LATTICE ION TRAP: CLASSICAL AND QUANTUM DESCRIPTION OF A POSSIBLE COLLISION MECHANISM FOR DEUTERONS IN METAL LATTICES

NUCLEAR REACTIONS IN SOLIDS

KEYWORDS: *ions, interaction in solids*

VITTORIO VIOLANTE* *ENEA, Dipartimento Energia*
Divisione Fusione, Centro Ricerche Frascati, C.P. 65 - 00044 Frascati, Rome, Italy

AMALIA TORRE and GIUSEPPE DATTOLI
ENEA, Dipartimento Innovazione, Divisione Fisica Applicata
Centro Ricerche Frascati, C.P. 65 - 00044 Frascati, Rome, Italy

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The dynamics of deuterons inside a palladium lattice around tetrahedral sites at high deuterium concentration is studied by using both a classical description and a quantum mechanical representation, and the results are compared. The classical representation takes advantage of the similarity between the electrodynamic confinement of charged particles stored in a quadrupolar radio-frequency trap and the palladium lattice. The quantum mechanical description of the dynamics of a charged particle interacting with another charged particle within a lattice radio-frequency trap is carried out by solving the time-dependent Schrödinger equation with a numerical procedure. Both descriptions produce an interaction effect between the deuterons inside the metal lattice.

I. INTRODUCTION

The electrodynamic confinement of charged particles stored in a radio-frequency (rf) electric quadrupole trap has been widely studied by several authors.[1–7] A remarkable similarity between the aforementioned quadrupole rf trap and the lattice structure of some metals like palladium and nickel allowed a classical study of the dynamics of two deuterons moving within the lattice around tetrahedral sites.[8] The hydrogen isotopes within a metal lattice like the palladium one can be considered as ions because of the higher electro-negativity of the host metal atoms.

In the proposed model it has been supposed that the alternating signal of a lattice rf trap can be generated by the motion of the electrons of the metal atoms close to Fermi energy. The motion of the electrons can be traced back to an oscillating electron cloud producing an electric field.

Electronic oscillations (surface plasmons) take place at metal/electrolyte (or metal/gaseous) interfaces and can be enhanced by surface roughness.[9–11]

A quantum description of the charged-particle dynamics within an rf trap (i.e., Paul trap) has been recently proposed based on the theory that the harmonic oscillator has a time-dependent frequency,[12] and the solution of the problem has been carried out by means of an operator constant of the motion. In the case under study, the particle dynamics within the lattice trap cannot be described in terms of a harmonic oscillator with a time-dependent frequency because of the interaction with the other charged particle that introduces an anharmonicity in the motion when the distance between the particles becomes very short and the repulsive effect dominates.

In this paper we propose a quantum mechanical description of the dynamics of a charged particle interacting with another charged particle within a lattice rf trap by solving the time-dependent Schrödinger equation with a numerical procedure.

II. SUMMARY OF THE CLASSICAL DESCRIPTION

The basic hypothesis of the model is that the alternating signal of the lattice rf trap can be generated by the

*E-mail: violante@frascati.enea.it

motion of electrons close to Fermi energy. The electron motion can be traced back to an oscillating electronic cloud over the palladium atoms that produces an electric field because of charge separation. A coherent mechanism of the electron cloud's behavior is proposed for the model because no phase is subject to random noise.

In the following, the palladium atoms, oscillating at acoustic frequency, are supposed to be at rest (adiabatic approximation) compared with the deuterium atoms, which oscillate in the range of the optical frequencies in the metal-hydrogen lattice (e.g., palladium-deuterium lattice). However, the plasma frequency of the deuterons is about two orders of magnitude less than the electron plasma frequency. Therefore, their dynamics are studied only by considering the forces acting in the lattice space around the tetrahedral sites. The forces are produced by the charge separation due to the electron cloud oscillations. In other words, the electrons are seen by the deuterons just as an alternating signal.

Figure 1 shows the palladium lattice cell: The octahedral sites (occupied by hydrogen and/or its isotopes in beta phase) are between the vertices of the cubic structure; the tetrahedral sites, which could be available for deuterons above $x = 0.9$ (Ref. 13), belong to the intersection between the (101 and $(10\bar{1})$ planes. The electron cloud spatial oscillations around the palladium atoms produce, in both planes, an oscillation of the charge density that creates an electric field.

