Material Science Studies

QUANTUM MECHANICAL DESCRIPTION OF A LATTICE ION TRAP: Deuteron Approaching Mechanism in Condensed Matter

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1. Introduction

The electrodynamic confinement of charged particles stored in a radio-frequency electric quadrupole trap has been widely investigated by several authors [1,2]. A remarkable similarity between the above mentioned quadrupole radio-frequency trap and the palladium lattice structure allowed a classical study of the dynamics of two deuterons moving within the Pd lattice around tetrahedral sites [3,4]. The theory of the harmonic oscillator with time dependent frequency has been reviewed by introducing an operator which is a constant of the motion [5]. In this paper a quantum description of a deuteron dynamics and its interaction with an other one inside the lattice ion trap is carried out taking advantage of an oscillating behaviour that can be traced back to a quantum harmonic oscillator. The calculations show, in both treatments, a reduction of the mean distance between the particles.

2. Quantum description of the oscillator with time-dependent frequency

The Hamiltonian for a particle of mass m, momentum $\bar{p}$ and position $\bar{x}$ moving as an harmonic oscillator with time-dependent frequency $\bar{\varpi}=\bar{\varpi}(t)$ can be written in terms of dimensionless position x and momentum p as in the following expression:

$$H=\frac{1}{2}p^2+\frac{1}{2}\omega^2(t)x^2 \tag{1}$$

where:

$$\bar{x}=\sqrt{\frac{\hbar}{m\omega_0}}x;\ \bar{p}=\sqrt{\hbar m\omega_0}p\ ; \tag{2}$$

$$\omega(t)=\frac{\varpi(t)}{\omega_0} \tag{3}$$

The introduction of the dimensionless position and momentum operators $\hat{x}$ and $\hat{p}$ satisfying the commutation relation:

$$[\hat{x},\hat{p}]=i \tag{4}$$

leads the transition to quantum mechanics. The quantum mechanical harmonic oscillator, with time-dependent frequency

$$\hat{H}=\frac{1}{2}\hat{p}^2+\frac{1}{2}\omega^2(t)\hat{x}^2 \tag{5}$$

can be solved by defining the operator:

$$\hat{A}(t)=\frac{i}{\sqrt{2}}[\varepsilon(t)\hat{p}-\dot{\varepsilon}(t)\hat{x}] \tag{6}$$

which is a linear combination of the position and the momentum operators with time dependent coefficients. The time dependent function ε(t) satisfies the Newton equation of motion for the corresponding classical oscillator subjected to the appropriate initial conditions:

$$\ddot{\varepsilon}(t)+\omega^2(t)\varepsilon(t)=0 \tag{7}$$

It can be shown that the operator $\hat{A}(t)$ is a constant of motion:

$$\frac{d\hat{A}}{dt}=0 \tag{8}$$

With the following choice of the initial conditions:

$$\varepsilon(0)=1;\dot{\varepsilon}(0)=i \tag{9}$$

the operator $\hat{A}$ leads to:

$$\hat{A}(t=0)=\frac{1}{\sqrt{2}}(\hat{x}+i\hat{p}) \tag{10}$$

Then for t=0 the operator is identical to the annihilation operator $\hat{a}$ of the time-independent harmonic oscillator. It has been demonstrated [5] that:

$$[\hat{A}(t),\hat{A}^{+}(t)]=1 \tag{11}$$

In the following it will be shown that the ground state $|0;t\rangle$ and the excited states $|n;t\rangle$ of a deuteron behaving as a harmonic oscillator with time-dependent frequency can be obtained by using the constant of the motion $\hat{A}(t)$.

