



Quantum states of H_2^+ and H_2 in an icosahedral potential well

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Abstract. We investigate the potential energy surfaces (PESs) of the hydrogen-based cation H_2^+ and the neutral molecule H_2 confined inside an infinite potential well in the shape of a regular icosahedron. The numerical computations are performed using the diffusion Monte Carlo method and are based on an analytical technique for obtaining simple equations of the surfaces of convex polyhedra proposed by S. Onaka. Different states and different orientations of the molecules inside the confining potential well, as well as various sizes of the latter, are studied. We provide a detailed symmetry analysis and consistent labeling of the H_2^+ states considered. The results show that the icosahedral confinement is closely isotropic in its inner region, leading to PESs that develop pronounced minima, as in the case of simpler confinement geometries. Shape-specific effects can be evidenced when the nuclei are in contact with the confining wall.

1 Introduction

In recent years, there has been a great amount of interest in the study of quantum systems, such as atoms and small molecules, confined within infinitely deep potential wells in three spatial dimensions [1–14]. Very detailed and relatively recent reviews of the state of the art can be found in [15, 16]. In fact, the idea of confining atomic and molecular systems using a potential well derives from a long tradition in quantum mechanics [17–19], and it was introduced to simulate atoms under very high pressure conditions.

The confinement of a molecular system in a potential well produces a series of effects that have been characterized in various works over the last 20 years [20–22]; in particular, it has been shown that, because of the confinement, the strength of the bond increases and the excited repulsive states behave as bound ones [11–13]. These studies can be compared with others, developed in recent decades, that simulate a specific molecular system that act as a cage and produce the confinement effect, like crystalline cavities, fullerenes and nanotubes [23–25]. The confinement of a molecular

system by means of a potential well allows one to analyze and discuss the essence of the effects produced by a molecular cage, getting rid of the specific details of the intricate interaction between the atoms of the system and those of the cage.

Results related to confining systems with symmetries different from the simplest ones (e. g., the sphere) can represent a model of more realistic scenarios. In this regard, we remark that the studies presented so far mostly refer to spherical or ellipsoidal three-dimensional potential wells [1–7, 20, 21], with very few exceptions [8–10, 14, 26, 27] that, however, mostly involve cylindrical, cubic and octahedral wells.

In particular, there are no significant results in the literature about molecular systems confined within an ideal icosahedral well. In our opinion, this is a shortcoming that has to be amended, for more than one reason. Firstly, the icosahedron has a great intrinsic interest as the Platonic polyhedron having (together with its dual polyhedron, the dodecahedron) the highest degree of symmetry, I_h , where the number of all symmetry operations, that is the order of the group, is equal to 120. Moreover, the icosahedral geometry represents a model for the interaction potential inside molecular cages exhibiting an icosahedral symmetry: among these, we may mention fullerenes, hydrogenated boron clusters like $\text{B}_{12}\text{H}_{12}^{2-}$, and many others [28]. Finally, the icosahedron has a deep connection with the

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algebraic applications of group theory and with the mathematical methods of quantum chemistry [29, 30].

In this work, we present detailed calculations, performed with the diffusion Monte Carlo (DMC) method, related to the energies of quantum states of the ionic molecule H_2^+ and the neutral molecule H_2 confined within an icosahedral potential well. Hydrogen-based species are essential in the context of confined systems; H_2^+ and H_2 , in particular, are the subject of the vast majority of the works published concerning geometrical confinements [4, 6, 11, 31–33], both because of their simplicity as well as in view of the growing interest in hydrogen storage and quantum computing, because of the analogy among H_2^+ and more complex systems confined by a crystal field. For example, Kang et al. [34] claim that quantum calculations of confined H_2^+ may be meaningful to the realization of a charge qubit with double donor systems.

We underline the fundamental motivation of this study: the icosahedron is a Platonic polyhedron never considered as the shape of an infinite potential well. We show that a combination of unbiased DMC and Onaka's analytical method allow us to study this complex system straightforwardly. Although there are numerous real systems in which molecules are confined within molecular cages in the shape of an icosahedron [35], these real objects represent an indirect motivation for our study, and in any case their potential well is very different from an ideal icosahedral well. We believe that our calculations may provide new insights, e.g. the role of the numerous symmetries, subgroups of I_h , that are obtained by the molecule rotation.