For simplicity's sake we consider that the charges acting in the (101) plane are midway between palladium atoms 1 and 2 and between 3 and 4 (see Fig. 1), and the charges acting in the $(10\bar{1})$ plane are just atoms 5 and 6.

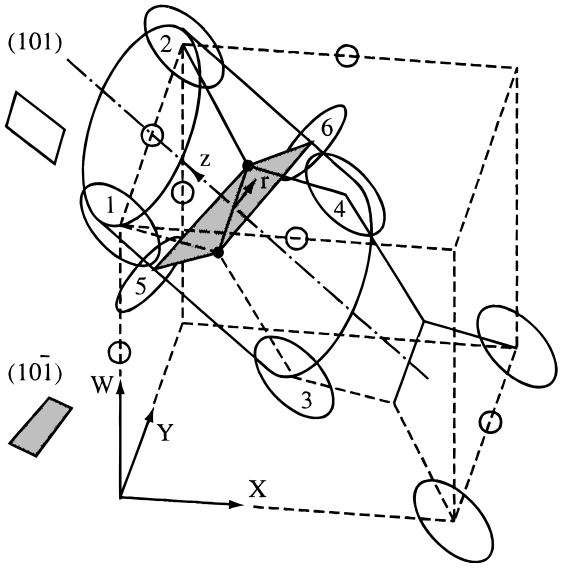

Fig. 1. Palladium lattice cell with palladium atoms (large circles) and octahedral and tetrahedral positions (small circles). The axes of the system of coordinates are r and z.

Let E_z and E_r be the effective components of the electric field for ion dynamics in the $[101]$ and $[10\bar{1}]$ directions, respectively. When the oscillation direction moves away from the plane direction, the oscillating charge density decreases within the plane; therefore, the signal across the plane is also reduced. This effect can be taken into account in the calculations by introducing a factor that ranges between 0 and 1 in the peak signal; then, when the electric peak signal reaches its maximum value in one plane, it is zero in the other and vice versa because of the orthogonality between the planes. Such a situation leads to sinusoidally time-varying forces whose strength is proportional to the distance from a central origin. The trap geometry reveals a cylindrical symmetry, as can be seen in Fig. 1, and the model will be developed in the trap coordinates system.

In this paper we consider that one particle (particle 2) is at rest (e.g., in a tetrahedral site), and the other one (particle 1) enters the trap with a random energy (close to the thermal one because it can be considered to enter the trap by diffusion) as well as random direction and position. The particle at rest can be allowed to be in motion when the interaction energy with the other one becomes larger than its bound energy with the lattice (i.e., $\sim$1 eV).

The motion equations in dimensionless form in the trap coordinates system are[3,7] as follows:

$$\frac{d^2\bar{r}_1}{dx^2} = (1-\alpha)\,\frac{4q_1}{m_1\Omega^2}\,\frac{\bar{r}_1}{l_0^2}\,V_{acr}\cos(2x) + \frac{4q_1q_2}{m_1\Omega^2}\,\frac{|\bar{r}_1-\bar{r}_2|\hat{k}_{12}}{[(r_1-r_2)^2+(z_1-z_2)^2]^{3/2}}\,\beta \quad , \quad (1)$$

$$\frac{d^2\bar{z}_1}{dx^2} = -2\alpha\,\frac{4q_1}{m_1\Omega^2}\,\frac{\bar{z}_1}{l_0^2}\,V_{acz}\cos(2x) + \frac{4q_1q_2}{m_1\Omega^2}\,\frac{|\bar{z}_1-\bar{z}_2|\hat{k}_{12}}{[(r_1-r_2)^2+(z_1-z_2)^2]^{3/2}}\,\beta \quad , \quad (2)$$

$$\frac{d^2\bar{r}_2}{dx^2} = (1-\alpha)\,\frac{4q_2}{m_2\Omega^2}\,\frac{\bar{r}_2}{l_0^2}\,V_{acr}\cos(2x) + \frac{4q_1q_2}{m_2\Omega^2}\,\frac{|\bar{r}_1-\bar{r}_2|\hat{k}_{21}}{[(r_1-r_2)^2+(z_1-z_2)^2]^{3/2}}\,\beta \quad , \quad (3)$$