The time independence of the commutator (11) ensures that the Hamiltonian has a state $|0;t\rangle$ analogous to the ground state of the time-independent harmonic oscillator. The analogy allows us to define:

$$\hat{A}(t)|0;t\rangle=0\ , \tag{12}$$

leading, for the position representation $\psi_0(x,t)\equiv\langle x|0;t\rangle$ of the ground state, to the differential equation:

$$\langle x|\hat{A}(t)|0;t\rangle=\frac{i}{\sqrt{2}}\left[-i\varepsilon(t)\frac{d}{dx}-\dot{\varepsilon}(t)x\right]\psi_0(x,t)=0 \tag{13}$$

The resulting expression for the probability distribution in coordinate space is:

$$P_0(x,t)\equiv|\psi_0(x,t)|^2=\frac{1}{\sqrt{\pi}|\varepsilon(t)|}\exp\left(-\frac{x^2}{|\varepsilon(t)|^2}\right) \tag{14}$$

For the excited states the probability distribution in coordinate space is [5]:

$$P_n(x,t)\equiv|\psi_n(x,t)|^2=\frac{1}{\sqrt{\pi}|\varepsilon(t)|}\frac{1}{2^n n!}H_n^2\left(\frac{x}{|\varepsilon(t)|}\right)\exp\left(-\frac{x^2}{|\varepsilon(t)|^2}\right) \tag{15}$$

where H_n is the nth Hermite polynomial. Then, if we can obtain the value of the function ε(t) at a time t, the equations (14) and (15) allow us to estimate the probability that two particles are at a distance x after a time t for a system in the ground state or in an excited state respectively.

3. Lattice ion trap classical description

The model of the "lattice ion trap" has been carried out in ref. [3,4] to study the dynamics of two deuterons moving within the Palladium lattice space around the tedrahedral sites. The space around the tetrahedral sites can be seen as a quadrupole trap for the deuterons; then the effect of the electrodynamic containment on its dynamics can be studied by means of the equations of motion. The alternating signal of the lattice radiofrequency trap is assumed to be generated by the motion of electrons close to the Fermi energy: the electron motion can be traced back to an oscillating electronic cloud that produces an electric field because of the charge separation due to the oscillation. A coherent mechanism of the electron cloud is proposed for the model, since no phase is subject to random noise. Fig.1 shows the palladium lattice cell. The octhaedral sites are in the middle between the vertexes of the cubic structure. The tetrahedral sites, that could be available for deuterons above x=0.95, belong to the intersection between the (101) and the $(10\bar{1})$ planes. The similarity between a quadrupolar ion trap and the system shown in Fig.1 allows us to consider, for simplicity's sake, that the charges acting in the (101) plane are midway between Pd atoms 1 & 2, and 3 & 4, and the charges acting in the $(10\bar{1})$ plane are just atoms 5 and 6. The projection in the x-w plane gives a simplified two-dimensional view of the spatial oscillations of the electron clouds (see Fig.2). Their displacements in both (101) and $(10\bar{1})$ planes are oscillations of charge density producing an alternating potential difference that generates an electric field. Let z and r be the [101] and $[10\bar{1}]$ directions respectively, then E^z and E^r are the effective components of the electric field for the ion dynamics. The electric field in each plane achieves its maximum value when it is minimum in the other one, because of the orthogonality of the planes. Such a situation leads to sinusoidally time varying forces whose strengths are proportional to the distance from a central