2 Method

2.1 Diffusion Monte Carlo

Confinement problems having a significant novelty character are best addressed and solved via the diffusion Monte Carlo (DMC) technique [11, 32, 36, 37], which is based on the formal replacement of the Schrödinger equation with a reaction–diffusion equation in an imaginary time coordinate, whose short-time propagator is given by:

$$G(\mathbf{R} \leftarrow \mathbf{R}', \tau) \approx (2\pi\tau)^{-\frac{3N}{2}} \exp\left[\frac{-(\mathbf{R} - \mathbf{R}')^2}{2\tau}\right] \times \exp\left[\frac{-\tau(V(\mathbf{R}) - V(\mathbf{R}') - 2E_T)}{2}\right] \quad (1)$$

where N is the number of quantum particles in the system and τ is a numerical step. The diffusion equation (the first exponential term) is solved by carrying out the corresponding stochastic process via a cloud of mathematical points (*walkers*) in a set \mathbf{R}_i that move randomly in the $3N$ -configuration space by small time steps based on the short-time diffusion propagator. In

addition, according to the second exponential term of Eq. (1), the walkers can disappear in regions of high potential energy, while those who are in regions of low potential energy can multiply. The estimated energy E_T , the so-called energy offset that controls the total population of the walkers, is adapted by a relaxation method until the numerical equilibrium of the population of walkers is reached: the obtained estimate is the one of the lowest energy state compatible with the assigned constraints.

For simple quantum systems, some excited states with distinct symmetries can be determined by knowing the relative nodal surfaces: basically, the walkers' diffusion is limited to a single region of space where the wavefunction remains positive. In order to constraint the wavefunctions to vanish at the nodal surface, the walkers that come into contact with it are removed from the simulation. With the same method, the surface of an infinite potential well of the desired shape is introduced, thereby implementing a Dirichlet boundary condition.

The use of the Cartesian coordinates represents a straightforward advantage of the DMC method, since a change of the confinement shape can be realized with very few modifications to the calculation program.

Several programs to perform DMC calculations are available. The calculations presented in this work have been performed using the open-source program *DMC_Basic* [38], which is especially suited to confined quantum systems. This is a Fortran-language standard DMC program that allows one to find the ground state and symmetry-selected excited states of one- and two-electron systems confined in potential wells of any shape, with a very limited number of numerical parameters to be optimized (typically: the energy offset E_T , the time step τ and the number of walkers). The source code has been extended to treat the case of icosahedral confinement, following the prescriptions detailed in the next subsection.

The calculations of this work are performed within the Born–Oppenheimer approximation: the nuclei of the molecules are modeled as classical point-like sources of Coulomb potentials, placed in different locations inside the potential well. As their position varies, the potential energy surface (PES) of the molecule is determined. An alternative way would consist in performing calculations with mobile nuclei, i.e., adding three dimensions for each nucleus to the wavefunction. These calculations have been actually performed in the case of some confined systems [39, 40]; however, since in our case studies we are interested in the PESs, we need to specify the nuclear coordinates as independent variables. Furthermore, our method is greatly versatile with respect to the shape and symmetry of the potential well, as it does not employ variance reduction techniques. Therefore, the use of mobile nuclei would require excessive calculation times.

The DMC calculations are performed with an imaginary time step equal to 2×10^{-3} , totaling 10^5 time steps, during which the energy is updated and time-averaged, using 10^3 walkers in the three- or six-dimensional configuration space. The calculation of a typical PES, with

20 values of the internuclear distance, required a few to several minutes on a 2.8 GHz Intel Core i5 computer. The statistical variance of these runs was typically in the 10^{-3} a.u. range, low enough to produce smooth plots.

In all simulations, the zero value of the energy corresponds to the configuration in which all the particles are infinitely distant from each other: consequently, the dissociation limit of H_2^+ without confinement is at -0.5 a.u., while for H_2 it is at -1 a.u.

2.2 Equations of the icosahedral well

The icosahedron is a regular polyhedron limited by twenty faces (ten sets of parallel ones), that are identical equilateral triangles, each uniquely defining one plane. A generic point (x, y, z) is thus inside the icosahedron if and only if it is simultaneously in the twenty corresponding half-spaces, each one containing the origin of the coordinates. A detailed and explicit construction of such inequalities can be found in S. Onaka’s work [41]: here, the problem is generally addressed in the case of a convex surface that, depending on the value of a single parameter, smoothly interpolates between the surface of a given polyhedron and that of the inscribed sphere; the regular icosahedron is included among those limit cases. For our specific purposes, we employed Onaka’s construction with some minor modifications with respect to the original work: namely, we use Cartesian coordinates (more convenient in the DMC method, as mentioned in the previous section) instead of spherical ones, and we work with the inverses of the functions defined in Onaka’s original work, in order to avoid numerical overflows in the inner region. With the aforementioned modifications, the inner region of the potential well is characterized as follows: the point (x, y, z) is inside the icosahedron if all the following inequalities are *simultaneously* true:

