try to study the effect of the approximation of  $f_1(\vec{k})$  to the stopping power of dicluster:

# (i) The First approximation method to $f_1(\vec{k})$ :

If we take  $f_1(\vec{k}) = 1$ , then Eq. (20) becomes

Substitute Eq. (15) in Eq. (21) one can get, 1  $2\vec{k} \omega$ 

where

 $k_D^2 = \frac{4\vec{k}_F}{\pi}$ 

By substituting Eq. (22) into Eqs. (9a, 9b) respectively, then:

Or

Let  $\psi = \pi \vec{k}_F$ , then

Then the average rate of stopping power due to single charges at low velocity with no damping 
$$(\gamma \rightarrow 0)$$
 is given by the following Eq.

$$\left\langle -\frac{dW_s}{dx} \right\rangle_L = \frac{2e^2 \vec{v}}{3\pi} \left( z_1^2 + z_2^2 \right) I\left( \pi / \alpha r_s \right)$$
(27)

If we return to the substitution of Eq. (22) into Eq. (9b) one can get

The average stopping power due to correlation of charges becomes,

# (ii) The Second Approximation form to $f_1(\vec{k})$ :

A good approximation to the stopping power values obtained numerically by using the full (RPA) dielectric response function has been proposed by Lindhard and Winther [15]. Expanding the function  $f_1(\vec{k})$  and then,  $f_1(\vec{k})$  up to the second order in k and then,  $f_1(\vec{k})$  becomes [16].

The imaginary part of the (RPA) dielectric loss function is given by inserting Eqs. (13-15) and Eq. (31) into Eq. (12) as follows:

By substituting Eq. (33) into the stopping power of a single charges projectile expression, Eq. (9a), One can get:

By using the standard integral solution [91], one can get the final solution to Eq. (34) as follows:  $\Box$ 

$$f_{s}(\vec{k},\omega) = \frac{\left(z_{1}^{2} + z_{2}^{2}\right)v^{3}}{3\Pi^{4}} \left[ \ln\left(1 + \frac{4k_{F}^{2}}{(k_{D}^{2}/\Pi^{2})}\right) - \frac{1}{1 + \frac{(k_{D}^{2}/\Pi^{2})}{4k_{F}^{2}}} \right] \dots (35)$$

The average rate of the stopping power for the second approximation due to single charges with low velocity is given by the following Eq.

Let 
$$\chi^2 = \frac{1}{\pi \bar{k}_F}, \chi_1^2 = 1 - \frac{\chi^2}{3}, \chi_2^2 = 1 + \frac{2\chi^2}{3}$$
 .....(37)

One can get

To calculate the average energy loss per unit path length of the two correlated ions we substitute Eq. (33) into Eq. (9b) as follows:

The average correlated stopping power can be written as follows:

$$\left\langle -\frac{dW_c}{dx} \right\rangle_L = \frac{2e^2}{\pi v^2} f_c(\vec{k}, \omega) \qquad .....(40)$$
  
Or  
$$\left\langle -\frac{dW_c}{dx} \right\rangle_L = \frac{8e^2(z_1 z_2)\vec{v}}{3\pi \vec{r}_{12} \Pi^4} \int_0^{2\vec{k}_F} \frac{k^2 d\vec{k} \sin(\vec{k}.\vec{r}_{12})}{\left(k^2 + k_D^2 / \Pi^2\right)^2} \qquad .....(41)$$

Eqs. (36) and (41) has been solved numerically.

## **4.2** Calculation of Dicluster Stopping Power with Damping Process $(\gamma \rightarrow 0)$ For Slow Ions $\vec{v} < \vec{v}_F$ :

For an electron gas described by a complex dielectric function,  $\in (\bar{k}, \omega)$ , the stopping power for a carbon of velocity  $\vec{v}$  in the electron gas (or the stopping power of the electron gas) is given by the Eq. (6), and a dielectric function approximation for the of slow ions has been suggested by Ferrel et al. [18]. They employ an approximation form for,  $\in (\bar{k}, \omega)$ , the dielectric function of the metal, which is appropriate when energy transfer,  $\omega$ , is small compared with the Fermi energy of the metal.

