Erratum: Treatment of resonances in the scattering of a heavy positron by H_2 that are due to interaction with vibrationally excited quasibound states [Phys. Rev. A 82, 042702 (2010)]

E. A. G. Armour*

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In the published paper, I carried out a detailed, *ab initio* treatment of resonances in positron H_2 scattering, using the Kohn variational method. Such resonances have been observed in, for example, positron scattering by methyl halides [1,2]. Because a positron does not form a bound state with H_2, I increased the mass of the positron until it formed a very weakly bound state in this case. I stated that the resulting expression for the resonant contribution to $Z_{\text{eff}}(k)$ from a quasibound state was infinite when the resonance condition was satisfied.

I now realize that this was due to a mistake in my calculation. In this erratum, I correct this error. This makes it possible to calculate a width for the resonance in my treatment. This is compared with the width obtained by Gribakin and Lee [2], using the Breit-Wigner formula. The fact that all the Kohn coefficients tend to infinity at the resonance and not just d_1, the coefficient of the resonant quasibound state, was not taken into account in the paper. It is shown to follow from this that all the basis functions except the entrance channel function Ψ_{0a}, which has coefficient unity, contribute to $Z_{\text{eff}}(k)$ at the resonance, and not just the quasibound state whose energy is close to that of the system at the resonance.

Correction to my treatment. The Kohn equations are of the form given in Eq. (17) in the paper. x is a column vector containing the coefficients$\{x_i\}$ of the basis functions in the trial function that are to be determined, i.e., all the basis functions except the function Ψ_{0a}, which has asymptotic form as given in Eq. (13) in the paper.

It follows from Cramer's rule that

$$x_i = \frac{\det(A_{C,i})}{\det(A)}, \tag{1}$$

where $A_{C,i}$ is the matrix formed by replacing the ith column of A by $-b$. A is a $p \times p$ matrix, where p is the number of basis functions in the trial function other than the entrance channel function Ψ_{0a}. The order of the basis functions is adjusted so that the quasibound state of interest has a coefficient equal to x_p. Since this quasibound state is taken to be the lowest in energy, I denoted its coefficient by d_1, where the letter d was used to label the coefficients of the N_r quasibound states. It follows that $d_1 = x_p$.

Applying Cramer's rule and dividing the numerator and denominator of the resulting expression by A'_{pp}, where A'_{pp} is the cofactor of the element A_{pp} of the matrix A, we obtain

$$d_1 = -\frac{(\langle\Psi_{nr}|\hat{F}|\Psi_{0a}\rangle + \langle\Psi_{\text{lep},0}\chi_{01}|\hat{F}|\Psi_{0a}\rangle)}{\frac{1}{\mu_M}\langle\Psi_{nr}|\zeta_1+\omega_1\rangle + \left(E_{01} - E + \frac{1}{\mu_M}\langle\Psi_{\text{lep},0}\chi_{01}|\omega_1\rangle\right)}, \tag{2}$$

where the quantities on the right-hand side are as defined in the paper. Note that it is shown in the Appendix in the paper that the coefficients $\{g_i\}_{i=1}^{p-1}$ in Ψ_{nr} are such that $\langle\Psi_{nr} + \Psi_{\text{lep},0}\chi_{01}|\hat{H}_{\text{c.m.}} - E|\Psi_{nr} + \Psi_{\text{lep},0}\chi_{01}\rangle$ is stationary for variations of these coefficients.

The value of $Z_{\text{eff}}(k)$ is given by Eq. (31) in the paper. It follows that the contribution to $Z_{\text{eff}}(k)$ from the diagonal δ-function matrix element containing the resonant quasibound state $\Psi_{\text{lep},0}\chi_{01}$ under consideration is of the form

$$|B|^2 d_1^2 \langle\Psi_{\text{lep},0}\chi_{01}|\sum_{i=2}^{3}\delta(\mathbf{r_1}-\mathbf{r_i})|\Psi_{\text{lep},0}\chi_{01}\rangle.$$

As was pointed out in the paper, setting the denominator of the expression for d_1 in Eq. (2) equal to zero gives rise to an energy condition associated with a resonance. From the method used to obtain the expression for d_1 above, it follows that this denominator is equal to $\frac{\det(A)}{A'_{pp}}$. Since we are assuming that A'_{pp} is nonzero, it follows that if the resonance condition is satisfied, $\det(A) = 0$. Thus all the coefficients $\{x_i\}_{i=1}^{p}$, and not just $d_1 = x_p$ as stated in the paper, are infinite when the resonance condition is satisfied. Thus all basis functions, except Ψ_{0a}, will contribute to the resonance.