and

$$\frac{d^2\bar{z}_2}{dx^2} = -2\alpha\,\frac{4q_2}{m_2\Omega^2}\,\frac{\bar{z}_2}{l_0^2}\,V_{acz}\cos(2x) + \frac{4q_1q_2}{m_2\Omega^2}\,\frac{|\bar{z}_1-\bar{z}_2|\hat{k}_{21}}{[(r_1-r_2)^2+(z_1-z_2)^2]^{3/2}}\,\beta \quad , \quad (4)$$

where

$\bar{r}$ = radial coordinate

$\bar{z}$ = axial coordinates

indexes 1, 2 = particles 1 and 2, respectively

q_1, q_2 = charges of the particles

$\hat{k}_{12}, \hat{k}_{21}$ = unit vectors pointing, respectively, from particle 1 to particle 2 and vice versa

l_0 = trap characteristic length (the radius or the length from the central origin, which are assumed to be equal in this case)

β = Thomas-Fermi screening factor.[8]

Furthermore, V_{acr} and V_{acz} are the peak values of the alternating signal, having angular frequency Ω, in the directions [101] and [10$\bar{1}$], respectively:

$$V_{acr,z} = 4\pi n e \eta^2 \ , \tag{5}$$

where η is the maximum distance between the positive and negative centers of charge during the oscillations (i.e., the distance between the palladium atoms): $\eta = 2.83$ Å and $V_{acr,z} \sim 10^3$ V.

The particle dimensionless radial and axial coordinates and the dimensionless time are

$$\bar{r}_i = r_i / l_0 \quad \text{and} \quad \bar{z}_i = z_i / l_0 \ ,$$
$$x = \Omega t / 2 \ , \quad (i = 1,2) \ . \tag{6}$$

The frequency of the alternating signal can be evaluated by means of an approximation to an ideal electron plasma[14]:

$$\Omega \cong \frac{e}{m_e^{1/2}} n^{1/2} \approx (10^{16}\ \mathrm{s}^{-1}) \ , \tag{7}$$

where m_e is the electron mass and n is the electron plasma density. Assuming that the number of electrons at the Fermi level is equal to the density of state at such a level, we have ~7 electrons for atoms in palladium (~10 electrons for atoms in nickel)[15]; hence, $n \sim 10^{23}$.

The weak damping effect due to the average gradient of the energy barrier[8] has been neglected because it does not produce any significant effect on the particle dynamics.

Figure 2a shows the results of a classical study of a "collision" between two deuterons. We assume that particle 2 is at rest within a tetrahedral site [$\bar{r}_2(t = 0) = 0.5$, $\bar{z}_2(t = 0) = 0$], while particle 1 is entering the trap with initial position, direction, and energy evaluated randomly, but effective to have a collision. The initial position of such a particle is $\bar{r}_1(t = 0) = 0.5$, $\bar{z}_1(t = 0) = 1$. The initial conditions of the velocity components, chosen randomly, do not modify the dynamics of the particle, because if the particle is supposed to be initially at thermal energy, the effect of the trap force dominates.

We can see from Fig. 2 that the moving particle approaches the other particle at rest until their distance decreases to ~0.1 Å. Figure 2b shows the classically evaluated evolution of the energy of particle 1. Figure 3 shows the evolution of the radial and axial coordinates of the particle entering the trap, and it is clear that the motion develops mainly in the axial direction until the collision takes place. In this study the oscillation direction of the electron clouds is assumed to be mainly along the (101) plane.

III. QUANTUM MECHANICAL REPRESENTATION

In Sec. II we briefly discussed the classical modeling of particle dynamics in the trap by solving the equations of motion. We calculated that a charged particle

