Quadratic-linear B-spline grid for studying Ps-atom interactions in cavities

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The B-spline basis set was first introduced in 1946 [1] but has become ubiquitous in atomic physics since the 1990s [2, 3]. B-spline functions are square-integrable piecewise polynomials defined in a restricted domain (the *cavity*) over a set of non-decreasing points r_j (the *knot sequence*). The appropriate choice of knot sequence depends on the problem at hand. An exponential sequence, viz.,

$$r_j = r_0[\exp(\sigma j) - 1], \tag{1}$$

where r_0 and σ are constants, works well for describing electronic states of atoms and calculation of many-body-theory diagrams [2, 4]. However, it is ill-suited for describing continuum states of an electron (or positron) accurately.

We plan to use many-body theory to study Ps-atom interactions by calculating Ps states in the spherical cavity with the atom at the centre. This requires an accurate description of both the atomic bound states and the Ps continuum states. We also need to know the effect of the cavity wall on Ps, i.e., its effective radius. Though for us the cavity is a computational tool, for experimentalists it is a physical tool or even the object of study, e.g., where pore sizes are derived from Ps lifetime spectroscopy (see, e.g., [5, 6]).

It is known that an equispaced (linear) knot sequence can be used to describe states of free Ps in the cavity accurately [7]. Examining the atomic potential suggests that inside the atom an economical quadratic grid should be appropriate [3]. Thus, we propose the following grid for studying Ps-atom interactions:

$$r_j = Aj^2/(B + j), \tag{2}$$

where A and B are constants. For $j < B$, the dominant nature of the sequence is quadratic, while for $j > B$ it is linear. The value of B is chosen so that the change of the dominant nature occurs at $\sim$1 a.u. We refer to this knot sequence as the *quadratic-linear* grid.

In the present work we used a set 40 B-splines of order 6. Table 1 compares the energies of the ground-state orbitals of Ar using the exponential and quadratic-linear grids. The agreement is excellent: at least 6 significant figures. Table 2 likewise compares several energies of free Ps in the cavity. The agreement is at the level of 0.2% or better.

The next stage will be to use the quadratic-linear grid to build states of Ps in the field of the atom, treating it as a static potential source. Then we will proceed to describe the system using accurate many-body techniques.

Orbital	Exponential	Quadratic-linear
$1s$	-118.6103533	-118.6103516
$2s$	-12.3221526	-12.3221540
$2p$	-9.5714664	-9.5714662
$3s$	-1.2773533	-1.2773531
$3p$	-0.5910179	-0.5910175

Table 1: *Energies (in a.u.) of Ar orbitals using exponential and quadratic-linear grids.*

$nl(N, L)$	Linear	Quadratic-linear
$1s(1, 0)$	-0.216100	-0.216121
$1s(2, 0)$	-0.120167	-0.120246
$2s(1, 0)$	0.0239796	0.0239507
$1s(3, 0)$	0.0309400	0.0308777
$2p(1, 1)$	0.0768631	0.0768559

Table 2: *Energies of Ps in a cavity of radius 10 a.u. Internal state: nl, external state: (N, L).*

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