The case when $\det(A)$ is zero when applying the Kohn method is well documented; see [3,4]. This singular behavior is normally considered to be unphysical. In this case, it is physical because it is brought about by the existence of a quasibound state with energy close to the energy of the resonance. When $\det(A)$ is zero, in general no solution to the Kohn equations exists. However, a unique solution exists when $\det(A)$ is as close to zero as we please; see [4].

The fact that all the coefficients are infinite has two important consequences. First, $Z_{\text{eff}}(k)$ is finite at the resonance and exhibits behavior similar to that predicted by the Breit-Wigner formula in the vicinity of the resonance. Second, all basis functions except Ψ_{0a} contribute to the resonance.

Finite form of $Z_{\text{eff}}(k)$. The form of the normalization constant B in the expression for $Z_{\text{eff}}(k)$ was not considered in the paper. It is such that the zero angular momentum partial wave has the appropriate coefficient for an incident positron beam with one particle per unit volume. For this to be the case, the open-channel functions representing the positron beam and the associated cosine wave function must be expressible asymptotically in the form $(\frac{\sin(kr_1)}{kr_1} + \frac{\alpha\exp(kr_1)}{kr_1})\Psi_{\text{target}}$, where α is a constant. Thus

$$B = \frac{\sqrt{4\pi}}{1 - ia_{11}}, \tag{3}$$

where $a_{11} = x_1$ is the coefficient of the associated open-channel cosine wave function. It follows that the

*edward.armour@nottingham.ac.uk

contribution to $Z_{\text{eff}}(k)$ from the diagonal δ-function matrix element containing the resonant quasibound state, $\Psi_{\text{lep},0}\chi_{01}$, under consideration is of the form

$$\frac{4\pi[\det(A)]^2}{[\det(A_{C,1})]^2+[\det(A)]^2} d_1^2 \langle \Psi_{\text{lep},0}\chi_{01}| \sum_{i=2}^{3} \delta(\mathbf{r_1}-\mathbf{r_i})|\Psi_{\text{lep},0}\chi_{01}\rangle.$$

When $\hat{F}$ operates on Ψ_{0a} it is convenient to replace it, as in the paper, by V_p, the potential between the positron and the target. Now the denominator in the expression for d_1 in Eq. (2) is equal to $\frac{\det(A)}{A'_{pp}}$. Thus the contribution to $Z_{\text{eff}}(k)$ involving only the resonant quasibound state is of the form

$$4\pi \left[\frac{(\langle \Psi_{nr}+\Psi_{\text{lep},0}\chi_{01}|V_p|\Psi_{0a}\rangle)^2}{\left[\frac{1}{\mu_M}\langle\Psi_{nr}|\zeta_1+\omega_1\rangle + \left(E_{01}-E+\frac{1}{\mu_M}\langle\Psi_{\text{lep},0}\chi_{01}|\omega_1\rangle\right)\right]^2 + D^2} \right] \langle \Psi_{\text{lep},0}\chi_{01}|\sum_{i=2}^{3}\delta(\mathbf{r}_1-\mathbf{r}_i)|\Psi_{\text{lep},0}\chi_{01}\rangle,$$

where $D = \frac{\det(A_{C,1})}{A'_{pp}}$ and thus

$$D = -\langle \Psi_{1r}+\Psi_{0b}|V_p|\Psi_{0a}\rangle \frac{A'_{11}}{A'_{pp}}, \tag{4}$$

where

$$\Psi_{1r} = w_2\Psi_{0c} + \sum_{i=3}^{N+2} w_i\phi_{i-2} + \sum_{i=N+3}^{p} w_i \Psi_{\text{lep},0}\chi_{0j} \quad (j=i-N-2), \tag{5}$$