$$|g(X, Y, Z, \gamma, \gamma, \gamma)| < 1, \quad |g(X, Y, Z, -\gamma, \gamma, \gamma)| < 1, \\ |g(X, Y, Z, \gamma, -\gamma, \gamma)| < 1 \tag{2}$$

$$|g(X, Y, Z, \zeta, \eta, 0)| < 1, \quad |g(X, Y, Z, \zeta, -\eta, 0)| < 1 \tag{3}$$

$$|g(X, Y, Z, 0, \zeta, \eta)| < 1, \quad |g(X, Y, Z, 0, \zeta, -\eta)| < 1 \tag{4}$$

$$|g(X, Y, Z, \eta, 0, \zeta)| < 1, \quad |g(X, Y, Z, \eta, 0, -\zeta)| < 1 \tag{5}$$

where, for the sake of brevity, one defines the function

$$g(x, y, z, a, b, c) = ax + by + cz \tag{6}$$

the rescaled (dimensionless) spatial coordinates

$$X = \frac{x}{l\eta}, Y = \frac{y}{l\eta}, Z = \frac{z}{l\eta} \tag{7}$$

and the fixed parameters

$$\gamma = \frac{1}{\sqrt{3}}, \quad \eta = \sqrt{\frac{3 + \sqrt{5}}{6}}, \quad \zeta = \sqrt{\frac{3 - \sqrt{5}}{6}} \tag{8}$$

In these equations, l is the half-length of the edge of the cube in which the icosahedron is inscribed, as shown in Fig. 1.

By simple geometrical considerations, the edge of the icosahedron equals l divided by the golden ratio; this simple equality easily allows for using the length of the edge of the icosahedron as a parameter, instead of the one of the inscribing cube.

These inequalities are used to compute the quantum states of the ionic molecule H_2^+ and the neutral molecule H_2 . In the latter case, the DMC method allows us to compute the ground state energy of the singlet without any approximation: indeed, the method computes the lowest energy associated to the six-dimensional (two-particle) wavefunction $\psi = \psi(x, y, z, u, v, w)$ without factorization, thus fully including the correlation effects; the allowed region of the configuration space is simply obtained by imposing the positions (x, y, z) and (u, v, w) to satisfy the prescription above.

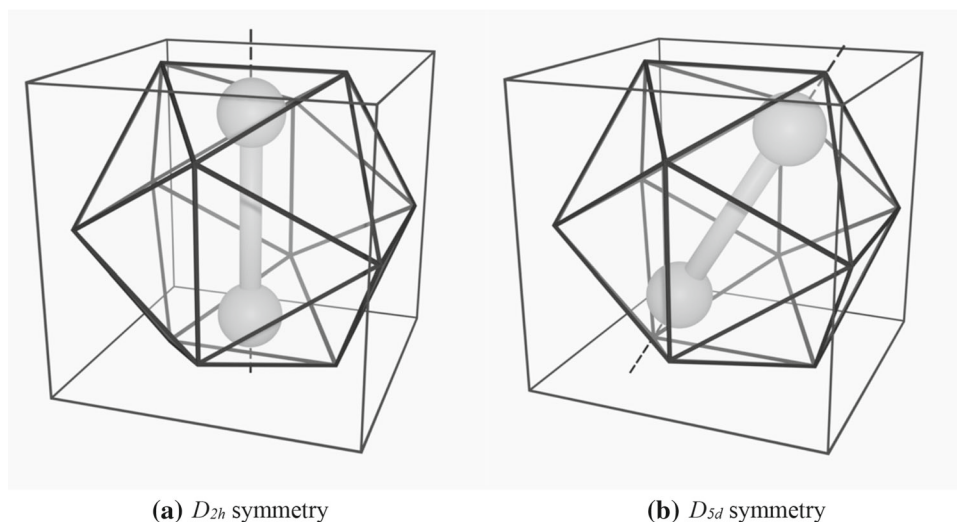
2.3 Symmetry considerations

As regards the ionic molecule H_2^+ , it is possible to identify various excited states by means of the relative nodal surfaces, which are known a priori in the case of this system. The main difficulty is that the nodal planes must also be valid for the confined system; consequently, these planes must be detected via symmetry considerations.

The icosahedron has a symmetry group I_h , the largest among those that can represent molecular symmetries, with order equal to 120. When a diatomic molecule is placed inside an icosahedron, with its center of mass coinciding with the geometrical center of the icosahedron, the resulting structure is described by a symmetry subgroup of I_h that depends on the orientation of the molecular axis. The order of the subgroup must be divided exactly into 120: the result of the division is the number of all structures that are equivalent, by symmetry, to the one considered [42]. For example, the geometry shown in Fig. 1 on the left has symmetry D_{2h} , whose order is 8. There are 15 equivalent geometries of this type, corresponding to situations where the molecular axis is perpendicular to two opposite edges.