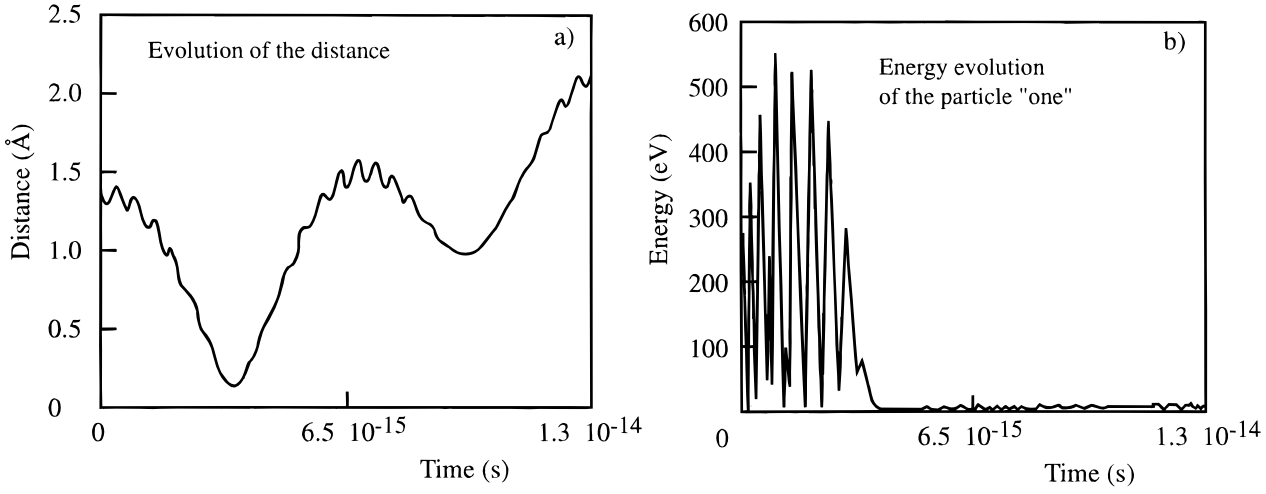

Fig. 2. (a) Evolution of the distance of the deuterons. (b) Deuteron energy evolution in the trap.

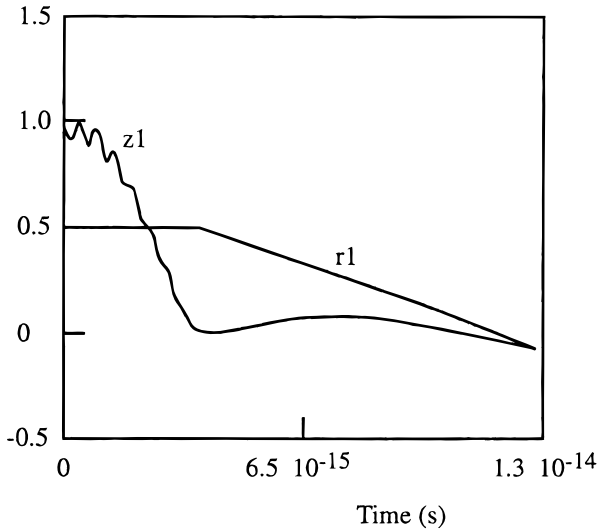

Fig. 3. Evolution of the radial and axial coordinates of the particle entering the trap.

moving in the trap can reach an energy of some hundreds of electron volts (see Fig. 2b). Then the particle gains hundreds of photons from the lattice trap because the electromagnetic signal frequency is 10^{16} s^{-1}; in this case, the particle dynamics can be classically approximated. On the other hand, as can be easily seen, the energy of the field in the trap is of the order of 10^4 photons because of the very high peak value of the electric field; therefore, the field can also be classically approximated. However, when the distance between the colliding particles becomes small, the momentum of particle 1 also diminishes, and its De Broglie wavelength becomes the same as the distance between the particles (i.e., $\sim 10^{-1}$ Å). A quantum mechanical analysis is then carried out to complete the description of the particle dynamics and to see if there are significant differences between the classical and the quantum mechanical description of the particle dynamics.

Based on the classical trajectory, we have seen (see Fig. 3) that the motion of particle 1 until the collision

