PERGAMON

International Journal of Hydrogen Energy 28 (2003) 125–129

International Journal of HYDROGEN ENERGY

www.elsevier.com/locate/ijhydene

Quantum collision states for positive charges in an octahedral cage

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Abstract

One-electron energy levels are studied for a configuration of two positive charges inside an octahedral cage, the vertices of the cage being occupied by atoms with a partially filled shell. Although ground states correspond to large separations, there are relatively low-lying states with large collision probabilities. Electromagnetic radiation fields used to excite the quantum collisional levels may provide a means to control nuclear reactions. However, given the scale of the excitation energies involved, this mechanism cannot provide an explanation for the unexplained "cold fusion" events.

PACS: 31.50.+w

1. Introduction

Inducing collision or near-collision states of like charged particles means overcoming the strong Coulomb repulsion at small distances, a very challenging task indeed. However, to master these events would have plentiful of potential applications in chemical processes and in the control of nuclear reactions. The traditional way to overcome the Coulomb repulsion is by endowing one or both particles with sufficient kinetic energy, either by acceleration or by thermal means. There are, however, subtler means to achieve this goal, which must obviously involve some other particles of opposite charge.

Classical configurations of particles of different charges in a close neighborhood are unstable and cannot provide a steady shielding effect. Turning to quantum mechanics, one also knows that static shielding effects of ground-state atomic orbitals, operative at atomic scales, do not provide adequate shielding at nuclear scale distances. However, quantum mechanics has some other subtler effects, namely the appearance of well-defined excited levels with wave functions located around some of the unstable classical orbits (*scars* [1]). A particularly interesting case corresponds to configurations related to unstable saddle points of the potential (*saddle scars* [2]). As opposed to the classical case, where it is always difficult to make use of unstable orbits (except in a few low-dimensional cases [3]), when these orbits have a scarred quantum counterpart, these states may be easily addressed and maintained by resonant excitation at the appropriate energy.

In this paper one computes the electronic states for a configuration of two positive charges in an octahedral cage. As expected, a static calculation leads to a lowest energy state with widely separated positive charges. However, when a dynamical degree of freedom is included for the positive charges, one finds relatively low-lying excited states with a large collision probability. These calculations are described in the next section. Finally, the last section is dedicated to the experimental implications of the results for the control of nuclear reactions and to a discussion of other related and unrelated results concerning similar questions.

2. Two charges in an octahedral cage

One considers two positive charges inside an octahedral cage. Atoms with a filled closed shell and some partially filled d-levels lie in the six vertices of the octahedral cage.

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0360-3199/02/$ 22.00
PII: S0360-3199(02)00024-1

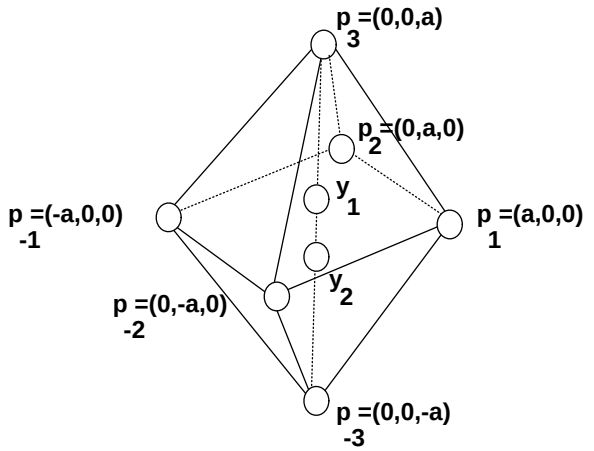

Fig. 1. Two charges in an octahedral cage.

The atoms at the vertices are assumed to be fixed and the two positive charges are symmetrically placed on the diagonal (see Fig. 1).

Two distinct cases are studied. In the first, the positive charges are assumed to be fixed and in the second, they are allowed to move symmetrically along the diagonal.

The one-electron energy levels inside the octahedral cage were studied assuming, as an approximation, that the available orbitals are:

(i) The d-orbitals centered at the vertices having $m = 0$ projection towards the interior of the octahedron, namely

$$\chi^{(d)}_{\pm i} = N_1 r_2^{-3/2} \left\{ 3 \left(\frac{(\vec{x} - \overrightarrow{p_{\pm i}}) \cdot \mathrm{e}_i}{|\vec{x} - \overrightarrow{p_{\pm i}}|} \right) - 1 \right\} g_{nd} \left(\frac{|\vec{x} - \overrightarrow{p_{\pm i}}|}{r_2} \right) \tag{1}$$

$\vec{x}$ being the coordinate of the electron, $\overrightarrow{p_i}$ the coordinates of the vertices and g_{nd} a radial function for d-states. The normalization constant N_1 is fixed by normalizing the function in the volume of the octahedron. The effective radius r_2 takes into account the shielding effect of the closed shell.