and

$$w_i = \frac{A'_{i1}}{A'_{11}} \qquad (A'_{11}\neq 0). \tag{6}$$

It can be shown in a way similar to that used in the case of $\{g_i\}_{i=1}^{p-1}$ that the choice of $\{w_i\}_{i=2}^{p}$ imposes the condition that the resulting wave function $\Psi_{1r}+\Psi_{0b}$ is such that $\langle\Psi_{1r}+\Psi_{0b}|\hat{H}_{\text{c.m.}}-E|\Psi_{1r}+\Psi_{0b}\rangle$ is stationary with respect to variations of the $\{w_i\}_{i=2}^{p}$.

Comparing the denominator in this expression with the denominator in the Breit-Wigner formula, we can see that $2|D|$ can be interpreted as the width of the resonance brought about by the quasibound state at the energy value that makes the other term in the denominator zero. This contribution is closer to the Breit-Wigner form used by Gribakin and Lee [2] than the incorrect form for this contribution given in the published paper. The form of the width in my treatment differs from its form in [2]. It contains a V_p matrix element as a factor, together with the $\frac{A'_{11}}{A'_{pp}}$ factor. Gribakin and Lee's form is quadratic in V_p. Also the wave function on the left side of the matrix element in my treatment is $\Psi_{1r}+\Psi_{0b}$, whereas in [2] it is the resonant quasibound state. Ψ_{1r} contains the resonant quasibound state $\Psi_{\text{lep},0}\chi_{01}$ but it also contains all the basis functions in the trial function, except Ψ_{0a} and Ψ_{0b}. We have calculated above the contribution to the resonant value of $Z_{\text{eff}}(k)$ that comes from the quasibound state $j=1$ itself. However, in my treatment all other functions in the wave function, except Ψ_{0a}, will also contribute resonantly to the value of $Z_{\text{eff}}(k)$. In addition to diagonal contributions involving only one such basis function, there will be contributions from all possible cross terms involving two basis functions other than Ψ_{0a}.

The Breit-Wigner formula implies that the dominant contribution to $Z_{\text{eff}}(k)$ in the vicinity of the resonance comes from the resonant quasibound state with $j=1$. This would be the case in my treatment if $|\frac{d_1}{x_i}|$ was large in this region if $i\neq p$. I am unable to prove this. What I can do is prove a corresponding stationary result for any basis function, other than Ψ_{0a}, to the stationary result that I proved earlier for $\Psi_{0,\text{lep}}\chi_{01}$ in the paper. This states that for any basis function η_i (say), other than Ψ_{0a}, $\langle\Psi_{ir}+\eta_i|\hat{H}_{\text{c.m.}}-E|\Psi_{ir}+\eta_i\rangle$ is stationary with respect to variations of the coefficients in Ψ_{ir}. Ψ_{ir} is a linear combination of all the basis functions, except Ψ_{0a} and η_i, with coefficient v_l equal to $\frac{A'_{li}}{A'_{ii}}$. The proof is similar to the proof given in the paper for the case when η_i is the wave function of the quasibound state with $j=1$. The numerator of the expression for the coefficient x_i is

$$-\langle\Psi_{ir}+\eta_i|V_p|\Psi_{0a}\rangle\frac{A'_{ii}}{A'_{pp}},$$

and the denominator is as in Eq. (2).

Conclusion. I have corrected a mistake in the published paper. This makes it possible to show that $Z_{\text{eff}}(k)$ is not infinite when the resonance condition is satisfied. In the vicinity of the resonance, it has a form similar to the Breit-Wigner form. However, the expression for the width of the resonance is not the same as in the Breit-Wigner formula [2]. It is shown that all basis functions except the entrance channel Ψ_{0a} and not just the resonant quasibound state $\Psi_{\text{lep},0}\chi_{01}$, as stated in the paper, contribute to $Z_{\text{eff}}(k)$ at the resonance. Finally, I point out that a result proved in the paper for the basis function $\Psi_{\text{lep},0}\chi_{01}$ can be extended to all basis functions except Ψ_{0a}.

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