Eq. (18) is a simple generalization of the longitudinal dielectric function of an electron gas as derived from the hydrodynamic model [13]. It is chosen so that the next Eqs. (53,55) of single and correlated stopping power respectively agree with Lindhard dielectric function, to first order. The presence of the factor  $\theta(2\bar{k}_F - \bar{k})$ accounts, hence particle-hole excitations of small energy cannot correspond to a momentum transfer much greater than  $2\vec{k}_F$ . The term containing  $\gamma$  as a factor describes damping of collective states and may be taken from experiments for a given metal.

By substituting the imaginary part, into Eqs. (9a,9b) then the average stopping power for single ions can be represented by the following equations:

by the following equations:

$$f_{s}(\vec{k},\omega) = \int_{0}^{2\vec{k}_{F}} \frac{dk}{\vec{k}} \int_{0}^{\vec{k}\cdot\vec{v}} \omega d\omega \times \\ \operatorname{Im}\left[\frac{-1}{1+\omega_{p}^{2}/\left\{s^{2}k^{2}\left[1-i\pi\theta(2\vec{k}_{F}-\vec{k})/2\vec{k}\cdot\vec{v}}\operatorname{Im}\left(\frac{-1}{\epsilon(\vec{k},\omega)}\right)^{2}\right)\right\}}\right] \left(z_{1}^{2}+z_{2}^{2}\right) \dots (42)$$
Therefore

Therefore

$$\left\langle -\frac{dW_s}{dx} \right\rangle_L = \frac{2e^2}{\pi v^2} \int_0^{2\bar{k}_F} \frac{d\bar{k}}{\bar{k}} \int_0^{\bar{k}.\bar{v}} \omega d\omega \times \operatorname{Im}\left[\frac{-1}{1+\omega_p^2/\left\{s^2k^2\left[1-i\pi\theta(2\bar{k}_F-\bar{k})/2\bar{k}.\bar{v}\right]-\omega(\omega-i\gamma)\right\}}\right] \left(z_1^2+z_2^2\right) \quad \dots \dots (43)$$

Also the average Stopping Power for the correlated ions is given as follows:

$$f_{c}(\vec{k},\omega) = \int_{0}^{2\vec{k}_{F}} \frac{dk}{\vec{k}} \int_{0}^{\vec{k}\vec{v}} \omega d\omega \times \\ \operatorname{Im}\left[\frac{-1}{1+\omega_{p}^{2}/\left\{s^{2}k^{2}\left[1-i\pi\theta(2\vec{k}_{F}-\vec{k})/2\vec{k}.\vec{v}\right]-\omega(\omega-i\gamma)\right\}}\right] \frac{\sin(\vec{k}.\vec{r}_{12})}{\vec{k}.\vec{r}_{12}} \dots (44)$$

Then 
$$\left\langle -\frac{dW_c}{dx} \right\rangle_L = \frac{2e^2}{\pi v^2} \int_0^{2\bar{k}_F} \frac{d\bar{k}}{\bar{k}} \int_0^{\bar{k}.\bar{v}} \omega d\omega \times$$

$$\operatorname{Im}\left[\frac{-1}{1+\omega_{p}^{2}/\left\{s^{2}k^{2}\left[1-i\pi\theta(2\vec{k}_{F}-\vec{k})/2\vec{k}.\vec{v}\right]-\omega(\omega-i\gamma)\right\}}\right]\frac{\sin(\vec{k}.\vec{r}_{12})}{\vec{k}.\vec{r}_{12}} \dots (45)$$

Eqs. (43) and (45) have been solved numerically.