(ii) The s-orbitals centered at the positive charges y_1 and y_2

$$\chi^{(s)}_j = N_0 \exp\left(- \frac{|\vec{x} - \overrightarrow{y_j}|}{r_1} \right) \tag{2}$$

with the same prescription as above for the computation of the normalization constant N_0.

When the positive charges are allowed to move symmetrically along the diagonal, one also uses a basis of Legendre polynomials in the z-coordinate

$$z = |\overrightarrow{y_1} - \overrightarrow{y_2}|. \tag{3}$$

With N polynomials one has a (non-orthogonal) basis of $8N$ functions.

This setting is recognized to be too simple to obtain accurate numerical values of energy levels for a realistic situation of positive charges confined in a metallic lattice. Nevertheless, it seems to be qualitatively correct and to provide a reasonable control on the nature of the excited states, which is the main objective.

The Hamiltonian is

$$aH = -\frac{\hbar^2}{2m_e a} \Delta_x - \sum_{j=1}^{2} \frac{\hbar^2}{2M_+ a} \Delta_{y_j} - \frac{e^2}{4\pi\varepsilon_0} \sum_{k=-3}^{3} \frac{Z_{\mathrm{eff}}}{|\vec{x} - \overrightarrow{p_k}|} + \frac{e^2}{4\pi\varepsilon_0} \left(- \sum_{j=1}^{2} \frac{1}{|\vec{x} - \overrightarrow{y_j}|} + \frac{1}{|\overrightarrow{y_1} - \overrightarrow{y_2}|} + \sum_{j=1,2;\ k=-3,\ldots,3} \frac{Z_{\mathrm{eff}}}{|\overrightarrow{y_j} - \overrightarrow{p_k}|} \right) \tag{4}$$

all distances being measured in units of a reference value a (one half the octahedron diagonal). Eq. (4) may be rewritten as

$$H' = \frac{4\pi\varepsilon_0 a}{e^2} H = -\frac{0.264}{a(\text{Å})} \left(\Delta_x + \sum_{j=1}^{2} \frac{m_e}{M_+} \Delta_{y_j} \right) - \sum_{k=-3}^{3} \frac{Z_{\mathrm{eff}}}{|\vec{x} - \overrightarrow{p_k}|} - \sum_{j=1}^{2} \frac{1}{|\vec{x} - \overrightarrow{y_j}|} + \frac{1}{|\overrightarrow{y_1} - \overrightarrow{y_2}|} + \sum_{j=1,2;\ k=-3,\ldots,3} \frac{Z_{\mathrm{eff}}}{|\overrightarrow{y_j} - \overrightarrow{p_k}|}, \tag{5}$$

where m_e being the electron mass, the relation

$$\frac{\hbar^2}{2m_e a} \frac{4\pi\varepsilon_0}{e^2} = \frac{0.264}{a(\text{Å})} \tag{6}$$

has been used, with a expressed in Angstroms.

2.1. Static charges

Here one studies the energy spectrum as a function of the separation of the two positive static charges located at $y_1 = (0, 0, l)$ and $y_2 = (0, 0, -l)$. The rescaled Hamiltonian H' in the static case may be split into two pieces $H' = H_x + H_0$

$$H_x(l) = -\frac{0.264}{a(\text{Å})} \Delta_x - \sum_{k=-3}^{3} \frac{Z_{\mathrm{eff}}}{|\vec{x} - \overrightarrow{p_k}|} - \sum_{j=1}^{2} \frac{1}{|\vec{x} - \overrightarrow{y_j}|},$$

$$H_0(l) = \frac{1}{2l} + \sum_{j=1,2;\ k=-3,\ldots,3} \frac{Z_{\mathrm{eff}}}{|\overrightarrow{y_j} - \overrightarrow{p_k}|}. \tag{7}$$