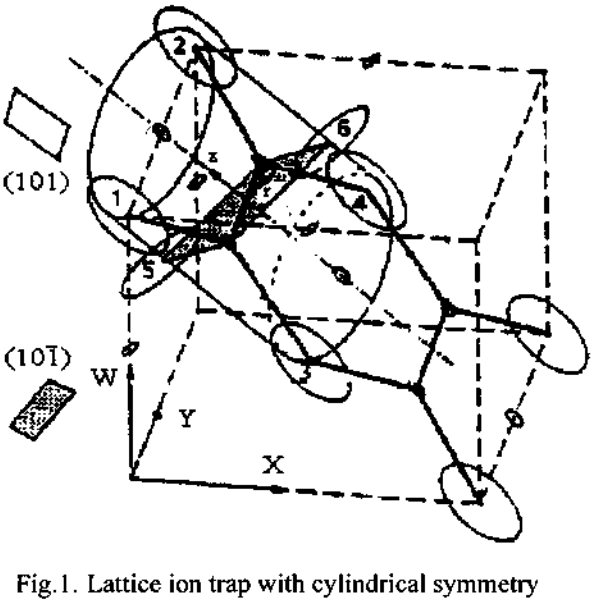

Fig.1. Lattice ion trap with cylindrical symmetry

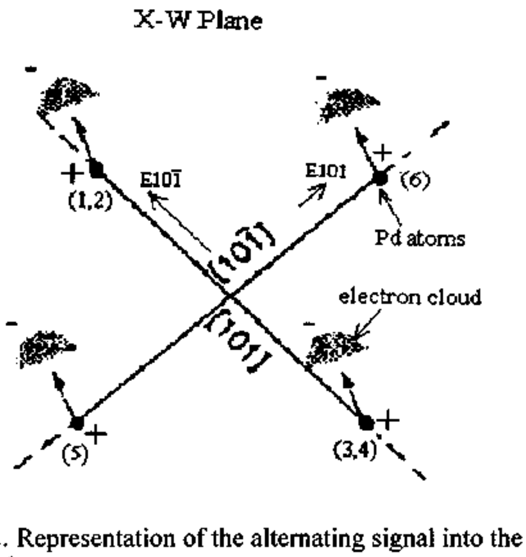

Fig.2. Representation of the alternating signal into the x-w plane

origin (in this case the intersection between the r and z axes) . The trap can be considered to have a cylindrical symmetry as shown in Fig.1. In order to link our system with the above mentioned quantum description of the Paul trap we will consider that one deuteron is located approximately in the midway between tetrahedral sites (i.e. the origin of the trap coordinate system) and the other one leaving the octahedral site (at the time t=0) and moving within the trap (i.e. $z(t=0)=l_o$).

Considering the cylindrical symmetry of the system, and introducing the following dimensionless variables:

$$\bar{r}=\frac{r}{l_0};\bar{z}=\frac{z}{l_0};\eta=\frac{t}{2\tau}, \tag{16}$$

the balance of the forces leads to the following equations of motion:

$$\begin{aligned}\frac{d^2\bar{r}}{d\eta^2}&=\frac{4\tau^2}{m}\bar{r}[e^2\frac{1}{(r^2+z^2)^{3/2}}\beta+\frac{(1-\alpha)eV_{acr}}{l_0^2}\cos(2\Omega\tau\eta+\frac{3}{2}\pi)]\\ \frac{d^2\bar{z}}{d\eta^2}&=\frac{4\tau^2}{m}\bar{z}[e^2\frac{1}{(r^2+z^2)^{3/2}}\beta-\frac{2\alpha eV_{acz}}{l_0^2}\cos(2\Omega\tau\eta)]\end{aligned} \tag{17}$$

where β is the Thomas Fermi screening term, V_{acr} and V_{acz} are the peak values of the alternating signal having angular frequency Ω , l_0 is the trap characteristic length (the radius or the distance from the symmetry point, which are equal in this case), r and z are the coordinates (in the trap coordinate system) of the deuteron moving in the trap, α is a random number, ranging between 0 and 1, taking into account the direction of oscillation (α can also change after a time interval of the order of the oscillation period), *e* is the electron charge, and *m* the particle mass.Time τ is the characteristic time of the moving deuteron: the ratio between l_0 and the initial velocity of the particles. This choice allows us to use always 1 as initial normalized velocity, whatever the initial velocity of the particle is. For instance if the initial energy of the moving deuteron is 0.1 eV its initial velocity is $\sim 3.1 \times 10^3$ m/s and $\tau \sim 4.5\times10^3$ s. Then if we change the initial deuteron velocitiy (energy) respect to which the normalization is carried out τ changes too: the information concerning the initial energy of the moving deuteron is given simply by using a proper value of τ in the equations (17). The terms on the right side of eq. (17) are due to the Coulomb interaction and the trap force respectively. The damping force that can be produced by the gradient of the energy barrier around the tetrahedral sites can be neglected in this approximation, since, as it can be easily seen, it is a low weight term in the equations of motion. The frequency of the alternating signal can be evaluated by means of the approximation to an ideal electron plasma [3,4]. The peak value of the alternating signal can be calculated on the basis of the electric field, in the classical approximation, associated with the plasma oscillation: $V_{acr,z}=4\pi ne\xi^2$, where ξ is the maximum distance between the positive and negative centres of charge during the oscillations: i.e. the distance between the Pd atoms.

