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Helium atom under pressure

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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 $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ with respect to this nucleus. In atomic units, the Hamiltonian of the helium atom reads

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

where $\boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ and Δ_1 and Δ_2 are the Laplacians with respect to $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$. 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

$$H\psi(r_1, r_2, r_{12}) = E\psi(r_1, r_2, r_{12}) \tag{2}$$

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

$$u = \frac{r_1 - r_2 + r_{12}}{2R - r_1 - r_2 + r_{12}}, \quad v = \frac{-r_1 + r_2 + r_{12}}{2R - r_1 - r_2 + r_{12}}, \quad w = \frac{r_1 + r_2 - r_{12}}{2R}. \tag{3}$$

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$\approx 10^3 \sim 2\times10^4$) 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.

R	E	$\langle r_{12} \rangle$	$\langle r_1 \rangle = \langle r_2 \rangle$	P
0.1	906.562 422 919 888	0.069 580 382 884 2	0.049 501 246 340 1	1.507 426 738 64[5]
1.0	1.015 754 976 048 4	0.643 664 253 878	0.441 796 632 103 3	9.510 085 662 1 [-1]
10.0	−2.903 724 375 687	1.422 070 172 936	0.929 472 251 212	2.711 [-12]

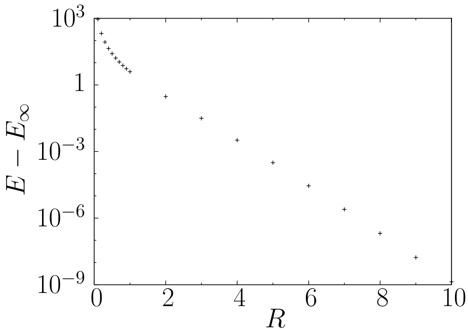

Figure 1. Difference between the ground-state energies of confined helium (E) and of free helium (E_∞) as a function of the confinement radius R. Atomic units are used.

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

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

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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