The l-dependent energy spectrum of H_x in the basis $\{\chi^{(s)}_j, \chi^{(d)}_{\pm i}\}$ (Eqs. (1) and (2))

$$\lambda_1(l), \lambda_2(l), \ldots, \lambda_8(l)$$

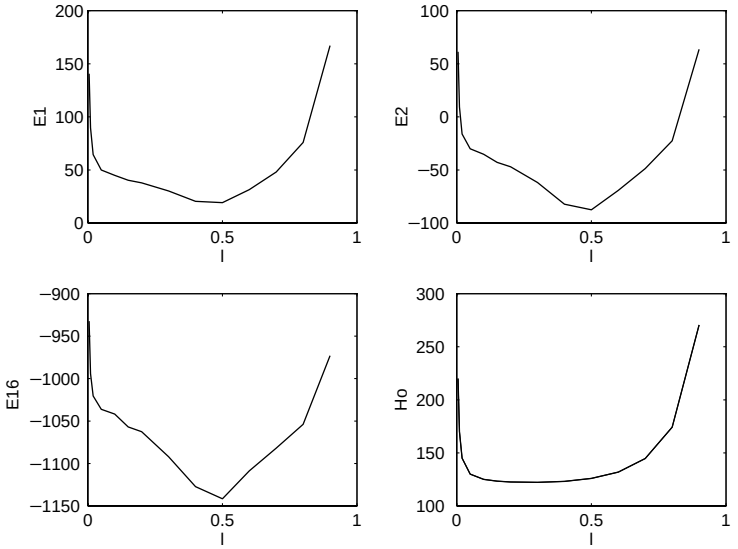

Fig. 2. Energy of 1, 2 and 16 electron configurations and static energy.

has been computed. In Fig. 2, one shows the energy of 1, 2 and 16 electrons (not corrected for electron–electron interactions), that is

$$E_1(l) = \lambda_1(l) + H_0(l),$$

$$E_K(l) = \sum_{i=1}^{K/2} 2\lambda_i(l) + H_0(l), \quad K = 2, 16 \tag{8}$$

as a function of l. The last plot in Fig. 2 shows $H_0(l)$. All results drawn in the figures of this paper correspond to $Z_{\text{eff}} = 10$ and $a = 2.05$ Å. Qualitatively similar results are obtained for other values of the constants.

One sees that, for all the electron configurations, the minimum energy occurs for a large separation of the positive charges at y_1 and y_2. For comparison, the energy for two electrons and two positive charges in empty space (an isolated molecule) was also computed for the same parameters. The result is shown in Fig. 3. One concludes that the octahedral cage and the d electron levels have the effect of increasing rather than decreasing the separation of the positive charges. This conclusion is similar to the result of Sun and Tománek [4] that, using a density-functional calculation, concluded that the equilibrium distance between two deuterium atoms in a palladium lattice is larger than the gas value.

The fact that the minimum energy is obtained for very large separations does not preclude the existence of low lying excited states, with large occupation probabilities at zero separation. To clarify this point one needs to solve the problem allowing, at least, the two charges to move along the z-axis.

Why a dynamical calculation may provide information qualitatively different from the static case is easy to understand. A static calculation is equivalent to constrain the wave functions in the relative coordinate to be a delta-function at $z = 2l$. If l is small, this means that the two positive charges are all the time very close to each other, independent of the position of the electrons. For the dynamic case the situation is different, because one may have high probabilities at $z = 0$ if they correspond to configurations where there is also a high probability for the electrons to be near the origin of the octahedron.

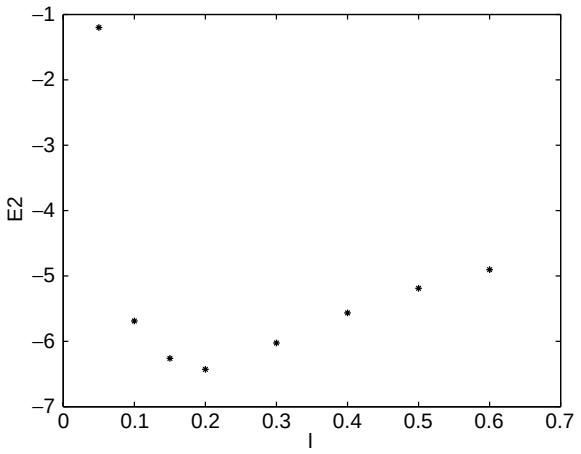

Fig. 3. Energy of an isolated molecule.