4. Quantum description of two deuterons in the trap

Now we apply the previous described quantum theory of the harmonic oscillator with time dependent frequency to the moving deuteron which oscillates inside the lattice radio-frequency trap, as can be seen observing the evolution of its trajectory.

As we stated before, the function $\varepsilon(t)$ satisfies the Newton equation of motion for our corresponding classical problem:

$$\ddot{\varepsilon}(t) = \left[a_{r,z}(t) + q_{r,z}\cos\left(2\Omega\tau\eta + \phi_{r,z}\right)\right]\varepsilon(t) \tag{18}$$

where $a_{r,z}(t)$ represents the interaction term in the corresponding eq. (17), q_r and q_z are the coefficients of the cosine term in the eq. (17).

The equation (18) corresponds to the equation systems (17) and results to be formally identical to eq. (7), since also $a_{r,z}(t)$ is a function of the time; therefore the term inside the square brackets corresponds to $\omega^2(t)$. Then $\varepsilon(t)$ plays the role of the distance between the particles, whose components are r and z. It is important to underline that $a_{r,z}(t)$ contains the distance between the particles (i.e. $\varepsilon(t)$) and is a not linear term. If the distance between the particles is larger than the screening length (~0.4Å), $a_{r,z}(t)$ is negligible with respect to the cosine term, and the particle motion can be traced back to an harmonic oscillator. When the distance decreases below the screening length, the interaction term $a_{r,z}(t)$ becomes the dominant one and the oscillator becomes anharmonic. Therefore, for distances below the screening length we can roughly approximate the problem to a diffusion one. The interaction probability can be evaluated by means of the momentum value of the moving particle when its distance from the particle at rest is equal to the screening length. The scattering angle can be calculated on the basis of the *r* and *z* values after the interaction. We can apply the following relationship:

$$dw_{fi} = \left(\frac{z_1 z_2 e^2 m}{2p^2 \sin^2 \theta/2}\right)^2 \frac{p}{L^3 m} d\Omega \tag{19}$$

where Ω is the solid angle, w_{fi} the transition probability for unit time and θ the scattering angle.The interaction probability, for distances below the screening length, can be obtained by integrating w_{fi} over the time interval required by the particle, having momentum p, to move towards a distance of the order of the screening length (~0.1Å)

$$P_{\text{int}} = \int_0^{\Delta t} w_{fi} dt \tag{20}$$

Going back to the quantum description of the harmonic oscillator having a time dependent frequency, we can write the following positions:

$$z \equiv \text{Re}\,\varepsilon, \quad r \equiv \text{Im}\,\varepsilon \tag{21}$$

We have to satisfy the initial conditions (9) that can be simply imposed by taking advantage of the choice for the dimensionless time as explained above. Condition (3) is given by assuming $\omega_0 = 1/2\tau$. The initial conditions (9), with position (21), can be rewritten as follows:

$$z(0) \equiv \text{Re}\,\varepsilon = 1;\ r(0) \equiv \text{Im}\,\varepsilon = 0;\ \dot{z}(0) \equiv \text{Re}\,\dot{\varepsilon} = 0;\ \dot{r}(0) \equiv \text{Im}\,\dot{\varepsilon} = 1 \tag{22}$$

The solution of the classical motion equations with conditions (22) is obtained by numerical integration.