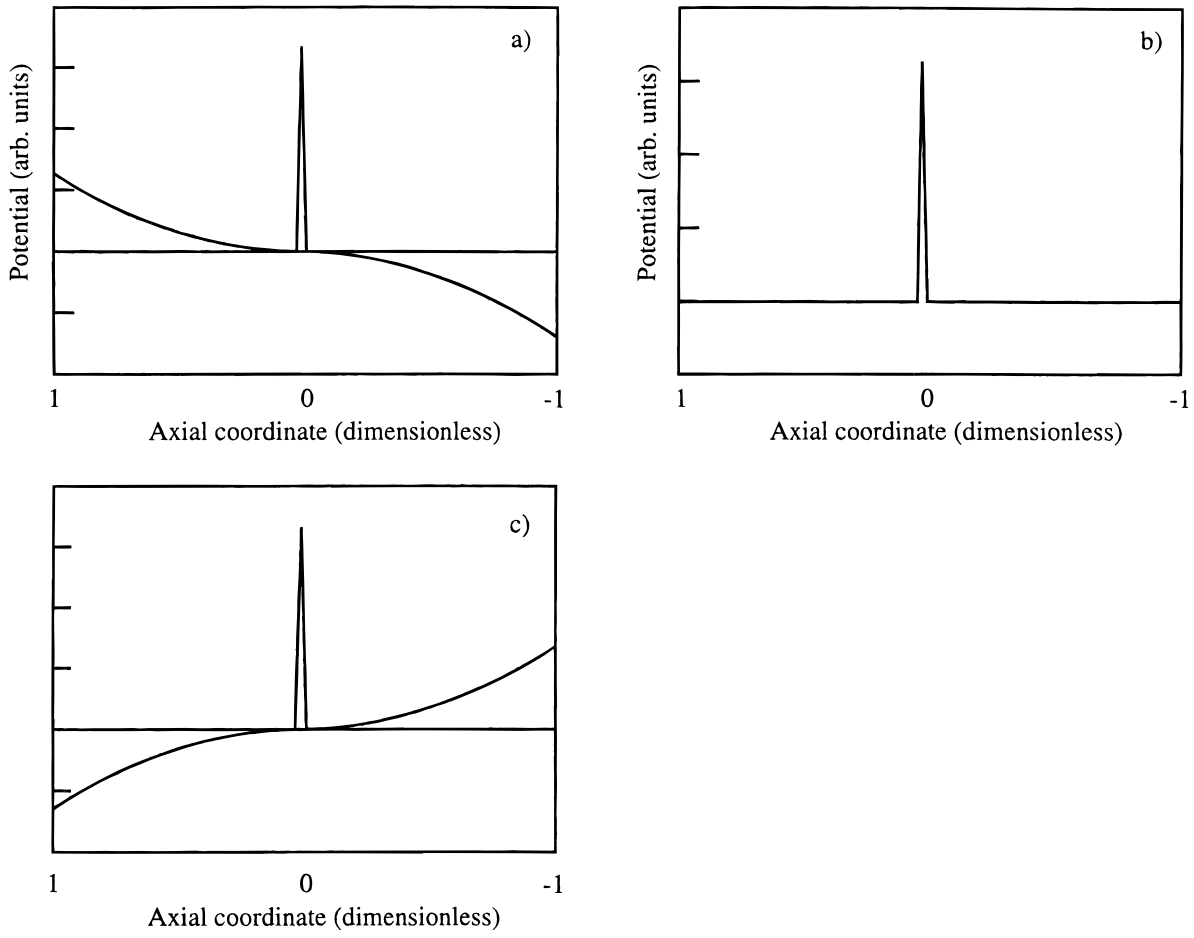

Fig. 4. Potential shape along the *z* axis for three consecutive time steps.

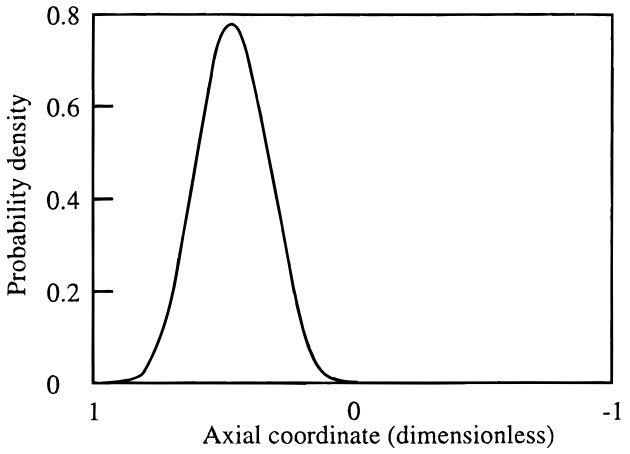

Fig. 5. Initial probability density distribution.

can be approximated by a motion along the z axis. Consequently, the quantum description can be reasonably obtained by studying, in one dimension, the interaction of a wave packet with the system potential.