Of course, situations of this type are energetically favorable only if the overall potential of positive and negative charges has local minima near $z = 0$. In particular, if these are saddle points of the potential, it is known that the unsta-

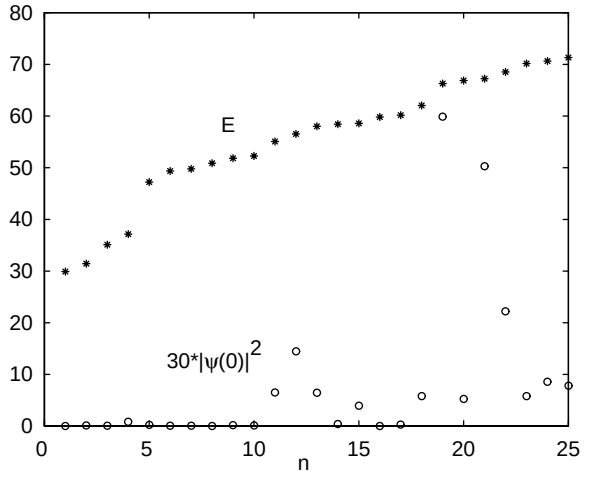

Fig. 4. One-electron spectrum and projected squared wave-function at $z = 0$.

ble classical equilibrium configurations manifest themselves as well defined quantum states [2].

2.2. Dynamic charges

Here one allows the positive charges at y_1 and y_2, to move symmetrically along the z-axis. By allowing just one additional dynamical degree of freedom, the problem is kept computationally simple, while at the some time a large enough basis may be used for the z degree of freedom. A basis of eight Legendre polynomials $P_n(z)$ in the z-coordinate is used. Together with the states defined in Eqs. (1) and (2) the basis has now 64 states. The one-electron spectrum that is obtained is plotted in the upper plot of Fig. 4. The lower plot shows the value of the projected squared wave-function $|\psi|^2$ at $z = 0$. M_+ is taken to be the deuterium mass and for Z_{eff} and a the values are the same as in the static case.

In all calculations, here and in the static case, care should be taken that the basis that is chosen is not an orthogonal basis. Denote by χ_α the electron basis states defined in Eqs. (1) and (2). Let the eigenvector of the Hamiltonian corresponding to the eigenvalue λ_k be

$$\phi^{(k)}(\vec{x}, z) = \sum_{\alpha n} c_{\alpha n}^{(k)} \chi_\alpha(\vec{x}, z) P_n(z).$$

The coefficient $c_{\alpha n}^{(k)}$ is obtained from

$$c_{\alpha n}^{(k)} = \sum_{\beta m} V_{\alpha n, \beta m} \frac{1}{\sqrt{\gamma_\beta}} A_{\beta m, k}$$

V being the matrix that diagonalizes the original basis and A the matrix that diagonalizes the Hamiltonian in the new orthonormalized basis. The factor γ_β is

$$\gamma_\beta = \sum_{\alpha\varepsilon} V^T_{\beta n, \alpha n}(\chi_\alpha, \chi_\varepsilon) V_{\varepsilon n, \beta n}.$$

Now the projected squared wave function on the z-axis is

$$|\psi^{(k)}(z)|^2 = \sum_{\alpha n, \beta m} c_{\alpha n}^{(k)*} c_{\beta m}^{(k)} P_n(z) P_m(z)$$

$$\int_\Sigma \chi_\alpha(\vec{x}, z) \chi_\beta(\vec{x}, z)\, \mathrm{d}^3 x$$

Σ being the octahedron volume.

On sees from the lower plot in Fig. 4 that, as expected, the ground state and the first excited states correspond to a vanishing collision probability for the positive particles. However, after the 10th excited state many levels appear that have a large value of the projected wave function at $z = 0$. These are *quantum collision states* which, when excited, lead the positive particles to configurations of close proximity. In an energy spectrum that, in the rescaled units of Eq. (5) varies from 27.7 to 30,000, the first states where $|\psi(0)|^2$ is appreciably different from zero lie only 26 units above the ground state. The meaning of this energy difference in physical units will be discussed in the next section. Fig. 5 shows the projected wave functions for the ground state and for levels 11 and 12.

3. Conclusions and experimental implications

Quantum collision states between like charged particles, in structures of the type studied in the previous section, cannot be useful unless the structure belongs to some lattice and a similar configuration is repeated throughout, at least, a large part of the lattice. That is, the lattice must act as a confining medium for the positive particle configurations.