In Onaka’s formulation, one of these orientations fixes the direction of the z axis, while the x axis is directed along the two edges in question. This choice of axes is then kept when the molecule is in a different geometric relation with the icosahedron, that is, the icosahedron has fixed relation to coordinates. The nuclei of the molecule are displaced. These excited states are correlated with those of the free molecule: therefore, they

Fig. 1 The geometry of the system under investigation. The molecular orientation shown on the left has D_{2h} symmetry, where many different nodal planes remain perfectly valid for the confined system and allow the identification of excited states of the H_2^+ molecule ion. The geometry corresponding to D_{5d} symmetry is shown on the right; the generic orientation investigated here still retains C_s symmetry. In the figure, the z axis is vertical, while the x axis is directed from left to right



can be named according to the corresponding correlation table [42]. The nodal plane considered must be the same in both cases.

To give a specific example, in the case of the free molecule H_2^+ the excited state Σ_u is the state of minimum energy such that the wavefunction vanishes on the plane perpendicular to the internuclear axis [11, 38]. When the overall system is in the configuration of Fig. 1a, this is still a symmetry plane for the whole system: therefore, it is possible to identify the excited state correlated with the free one, i.e., for large values of l . Its symmetry is B_{1u} , the irreducible representation of the z axis in D_{2h} , describing functions with a single nodal plane, the xy one: $\Sigma_u^+(D_{\infty h}) \rightarrow B_{1u}(D_{2h})$.

Some degenerate excited states of the free molecule (for example, Π_u) will not be degenerate in the case of the symmetry D_{2h} , since the latter only admits one-dimensional representations: the actual correlation is $\Pi_u(D_{\infty h}) \rightarrow B_{2u} + B_{3u}(D_{2h})$. For the most general geometry considered in this paper (see next section), the symmetry is C_s .

3 Results

The physical parameters in our case study are the half-edge l of the inscribing cube (see Fig. 1), the spherical angles θ, ϕ identifying the direction of the internuclear axes, and the internuclear distance d . For the sake of simplicity, in all simulations we set $\phi = 0$, corresponding to the situation where the molecular axis lies on the xz plane.

Figure 2 shows the potential curves of the confined H_2^+ molecule with the orientation corresponding to D_{2h} symmetry. We left as state labels those corresponding to the symmetry group of the free molecule ($D_{\infty h}$), in order to make the results more easily readable. Rigorously, the names of these states should be the names of irreducible representations of the group D_{2h} , namely

A_g, B_{1u}, B_{2u} and B_{1g} (in order of increasing energy); this should not cause any difficulty.

The results show that an increasing confinement produces a greater depth of the minimum of the potential well; however, for the confined molecule, it is not possible to define a dissociation limit, but rather a contact limit when the nuclei reach the surface of the well. We also stress the effect produced by confinement on the excited state potential curves: such states show qualitatively the characteristics of a bound state, producing deeper minima as the confinement increases.

As regards the H_2 system, the results of the ground state and three confinement dimensions are shown in Fig. 3.

From a qualitative point of view, a behavior similar to the ionic system is obtained. Here, though, we are in the presence of a traditional chemical bond, corresponding to a single Lewis bond: in the case of the icosahedral well, we can confirm the effect of confinement on a single bond discussed for other geometries.

Interestingly, the calculations highlight the isotropy of the icosahedron. The calculations carried out with regard to the D_{5d} symmetry, shown in Fig. 1b, led to results practically indistinguishable from those of the D_{2h} symmetry. A determination of this small energy differences is therefore to be addressed via deterministic approaches or by using importance sampling methods which, however, need to be developed ad hoc in the case of this geometry. As a consequence of the remarkable isotropy of the inner region of the icosahedron, the conclusions about the dissociation energy and vibrational energies of the confined molecule are substantially those of the spherical case.

In order to show some of the small effects due to orientation, and highlight the peculiar geometry of icosahedron, we performed a series of calculations corresponding to an extreme case: the one in which the nuclei are constantly in contact with the surface of the potential well. The internuclear distance is therefore completely determined by the geometry of the icosahedron as a function of the angle θ . As shown in the case of