The one-dimensional, time-dependent Schrödinger equation is

$$i\hbar\frac{\partial\psi}{\partial t} = \mathrm{H}\psi \ . \tag{8}$$

The Hamiltonian is

$$\mathrm{H} = -\frac{\hbar^2}{2m_1}\nabla^2 + V(z,t) \ , \tag{9}$$

where z is the position of the particle with mass m_1, and $V(z,t)$ is the potential, which combines the Thomas-Fermi screened potential between the interacting charged particles and the potential due to the trap force; then

$$V(z,t) = Q_{int} - \int F^{Trap}\, dz \ , \tag{10}$$

where Q_{int} is the screened interaction potential and F^{trap} is the rf trap force along the z direction. The potential shape along the z axis is shown in Figs. 4a, 4b, and

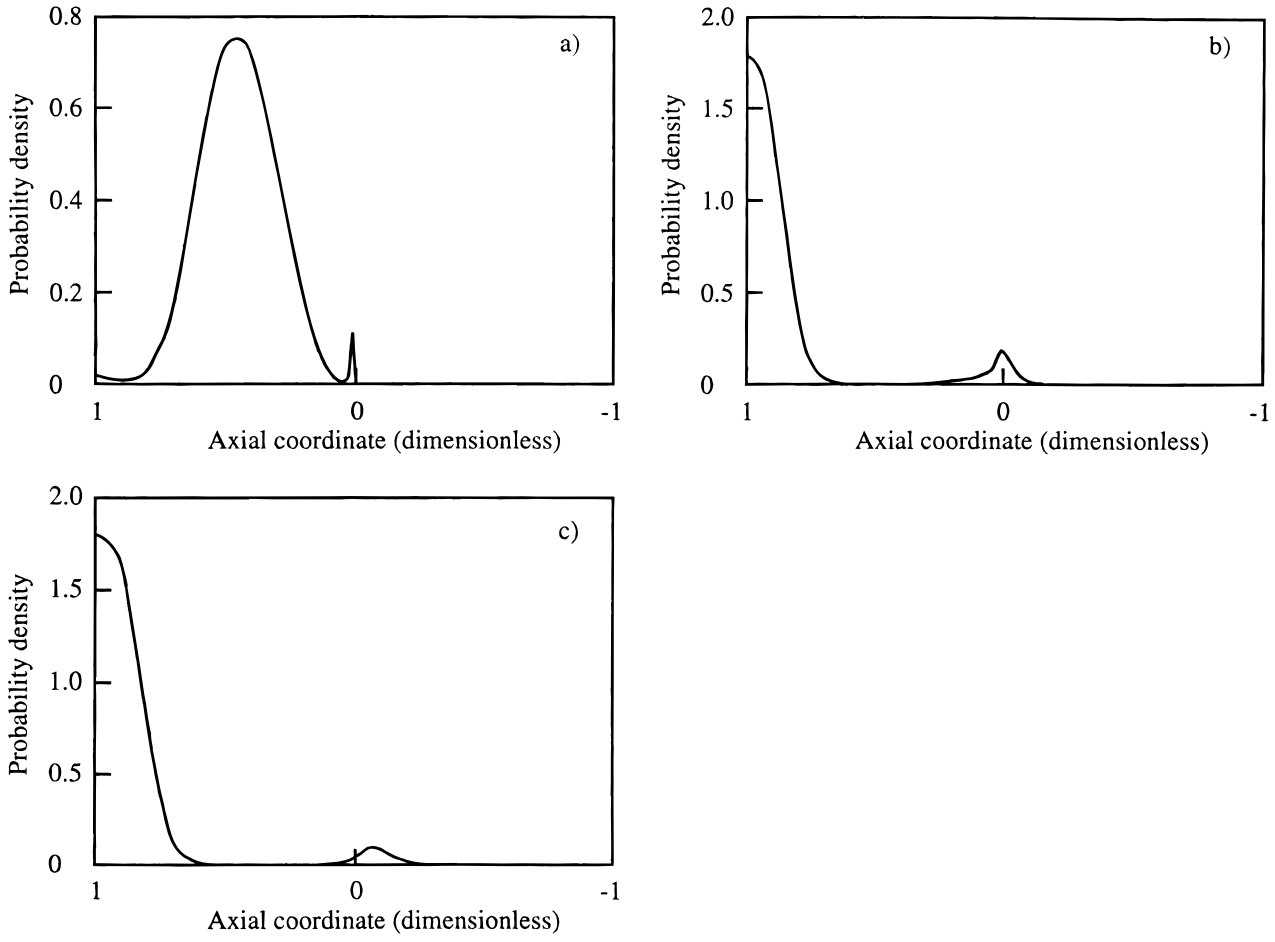

Fig. 6. Evolution of the square module of the wave function with the potential shape of Fig. 4a.

4c for three consecutive time steps $t_3 > t_2 > t_1$. The delta-like behavior of the potential in the middle of the system ($z = 0$) is due to the charged particle at rest.

The Schrödinger equation can be written in terms of the real and imaginary parts ψ_{re} and ψ_{im} of the wave function, resulting in the set of coupled equations

$$\hbar \frac{\partial \psi_{re}(t,z)}{\partial t} = \mathrm{H}\psi_{im}$$

and

$$\hbar \frac{\partial \psi_{im}(t,z)}{\partial t} = -\mathrm{H}\psi_{re} \ . \qquad (11)$$