To evaluate the potential usefulness of the quantum collision states for the practical achievement of reactions between the positive particles, the first step is to estimate, in physical units, the needed excitation energy when the length parameter a takes typical atomic values. For $a = 2.05$ Å, the factor $4\pi\varepsilon_0 a/e^2$ in Eq. (5) implies that an excitation energy of 182 eV corresponds to the 26 units of the adimensional Hamiltonian H' used in Section 2.2. That is, the excitation energies are in the high ultraviolet–low X-ray range. These are energies at least 100 times higher than thermal excitations. Therefore one should not expect the quantum collision states to be excited by thermal fluctuations. To make use of these states electromagnetic radiation fields, in the high ultraviolet–low X-ray range, should be used.

After a very controversial start, the so called *cold fusion* experiments were continued in several places in a much sober mood. Although some of the initial claims could not be confirmed, there are undeniably a few facts that defy chemical or thermodynamical explanations [5]. Among them are the abnormal isotope ratios [6,7] and a small but well measured excess power effect [8].

Given the scale of energies needed to excite the quantum collision states, discussed in this paper, it is not probable that they are at the origin of the cold fusion events. It is much more probable that the observed events arise from a mix-

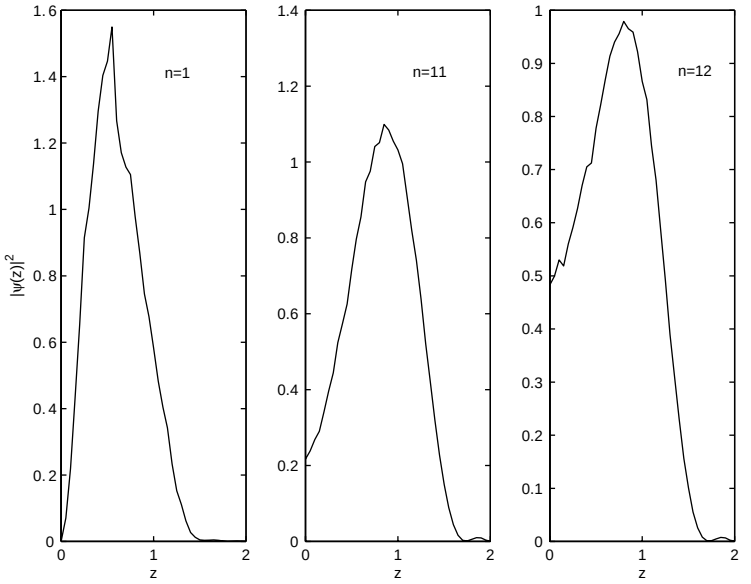

Fig. 5. Projected wave functions for the ground state and levels 11 and 12.

ture of exceptional causes. On one hand, when deuterium is absorbed by hydrogen storage materials, there is an expansion of the crystal lattice and cracks are expected to occur. Strong electric fields may occur in the cracks, accelerating the deuterons to nuclear fusion energies. This is consistent with the observation of protuberances and craters in cold fusion samples, these being often the sites where unexpected elements appear in high local concentrations.

On the other hand in hot spots caused by the (aggressive) electrolysis process, instead of an ordered structure, one might have a hot soup of electrons and deuterons and then, in this ergodic situation, it is known that three body collisions DeD have a small but non-negligible probability [9]. The occurrence of both situations, of course, will very much depend on the material structure of the samples.

Being probably due to a mixture of exceptional events, it is therefore natural for the cold fusion events to be hardly reproducible in any controllable way. It is the opposite situation that would be surprising. By contrast, the nuclear reaction control method that is being proposed here, is supposed to operate only when a large number of lattice cells is occupied by the right number of reactant nuclei and this in a regular manner to have well defined excitation levels. It is therefore a method that, if feasible, is fully controllable. A precondition for this scheme would be an accurate experimental determination of the excitation levels, to design the appropriate excitatory electromagnetic radiation field.

One might draw here a parallel with the current schemes for fusion by plasma confinement. There, charged particles are hopefully confined by magnetic fields, but confinement is not sufficient to achieve fusion. One needs to heat the plasma by radiofrequencies. A metallic lattice is a much softer confining device, but again one should not expect that just by confining the particles, many energetically useful fusion events would take place. That would be an unexpected miracle. To confine the deuterons, or other reactants, on a lattice seems a sound approach, but then some other mechanism, like the one discussed in this paper, must be found to induce the desired reaction. It is this approach that here (and elsewhere [10]) is called *hybrid fusion.*

Incidentally, both in the quantum collision-states method and in the ergodic situation (but not necessarily in crack acceleration) the dominant process for the deuteron fusion would be three-body DeD events, which would lead to a preferred channel [9]

$$D + e + D \rightarrow {}^4\mathrm{He}^*(20.1) + e \\ \downarrow \\ \rightarrow T + p.$$

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