Abstract. Hard-sphere confinement is used to study helium atoms under pressure. The confined-helium Schrödinger equation is solved with a high accuracy by a Lagrange-mesh method.

The effects of high pressure on a helium gas can be estimated by studying the helium atom in a hard confinement, i.e. confined at the centre of an impenetrable spherical cavity, for different cavity radii. Contrary to the free helium atom, the confined helium has not been described with a very high accuracy until recently, when we have developed a Lagrange-mesh method to study this system [1]. This method improves by several order of magnitudes the accuracy of previous approaches [2–4].

The outlines of the model are the following. The assumed-infinite-mass nucleus is fixed and the electrons are characterized by coordinates \( r_1 \) and \( r_2 \) with respect to this nucleus. In atomic units, the Hamiltonian of the helium atom reads

\[
H = -\frac{1}{2} \Delta_1 - \frac{1}{2} \Delta_2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}},
\]

where \( r_{12} = r_1 - r_2 \) and \( \Delta_1 \) and \( \Delta_2 \) are the Laplacians with respect to \( r_1 \) and \( r_2 \). The confinement is introduced by forcing the wave function into some spherical cavity of radius \( R (r_1, r_2 \leq R) \). The wave function \( \psi(r_1, r_2, r_{12}) \) of an \( S \) state must thus verify the Schrödinger equation

\[
H \psi(r_1, r_2, r_{12}) = E \psi(r_1, r_2, r_{12})
\]

and vanishes at \( r_1 = R \) and \( r_2 = R \). The coordinates \( (r_1, r_2, r_{12}) \) are advantageously replaced by the coordinates \( (u, v, w) \) defined over \([0,1]\) by

\[
u = r_1 - r_2 + r_{12}, \quad \frac{r_2 - r_{12}}{2R}, \quad \frac{r_1 - r_2}{2R}, \quad \frac{r_{12}}{2R}.
\]

The confinement implies that the wave function \( \psi(u, v, w) \) vanishes at \( u = 1, v = 1, \) and \( w = 1 \).

The Schrödinger equation is solved by the Lagrange-mesh method [5–7], an approximate variational approach taking the form of a system of mesh equations by computing the Hamiltonian and overlap matrix elements with a Gauss quadrature. Using the coordinates \( (u, v, w) \) is essential for an easy treatment of the confinement and an high accuracy of the Gauss quadrature. The ground-state energy and wave function are obtained by diagonalizing a rather large (matrix dimension \( \approx 10^3 \sim 2 \times 10^4 \)) but sparse matrix. Ground-state energies and mean interparticle distances for several confinement radii \( R \) are given in table 1. The pressure acting on the confined helium atom is also given in table 1. It is

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Table 1. Ground-state energy and mean interparticle distances of a helium atom confined in a sphere of radius $R$ and pressure acting on such a confined helium atom [1]. Atomic units are used. The powers of ten are indicated between brackets.

<table>
<thead>
<tr>
<th>$R$</th>
<th>$E$</th>
<th>$\langle r_{12} \rangle$</th>
<th>$\langle r_1 \rangle = \langle r_2 \rangle$</th>
<th>$P$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>906.562</td>
<td>0.069 580 382 884 2</td>
<td>0.049 501 246 340 1</td>
<td>1.507 426 738 64</td>
</tr>
<tr>
<td>1.0</td>
<td>1.015 754</td>
<td>0.643 664 253 878</td>
<td>0.441 796 632 103 3</td>
<td>9.510 085 662 1</td>
</tr>
<tr>
<td>10.0</td>
<td>-2.903 724</td>
<td>1.422 070 172 936</td>
<td>0.929 472 251 212</td>
<td>2.711 [-12]</td>
</tr>
</tbody>
</table>

Figure 1. Difference between the ground-state energies of confined helium ($E$) and of free helium ($E_\infty$) as a function of the confinement radius $R$. Atomic units are used.

calculated from the radius dependence of the energies $E(R)$ by the formula [2–4],

$$P = -\frac{1}{4\pi R^2} \frac{dE}{dR},$$

where the derivative is evaluated by a finite-difference formula. A similar accuracy is obtained for the energy and interparticle distances of the first excited singlet level and the lowest triplet level [1]. Although the Lagrange-mesh method can be applied easily for small and large radii, it is particularly efficient for small radii (smaller variational basis size and better accuracy). The dependence of the ground-state energy on the confinement radius $R$ is shown graphically in Fig. 1. For large confinement radii ($R \gtrsim 2$ fm), the confined helium energy tends nearly exponentially to the free helium energy. A parametrization of this curve could allow an easy evaluation of the pressure at very large radii, difficult to reach by direct calculations.

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References