### 5. Results and Discussion

The energy loss of a pair of charges in correlated motions through a degenerate electron gas is calculated in the present work, within the linear response approximation of Random Phase Approximation (RPA) to describe collective excitations, where the total stopping power incorporates both excitation effect - (dE / dx) while the correlated energy loss represents the correlation effect alone. For sufficiently low velocities the energy loss of correlated charges depends on the relation between the internuclear distance  $\vec{r}_{12}$  and the wavelength of the electrons at the Fermi surface  $\lambda_F$  or Wigner Seitz radius  $r_s$  where  $\vec{k}_F \alpha \frac{1}{r_s}$  and  $\vec{k}_F \alpha \frac{1}{\lambda_F}$  [19,20]. For  $\vec{r}_{12} \gg \lambda_F$  (or  $\vec{r}_s$ ) the interference effects on the correlated energy loss become negligible, as it is physically plausible. These results are demonstrated in Figs. (1-4) although the accuracy difference of the results of Figs. (1,2) and (3,4), this physical explanation agree with Arista's results in (1977) [19] and his conclusions.



Fig.(1): Total stopping power versus internuclear distance of Au ,C, Al and Cs targets for first approximation at low velocities (a)V=0.1 (b) V=0.5 (c) V=0.7 (d) V=1.2, with no damping targets.



Fig.(2):Correlated stopping power versus internuclear distance of Au, C, Al and Cs targets for first approximation at low velocities (a) V=0.1 (b) V=0.5 (c) V=0.7 (d) V=1.2, with no damping target.

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Fig.(3): Total stopping power versus internuclear distance of Au, C, Al and Cs targets for second approximation at low velocities (a) V=0.1 (b) V=0.5 (c) V=0.7 (d) V=1.2, with no damping targets.

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Fig.(4):Correlated stopping power versus internuclear distance of Au, C, Al and Cs targets for second approximation at low velocities (a) V=0.1 (b) V=0.5 (c) V=0.7 (d) V=1.2, with no damping targets.

Here two important features are noted: (i) the interference effect becomes negative and this may happen when  $\frac{2\vec{v}}{\omega_p} < \vec{r}_{12} < \frac{5\vec{v}}{\omega_p}$  [20] where the electrons excitations of the medium atoms being incoherent to cause increasing projectile energy rather than dissipating it, and vice versa in the case of  $\vec{v}_{12} = \vec{v}/\omega_p$  which names resonant or Plasmon excitations the highest transfer of projectile energy to the target electrons should happen and this belongs to the coherency of electrons excitations, (ii) The value in the united atom case ( $\vec{r}_{12} = 0$ ) takes maximum energy loss values where the projectile behaves as a unit charge of  $(z_1 + z_2)$  which may increase Coulomb screening or in other ward the stopping power, conversely in the case of  $\vec{r}_{12} > \frac{5\vec{v}}{\omega_p}$  the dicluster should be two separated particles of charge  $z_1e$  and  $z_2e$  and , where the correlated stopping power would approach to zero[20].

### 6. Conclusion

The stopping power for a dicluster projectile of different internuclear distances moves at low and high velocity to interact with a piece of material of different electron densities:

$$Au(r_s = 1.49), \quad C(r_s = 1.66), \quad Al(r_s = 2.12), \text{ and } Cs(r_s = 5.88)$$

Stopping power relationship consists of two components the first one originates from the single or close collision between interactions happens at high velocity range where high momentum transfer is achieved from ion to electron. The second contributed component is caused by the collective excitation for the waves of plasma; the adequate circumstance for these latter phenomena is the low dicluster velocity or low momentum transfer to the target medium electrons. This obtained behavior gives good results compared with the theoretical results of Arista and Ponce [14] for ionic dicluster interacts with channeling target foil.

A good relationships have been obtained from calculating the total stopping power by using Lindhard function of Random phase Approximation with no damping for first and second order of approximation at low velocities as used by Nagy and Echenique [65] and Plasmon Pole Approximation at high velocities. This study is comparable to the result of Arista [15].

The rise of dicluster internuclear distance decreases the correlated values of stopping power but this relation is related to the other parameters as that of electrons density, where their comparable condition ensure the maximum efficient of dicluster projectile-target interaction, as well as the effect of the dicluster velocity.

When dicluster internuclear distance approaches to zero to be unit atom then the vicinage effect being at the maxima value for the best performance of the two ions exchange the polarization of each one of them. This behavior reflected on the high loss energy per the unit length exerted by the dicluster.

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