The numerical solution has been carried out by means of the following finite difference scheme[16]:

$$\psi_{re}(t + 0.5\psi\Delta t, z_i) = \psi_{re}(t - 0.5\Delta t, z_i) + \Delta t \mathrm{H}\psi_{im}(t, z_i) \ ;$$
$$\psi_{im}(t + 0.5\Delta t, z_i) = \psi_{im}(t - 0.5\Delta t, z_i) - \Delta t \mathrm{H}\psi_{re}(t, z_i) \ . \qquad (12)$$

The integration is performed through the time interval

$$\Delta\tau \approx \frac{\hbar}{2\Delta E} \ , \qquad (13)$$

where ΔE is the energy lost by particle 1 during the collision.

Figure 5 shows the probability density distribution $|\psi|^2$ at initial time $t = 0$; the particle is supposed to move within the trap toward the tetrahedral site, where the other charged particle is at rest.

Figures 6a, 6b, and 6c refer to the potential shape shown in Fig. 4a, while Figs. 7a, 7b, and 7c refer to the potential shape shown in Fig. 4c.

Figures 6a, 6b, and 6c report the probability density $|\psi|^2$ at different times within the Eq. (13) interaction time in correspondence with the potential shape of Fig. 4a. It is evident that there is a nonzero probability that the moving particle approaches close to the other charge.

Correspondingly, in Figs. 7a, 7b, and 7c the square modulus $|\psi|^2$ of the wave function is plotted at three different times for the potential shape of Fig. 4c. Basically,

