VIBRATIONAL RESONANCES IN POSITRON ANNIHILATION WITH KRYPTON DIMERS

G. F. Gribakin and C. M. R. Lee

Department of Applied Mathematics and Theoretical Physics, Queen's University, Belfast, UK

Experimental measurements of annihilation with a positron beam at high resolution (25 meV) [1, 2], have shown resonances in the annihilation rate parameter, $Z_{\rm eff}$, of alkane molecules. These can be explained by the capture of positrons into vibrational Feshbach resonances, which also account for very large values of $Z_{\rm eff}$ observed.

To examine the effect of vibrations on positron scattering and annihilation, we consider a simple model of Kr_2 dimer using the zero-range potential (ZRP) method. In the previous paper [3] the interaction between the atoms in the dimer was treated using the harmonic approximation (HA). This approximation does not describe well the true potential for weakly bound van der Waals molecules such as Kr_2. In this work we model the molecular interaction with the Morse potential (MP), $U(R) = U_{\rm min}[e^{-2\alpha(R-R_0)} - 2e^{-\alpha(R-R_0)}]$, whose parameters can be obtained from the known values of R_0, $U_{\rm min}$ and ω for the dimer.

The positron-molecule wavefunction outside the atoms can be written in the form of a linear combination with coefficients A_n and B_n,

$$\begin{aligned}\Psi &= e^{i\mathbf{k}_0\cdot\mathbf{r}}\Phi_0(\mathbf{R}) + \sum_n A_n \Phi_n(\mathbf{R})\frac{e^{ik_n|\mathbf{r}-\mathbf{R}_1|}}{|\mathbf{r}-\mathbf{R}_1|} \\ &+ \sum_n B_n \Phi_n(\mathbf{R})\frac{e^{ik_n|\mathbf{r}-\mathbf{R}_2|}}{|\mathbf{r}-\mathbf{R}_2|},\end{aligned}$$

where $\mathbf{k}_0$ is the incident positron momentum, Φ_n is the nth vibrational state of the molecule, and $\mathbf{R} = \mathbf{R}_1 - \mathbf{R}_2$ is the interatomic distance. The two sums represent scattering events which leave the molecule in the nth excited state, and k_n is the corresponding positron momentum.

One can obtain a set of linear equations for the coefficients A_n and B_n, using the ZRP boundary condition. They can then be used to calculate $Z_{\rm eff}$ by the formula [3],

$$Z_{\rm eff} = Z_{\rm eff}^{(0)}\kappa_0^2 \sum_n (|A_n|^2 + |B_n|^2),$$

where κ_0 is the zero-range parameter and $Z_{\rm eff}^{(0)}$ is the $Z_{\rm eff}$ value for an atom at zero positron energy.

For parameters $R_0 = 7.56$ a.u., $U_{\rm min} = 17.2$ meV and $\omega = 2.42$ meV, the bound states for MP are $\varepsilon_0 = -4.10$ meV and $\varepsilon_1 = -1.45$ meV, whereas for HA they are $\varepsilon_0 = -4.51$ meV, $\varepsilon_1 = -2.30$ meV and $\varepsilon_2 = -0.11$ meV. So in MP we find a smaller binding energy than in HA. We also see that MP results in a greater vibrational frequency for the $\mathrm{e}^+\mathrm{Kr}_2$ complex than that of Kr_2, whereas HA suggests it to be less.

Figure 1 shows $Z_{\rm eff}$ for both approximations. Though the resonances are in different positions, the strength of the first resonance ($n = 2$ for MP, $n = 3$ for HA) remains almost the same. After thermal averaging of $Z_{\rm eff}$ over the Maxwellian positron energy distribution, the graphs of $\bar{Z}_{\rm eff}(T)$ for MP and HA become similar, with the resonance contribution being about an order of magnitude greater than the background.

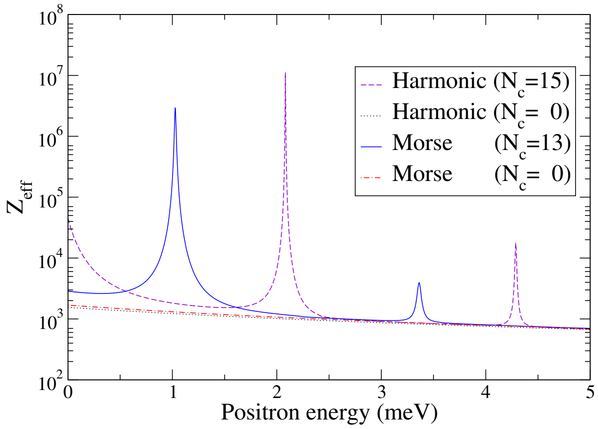

Fig. 1. Comparison of $Z_{\rm eff}$ for MP and HA, calculated using vibrational states with $n \le N_c$. $N_c = 0$ corresponds to the fixed nuclei approximation.

References

[1] S. J. Gilbert, L. D. Barnes, J. P. Sullivan and C. M. Surko, Phys. Rev. Lett. **88**, 043201 (2002).

[2] L. D. Barnes, S. J. Gilbert and C. M. Surko, Phys. Rev. A. **67**, 032706 (2003).

[3] G. F. Gribakin, Nucl. Instrum. and Methods B **192**, 26 (2002).