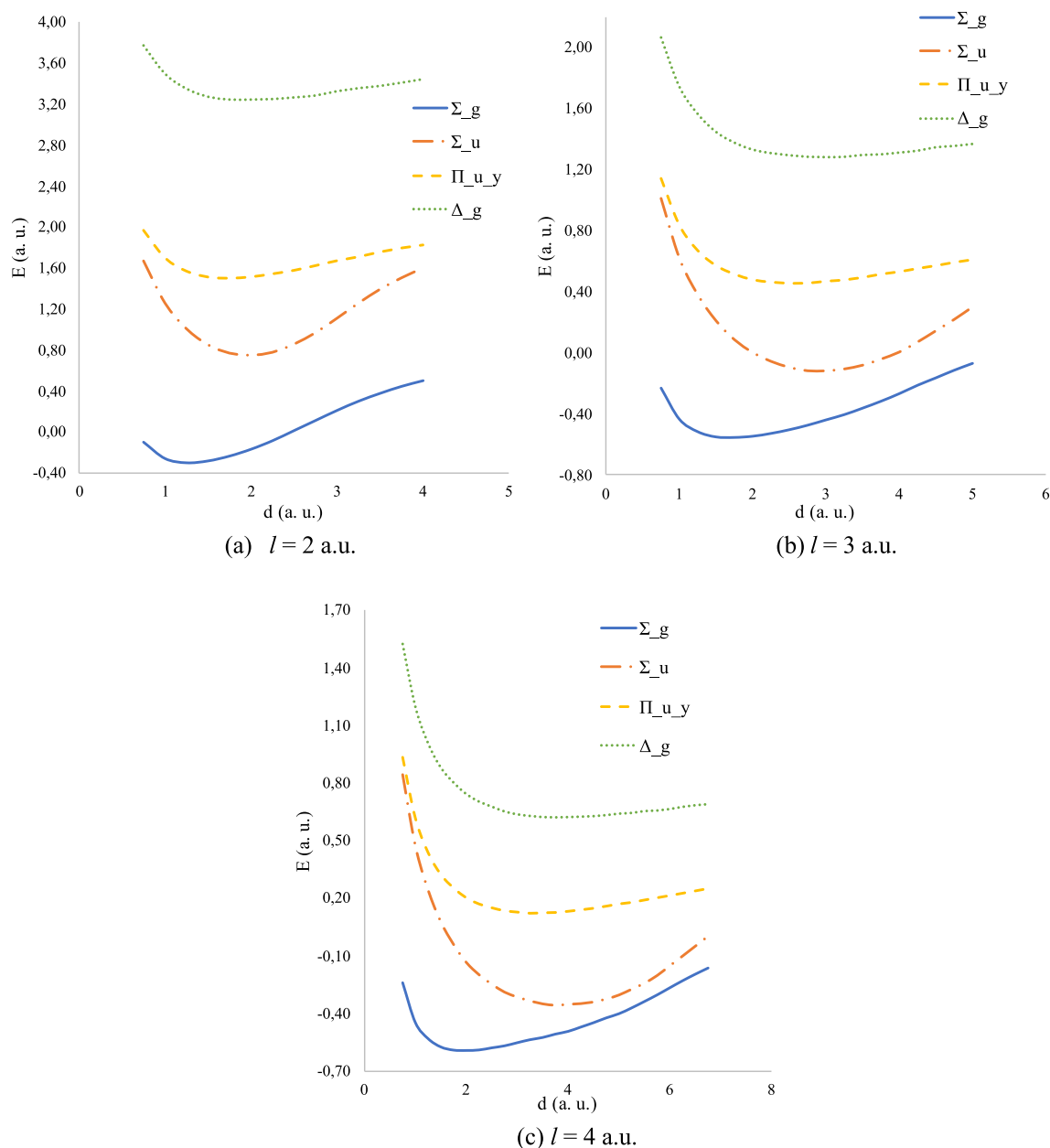


Fig. 2 Potential energy surfaces (PESs) of the ground state ${}^2\Sigma_g^+$ and three excited states (${}^2\Sigma_u^+$, ${}^2\Pi_u^+$, ${}^2\Pi_g^+$) of the H_2^+ ion enclosed in an icosahedral well, in the D_{2h} geometry, as a function of the internuclear distance d (atomic units), for three different values of the parameter l (the half-edge of the cube, as shown in Fig. 1)

spherical confinement [11], this limit case allows us to make semi-quantitative considerations related to the atomic states correlated with the molecular states for large dimensions of the potential well that produces the confinement. In this case, unlike in the case of spherical confinement, we expect the result to depend significantly on the direction of the molecular axis. The result of this calculation for the ${}^2\Sigma_g^+$ (${}^2A'$) state of H_2^+ is shown in Fig. 4.

The maximum of the energy is found in the D_{5d} geometry of Fig. 1b, while the minimum is found in the D_{3d} geometry where the two nuclei are in contact

with the centers of two opposite triangular faces. This shows that the main effect is due to the local shape of the contact surface.