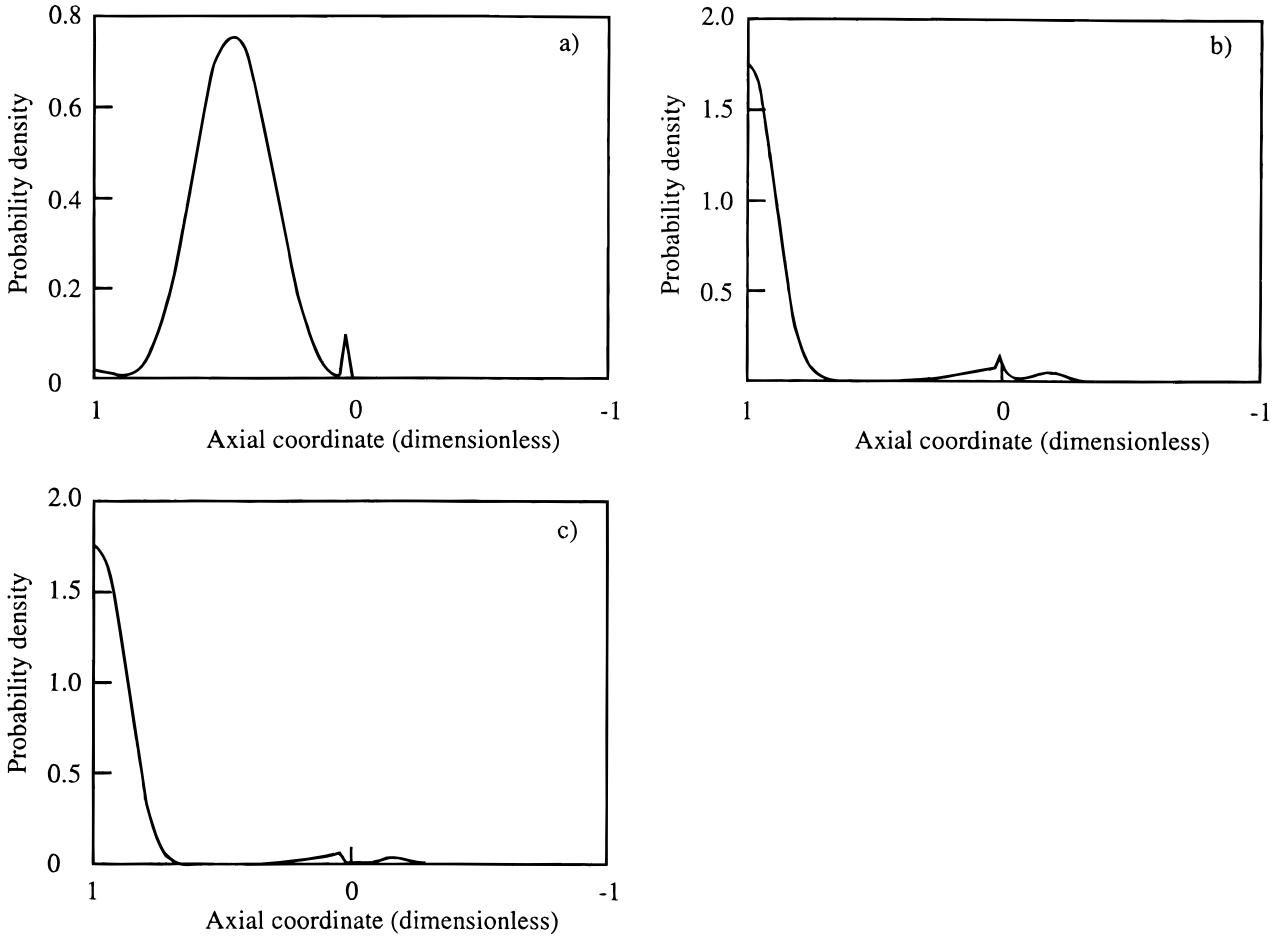

Fig. 7. Evolution of the square module of the wave function with the potential shape of Fig. 4c.

the trend of the probability density is similar even if the transmission effect is reduced for the potential of Fig. 4c, as a consequence of which the charge interacts with an increasing well in addition to the deltalike barrier.

IV. CONCLUSIONS

The proposed study is mainly designed to make a comparison between the results of a classical description and those arising from a quantum mechanical approach. However, the aforementioned quantum study should be considered preliminary because it is a first approach to the problem, and it has been carried out within the framework of some previously discussed limitations. Consequently, the results should be considered as indicative of a possible dynamics that in both representations (classical and quantum mechanical) reveals an interesting approaching mechanism of two deuterons embedded inside a metal lattice like palladium.

The comparative analysis shows that the classical description of the particle dynamics in the lattice can be considered a satisfactory and conservative approximation in accordance with the relatively high energy that the deuteron gains in the trap. The interesting aspect is that there is a reasonable agreement between the descriptions according to the relatively high energy that the particle achieves in the trap as previously mentioned.

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Vittorio Violante (chemical engineering degree, Naples University, Naples, Italy, 1979; PhD, new materials, Calabria University, Italy, 1992) is responsible for the Special Technology Section for Nuclear Fusion at ENEA Research Center of Frascati. He is involved in the ENEA research program for nuclear fusion; his field includes the interaction of hydrogen isotopes with materials, transport phenomena, and tritium fuel cycle.

Amalia Torre (PhD, physics, Naples University, Italy, 1983) is senior scientist at ENEA Frascati.

Giuseppe Dattoli (PhD, physics, Rome University, Italy, 1976) is director of the Theoretical Physics Group at ENEA Frascati. His main activity is free electron laser and classical and quantum optics.