5. Results and conclusions

The study is mainly oriented to a comparison between the results of a classical description and the results arising from a quantum mechanical approach, even if the analysis of the trapped deuterons is limited to some particular cases. We considered two different initial conditions, in terms of the

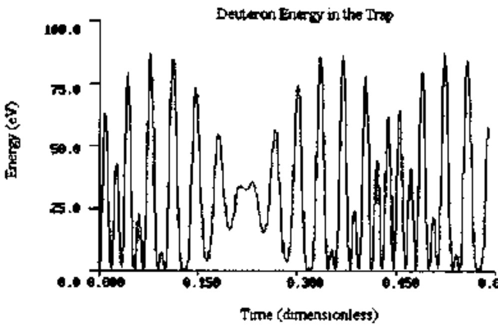

Fig. 3 Deuteron energy evolution in the trap

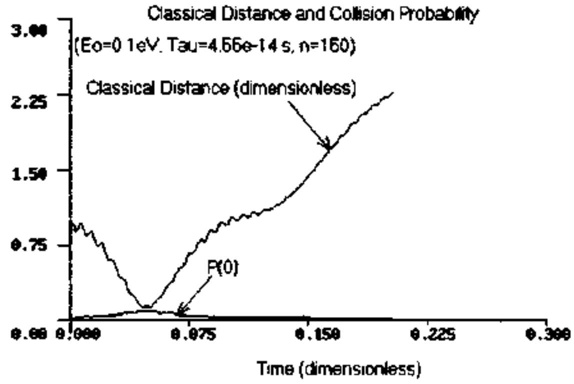

Fig.4 Evolution of the distance of the deuterons and collision probability (E_0=0.1 eV)

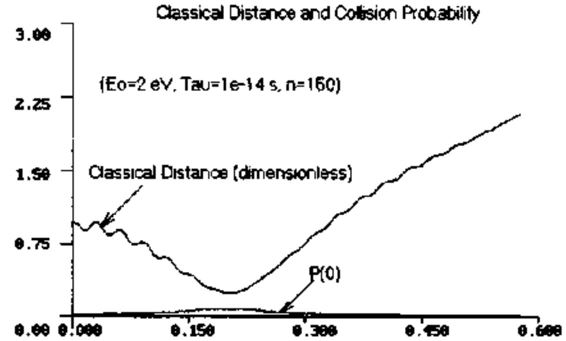

Fig 5 Evolution of the distance of the deuterons and collision probability (E_0=2 eV)

energy of the moving particles (i.e. of the τ value, such that the dimensionless initial velocity is always 1, as explained before). For the lattice cell parameters we consider in the model the β phase value.

Figure 3 shows the evolution of the moving deuteron energy classically evaluated. The average energy is some tenth of eV. The deuteron oscillation frequency is ranging between 10^{14} and 10^{15}. Therefore, from the oscillator energy calculation it follows:$(n+1/2)\hbar\omega=10^1$. Then a rough approximation gives n=150 to evaluate $P_n(x,t)$ with equation (15).

Figure 4 shows the calculation results for 0.1 eV as initial energy. The classical trajectory (the distance) and the probability to have the two particles at distance zero (collision) are plotted as a function of the dimensionless time. We can see that when the minimum distance between the particles, in the classical description, shows a minimum lower than 0.1 Å the quantum mechanical analysis produces a maximum collision probability. Figure 5 shows the results for an initial energy of 2 eV. In this case the initial conditions produce an approach, in the classical description, which is not effective for an interaction between the particles, but the quantum mechanical analysis gives a collision probability different from zero even if, in this case, the value is less than in the previous one. The oscillating behaviour of the deuteron moving inside the trap can be clearly observed in the classical trajectory evolution. 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. However the results obtained should be considered indicative, since some approximations have been introduced as well as the hypothesis that a deuteron is at rest in the midway between the tetrahedral positions (not exactly in the tetrahedral site as it should be), and since the problem is splitted in two separate regions.

In conclusion the approximation of the deuteron in the trap to an harmonic oscillator with time-dependent frequency and the approximation to a diffusion problem below the screening length gives a quantum mechanical description in reasonable accordance with the classical one. An interesting additional information is that the quantum mechanical description provides collision probabilities different from zero also when the classical description doesn't produce an effective approach to have an interaction between the particles.

The correlation existing between the classical and the quantum mechanical models allows us to extend to the quantum case all the considerations done in the classical description [3,4].

References

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