A qualitative interpretation of the result may be the following. A vertex produces a greater limitation of the available solid angle; therefore, the average electron-nucleus distance must increase, and this leads to a higher potential energy. For the same reason, the plane face yields a lower energy. These results are in good qualitative agreement with the discussion in [11] for the spherical well and for the results found in the case of

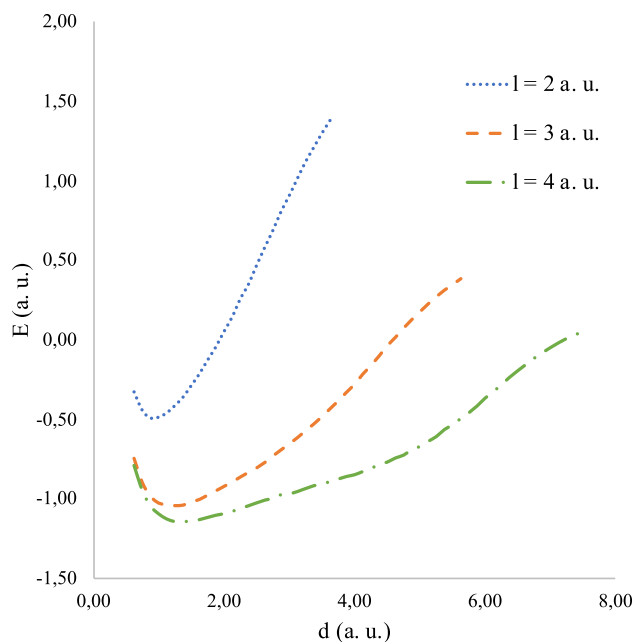


Fig. 3 Potential energy surfaces (PESs) of the ground state $1\Sigma_g^+$ of H_2 enclosed in an icosahedral well of different dimension l (the half-edge of the cube in Fig. 1) in the D_{2h} geometry, as a function of the internuclear distance d (atomic units)

the confinement of hydrogen atoms by dihedral surfaces (Ley-Koo et al. [15]).

4 Conclusions

In this work, the quantum states of H_2^+ and H_2 molecules confined within three-dimensional icosahedral potential wells have been determined, and some peculiarities produced by this potential well have been discussed. The results show that the confinement states present deeper minima in their potential curves, as it was demonstrated in the case of simpler confinement geometries. Moreover, some results concerning the effects of the orientation of the molecular axis, when the nuclei are very close to the confinement wall, have been presented.

The first contribution of this work lies in the methodology itself: the use of an analytical expression of the characteristic function of the icosahedron, in conjunction with the unbiased Diffusion Monte Carlo method, has allowed us to study this system straightforwardly.

Our results show that the inner region of the ideal icosahedral well behaves essentially isotropically, while more shape-specific effects can be evidenced when the nuclei are in contact with or very close to the boundary surface.

Given the importance of the icosahedron as a highly symmetrical Platonic polyhedron, the calculations carried out here have primarily a conceptual interest. At the same time, our results may serve as a starting point

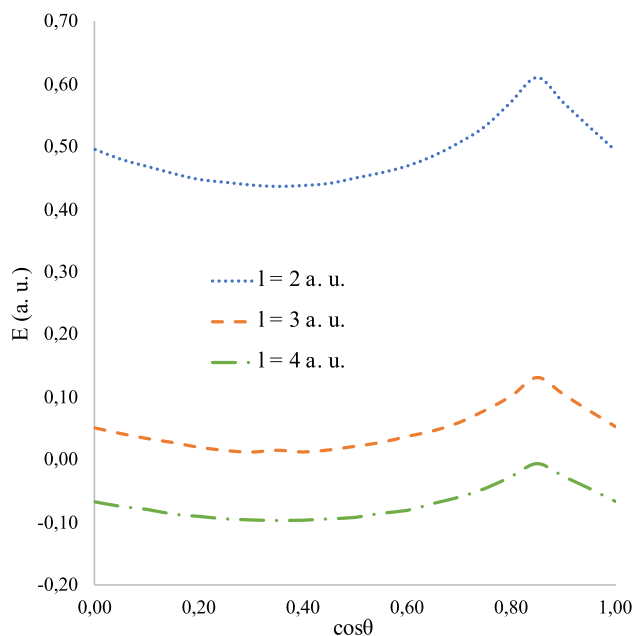


Fig. 4 The energy of the ground state $2\Sigma_g^+$ of H_2^+ enclosed in an icosahedral well of different dimension l (the half-edge of the cube in Fig. 1) in the limit case where the nuclei are constantly in contact with the icosahedral surface, as a function of $\cos\theta$ for $\phi = 0$

for investigating the features of icosahedral cages in inorganic chemistry and condensed matter physics: calculations for molecules confined within ideal icosahedral well represent an alternative to ab initio calculations, which show the role of the specific atoms of the cage, but for this very reason they are less general. Accordingly, the approach presented here may have a heuristic value to be evaluated in the future.

