Dipole transition of two-electron ions under pressure confinement

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Synopsis The energy values of atomic systems are modified when the system is placed in a confined domain. Within the finite domain, the ion experiences a thermodynamic pressure which pushes the energy levels towards continuum. Here we have performed explicitly correlated variational calculations in Hylleraas coordinates to estimate two-electron energy levels in ${}^1P^e$ state originating from $1snp$ configuration and $1s2p({}^1P^o) \to 1s^2({}^1S^e)$ transition wavelengths within such pressure confinement.

If a two-electron ion is placed within an impenetrable cavity keeping the nucleus (of charge Z and infinite mass) at the centre, then the non-relativistic Hamiltonian (in a.u.) may be written as

$$H = \sum_{i=1}^{2} \left[-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i} \right] + \frac{1}{r_{12}} + V_R(r_1, r_2) \qquad (1)$$

The confining potential $V_R(r_1, r_2)$ is expressed as

$$\begin{aligned} V_R(r_1,r_2) &= 0 \qquad 0 \le (r_1,r_2) \le R \\ &= \infty \qquad \text{otherwise} \end{aligned} \qquad (2)$$

A spatial restriction and hence a thermodynamic pressure is imposed on the system due to the confining potential. The wave function Ψ satisfies the boundary condition given by

$$\Psi(r) = 0 \qquad at \quad r \ge R \qquad (3)$$

The normalization condition $\langle \Psi | \Psi \rangle = 1$ is satisfied within the sphere.

We have estimated the $1s2p$ (${}^1P^o$) energy values of helium-like ions ($Z = 2, 3$). The variational equation is taken from Ref. [1]. The generalized eigenvalue equation $\underline{\underline{H}}\,\underline{C} = E\,\underline{\underline{S}}\,\underline{C}$ is solved where $\underline{\underline{H}}$ is the Hamiltonian matrix, $\underline{\underline{S}}$ is the overlap matrix and $\underline{C}$ is the column matrix consisting of linear variational parameters.

Under an adiabatic approximation, the pressure (P) inside the impenetrable cavity can be expressed according to the first law of thermodynamics as

$$P = -\frac{1}{4\pi R^2}\frac{dE_R}{dR} \qquad (4)$$

where E_R is the ground state energy of the ion inside the sphere of radius R.

In Fig. 1, we have shown the variation of energy value of $1s2p$ (${}^1P^o$) state of helium within pressure confinement. The energy value of the confined system is increasing with decrease in radius *i.e.* with increase of pressure.

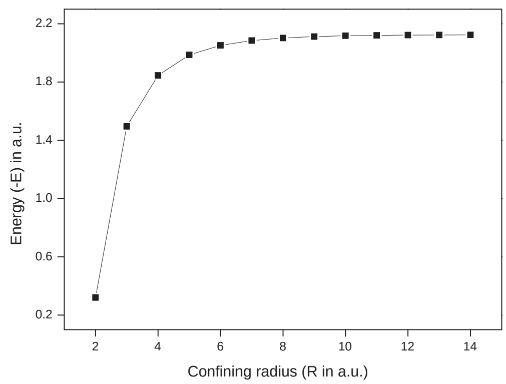

Figure 1. Energy value of $1s2p$ (${}^1P^o$) state of confined Helium.

We have also estimated the wavelengths corresponding to $1s2p({}^1P^o) \to 1s^2({}^1S^e)$ transitions under pressure confinement where the $1s^2({}^1S^e)$ energy values are taken from Ref. [2].

Table 1. Energy of $1s2p$ (${}^1P^o$) state and $1s2p({}^1P^o) \to 1s^2({}^1S^e)$ transition wavelengths of He placed under pressure confinement. x[y] denotes x × 10^y.

Radius (a.u.)	Energy (−E a.u.)	Transition wavelength (Å)	Pressure (Pa)
10.0	2.117 389	579.280	3.245[3]
7.0	2.084 815	556.239	2.886[5]
5.0	1.986 309	496.682	6.941[7]

Table 1 shows the energy values of $1s2p$ (${}^1P^o$) state and $1s2p({}^1P^o) \to 1s^2({}^1S^e)$ transition wavelengths of He placed under pressure confinement. We have also given the pressure 'felt' by the ion within the sphere.

References

[1] T. K. Mukherjee and P. K. Mukherjee 1994 *Phys. Rev. A* **50** 850 **635** 001001

[2] S. Bhattacharyya *et al.* 2013 *Phys. Scr.* **87** 065305

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