

**Cassidy *et al* Reply:** Recently we performed measurements and calculations concerning changes in the  $1S$ - $2P$  energy interval for positronium confined in small pores ( $\delta\varepsilon$ ) [1]. The calculated values of  $\delta\varepsilon$  were found to exhibit an unexpected dependence on the pore size that Green and Gribakin (GG) have suggested is an artifact of the calculation [2].

We broadly agree with the two simple analyses presented by GG; we also analytically expected the system should behave as  $1/R^3$  for large cavities (as mentioned in Ref [1]). However, the situation may not be as clear-cut as GG portray for cavity sizes less than  $\sim 5$  nm. Importantly, uncertainty in the cavity radius for which a  $1/R^3$  dependence should be expected meant that we had to defer to the calculations.

Based on subsequent work [3], we now believe that calculations should agree with the  $1/R^3$  dependence for diameters larger than  $\sim 5$  nm. However, depending on the shape of the potential chosen (i.e., the thickness of the skin and size of the step), we expect that there should be a different dependence somewhere between 1 nm and 4 nm, with a turning point that starts downward (as  $1/R$  or  $1/R^2$ , through to sharper than  $1/R^3$ ) before settling into the asymptotic regime [3]. Certainly, we do not expect that scaling a  $1/R^3$  dependence to our configuration interaction (CI) data at 2 nm will produce meaningful results. Indeed, so doing yields an implied value of  $\delta\varepsilon$  that is inconsistent with the measurement, as shown in Fig 1 of Ref. [2].

Having performed more analysis of the CI computations we agree with GG that the calculations are simply struggling at larger radii, resulting in the appearance of an unphysical downward trend. As we stated in the Letter, there were a number of convergence problems in the calculations, and we chose to report or interpret based on the wave functions as calculated. Based on follow-up work [3], our heuristic model advanced to justify the greater than  $1/R^3$  behavior seen in the CI calculations should only be applied in the intermediate regimes. The wave function

behavior in this regime is still under investigation, so we shall refrain from further comment on what GG call the “unlikely” mixing as exhibited in the CI wave functions.

We have also derived an expression similar to Eq. (1) in Ref [2], and found a prefactor for large diameter cavities [3]. We find that this agrees with (i) the measurement reported in Ref [1], (ii) the range deduced from the CI calculations (around 5–7 nm), and (iii) follow-up calculations [3].

In summary, GG have raised important points about the calculations described in [1]. Nevertheless, we expect that there will be interesting effects associated with positronium confinement, albeit for smaller radii than was originally suggested. The ostensibly simple system of a positronium atom confined in a small cavity has proven to be surprisingly complex, and warrants further theoretical and experimental investigation.

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