Author contributions

All authors contributed equally to the paper.

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Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors’ comment: The open-source *DMC_basic* code used in this paper is available on GitHub (https://github.com/SavinoLongoPhD/DMC_basic).]

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References

1. C. Laughlin, B.L. Burrows, M. Cohen, A hydrogen-like atom confined within an impenetrable spherical box. *J. Phys. B At. Mol. Opt. Phys.* **35**(3), 701 (2002)
2. T. Pang, Hydrogen molecule under confinement: exact results. *Phys. Rev. A* **49**(3), 1709 (1994)
3. M.E. Molinar-Tabares, G. Campoy-Güereña, Hydrogen molecular ion confined by a prolate spheroid. *J. Comput. Theor. Nanosci.* **9**(6), 894–899 (2012)
4. H.D.O. Batael, E. Drigo Filho, Ground-state energy for confined H₂: a variational approach. *Theor. Chem. Acc.* **137**(5), 1–6 (2018)
5. R. Colín-Rodríguez, C. Díaz-García, S.A. Cruz, The hydrogen molecule and the H⁺ 2 molecular ion inside padded prolate spheroidal cavities with arbitrary nuclear positions. *J. Phys. B At. Mol. Opt. Phys.* **44**(24), 241001 (2011)
6. H. Olivares-Pilón, S.A. Cruz, The H, H₂⁺, and HeH₂⁺ systems confined by an impenetrable spheroidal cavity: Revisited study via the Lagrange-mesh approach. *Int. J. Quantum Chem.* **117**(17), e25399 (2017)
7. S.B. Doma, F.N. El-Gammal, A.A. Amer, Ground-state calculations of confined hydrogen molecule H₂ using variational Monte Carlo method. *Mol. Phys.* **116**(14), 1827–1833 (2018)
8. T. Yildirim, A.B. Harris, Quantum dynamics of a hydrogen molecule confined in a cylindrical potential. *Phys. Rev. B* **67**(24), 245413 (2003)
9. S. Longo, G. Micca Longo, D. Giordano, Monte Carlo calculation of the potential energy surface for octahedral confined H₂⁺. *Rendiconti Lincei. Scienze Fisiche e Naturali* **29**(1), 173–177 (2018)
10. E. Ley-Koo, S. Rubinstein, The hydrogen atom inside boxes with paraboloidal surfaces. *J. Chem. Phys.* **73**(2), 887–893 (1980)
11. G. Micca Longo, S. Longo, D. Giordano, Spherically confined H₂⁺: 2Σg⁺ and 2Σu⁺ states. *Phys. Scr.* **90**(2), 025403 (2015)
12. G. Micca Longo, S. Longo, D. Giordano, Quantum states of confined hydrogen plasma species: Monte Carlo calculations. *Plasma Sources Sci. Technol.* **24**(6), 065019 (2015)
13. S.A. Cruz, D. Garrido-Aguirre, Confinement effects on the diatomic interaction potential. *Radiat. Eff. Defects Solids* **175**(1–2), 202–217 (2020)
14. G. Micca Longo, A.F. Cantatore, C. Stripoli, D. Giordano, S. Longo, Quantum states of hydrogen cations confined into spherical and nanotube-like potential wells: (*C*_{2h} and *C*_{2v}) and (*D*_{3h}). *Phys. Scr.* **96**(12), 125404 (2021)
15. K.D. Sen, K.D. Sen (eds.), *Electronic Structure of Quantum Confined Atoms and Molecules* (Springer, Cham, 2014), pp.1–253
16. E. Ley-Koo, Recent progress in confined atoms and molecules: superintegrability and symmetry breakings. *Revista mexicana de física* **64**(4), 326–363 (2018)
17. A. Sommerfeld, H. Welker, Künstliche Grenzbedingungen beim Keplerproblem. *Ann. Phys.* **424**(1–2), 56–65 (1938)
18. A. Michels, J. De Boer, A. Bijl, Remarks concerning molecular interaction and their influence on the polarisability. *Physica* **4**(10), 981–994 (1937)
19. S.R. De Groot, C.A. Ten Seldam, On the energy levels of a model of the compressed hydrogen atom. *Physica* **12**(9–10), 669–682 (1946)
20. S. Mateos-Cortés, E. Ley-Koo, S.A. Cruz, Hydrogen molecular ion inside penetrable prolate spheroidal boxes: electronic and vibrational properties. *Int. J. Quantum Chem.* **86**(4), 376–389 (2002)
21. J.F. da Silva, F.R. Silva, E.D. Filho, The effect of confinement on the electronic energy and polarizability of a hydrogen molecular ion. *Int. J. Quantum Chem.* **116**(7), 497–503 (2016)
22. H. de Oliveira Batael, E. Drigo Filho, J. Chahine, J.F. da Silva, Effects of quantum confinement on thermodynamic properties. *Eur. Phys. J. D* **75**(2), 1–9 (2021)
23. J. Soullard, R. Santamaria, S.A. Cruz, Endohedral confinement of molecular hydrogen. *Chem. Phys. Lett.* **391**(1–3), 187–190 (2004)
24. Y.X. Ren, T.Y. Ng, K.M. Liew, State of hydrogen molecules confined in C₆₀ fullerene and carbon nanocapsule structures. *Carbon* **44**(3), 397–406 (2006)
25. O.P. Charkin, N.M. Klimenko, D.O. Charkin, DFT study of molecules confined inside fullerene and fullerene-like cages. *Adv. Quantum Chem.* **58**, 69–114 (2009)
26. S. Longo, G. Micca Longo, K. Hassouni, A. Michau, S. Prasanna, Stochastic models of systems for nanotechnology: from micro to macro scale. *Nanotechnology* **32**(14), 145604 (2021)
27. R.A. Van Gorder, Compressed hydrogen atoms confined within generic boxes. *Proc. R. Soc. A* **478**(2268), 20220467 (2022)
28. S. Alvarez, Polyhedra in (inorganic) chemistry. *Dalton Trans.* **13**, 2209–2233 (2005)
29. O. Nash, On Klein's icosahedral solution of the quintic. *Expo. Math.* **32**(2), 99–120 (2014)
30. V. Aquilanti, C. Coletti, 3nj-symbols and harmonic superposition coefficients: an icosahedral abacus. *Chem. Phys. Lett.* **344**(5–6), 601–611 (2001)
31. R. Colín-Rodríguez, S.A. Cruz, The hydrogen molecule inside prolate spheroidal boxes: full nuclear position optimization. *J. Phys. B At. Mol. Opt. Phys.* **43**(23), 235102 (2010)
32. A. Sarsa, C.L. Sech, Study of quantum confinement of H₂⁺ ion and H₂ molecule with Monte Carlo. Respective role of the electron and nuclei confinement, in *Electronic*

Structure of Quantum Confined Atoms and Molecules. ed. by K.D. Sen (Springer, Cham, 2014), pp.227–253

33. G. Micca Longo, S. Longo, D. Giordano, Confined H(1s) and H(2p) under different geometries. *Phys. Scr.* **90**(8), 085402 (2015)
34. S. Kang, Y.M. Liu, T.Y. Shi, The characteristics for H₂⁺-like impurities confined by spherical quantum dots. *Eur. Phys. J. B* **63**, 37–42 (2008)
35. J. Hernández-Rojas, V. Monteseguro, J. Bretón, J.G. Llorente, Water clusters confined in icosahedral fullerene cavities. *Chem. Phys.* **399**, 240–244 (2012)
36. J.B. Anderson, A random-walk simulation of the Schrödinger equation: H+ 3. *J. Chem. Phys.* **63**(4), 1499–1503 (1975)
37. W.M.C. Foulkes, L. Mitas, R.J. Needs, G. Rajagopal, Quantum Monte Carlo simulations of solids. *Rev. Mod. Phys.* **73**(1), 33 (2001)
38. G. Micca Longo, C.M. Coppola, D. Giordano, S. Longo, The unbiased diffusion Monte Carlo: a versatile tool for two-electron systems confined in different geometries. *Eur. Phys. J. D* **75**(3), 1–7 (2021)
39. D. Skouteris, O. Gervasi, A. Laganà, Non-Born–Oppenheimer MCTDH calculations on the confined H₂⁺ molecular ion. *Chem. Phys. Lett.* **500**(1–3), 144–148 (2010)
40. A. Sarsa, J.M. Alcaraz-Pelegriña, C. Le Sech, S.A. Cruz, Quantum confinement of the covalent bond beyond the Born–Oppenheimer approximation. *J. Phys. Chem. B* **117**(24), 7270–7276 (2013)
41. S. Onaka, Simple equations giving shapes of various convex polyhedra: the regular polyhedra and polyhedra composed of crystallographically low-index planes. *Philos. Mag. Lett.* **86**(03), 175–183 (2006)
42. W.G. Fateley, N.T. McDevitt, F.F. Bentley, Infrared and Raman selection rules for lattice vibrations: the correlation method. *Appl. Spectrosc.* **25**(2), 155–173 (1971)