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Erratum to "Determination of Non–Adiabatic Scattering Wave Functions in a Born–Oppenheimer Model"

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We correct some typographical errors and mistakes in the published paper [1]. We freely use the paper's notation and equation numbering.

In Section 4, on the scattering properties of exact solutions to the molecular Schrödinger equation, we used too rough a definition of asymptotic states. We need to consider

$$\begin{aligned}\psi^{\sigma}(x,t,\epsilon,\pm)&\\ &= \sum_{j=1,\cdots,m} \phi_j(x) \int_\Delta \frac{Q(E,\epsilon)}{\sqrt{2k_j(\pm\infty,E)}}\, e^{-itE/\epsilon^2}\, c_j^{\sigma}(\pm\infty,E,\epsilon)\\ &\qquad\qquad \times e^{-i(xk_j^{\sigma}(\pm\infty,E)+\omega_j^{\sigma}(\pm\infty,E))/\epsilon^2}\, dE,\end{aligned}$$

instead of $\psi(x,t,\epsilon,\pm) = \sum_{\sigma=\pm} \psi^{\sigma}(x,t,\epsilon,\pm)$. With this definition, Proposition 4.1 should be replaced by

Proposition 4.1′ *Assume* **H1**, **H2**, **H3** *and* **C0**. *Then, for any* $0 < \beta < 1/2$, *we have the following* $L^2(I\!R)$*–norm estimate as* $t \to \pm\infty$,

$$\|\, \psi(x,t,\epsilon) \,-\, (\psi^-(x,t,\epsilon,\pm) + \psi^+(x,t,\epsilon,\mp))\,\| \;=\; O_\epsilon(1/|t|^{\beta}).$$

In eqn. (4.4), "$\psi(x,t,\epsilon,-) =$" should be replaced by "$\psi^-(x,t,\epsilon,-) \simeq$," and the qualification "for negative x's" should be added. Similarly, in the next sentence, the stipulation "for positive x's" should be added.

The proof of Proposition 4.1 should be amended as follows:
Equation (7.14) should begin with

$$\psi(x,t,\epsilon) - \psi^{\sigma}(x,t,\epsilon,\pm) = \sum_{j=1,2} \phi(x)\times$$

instead of "$\psi(x,t,\epsilon) - \psi(x,t,\epsilon,\pm) = \sum_{j=1,2\;\sigma=\pm} \phi(x)\times$," and every $L^2(I\!R)$ should be replaced by $L^2(I\!R^{\pm})$, where $I\!R^{\pm} = \{x \in I\!R : \pm x > 0\}$.

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At the end of the proof, one should add the sentence:
If $x \in I\!\!R^{\mp}$ and $\mathrm{sign}(t) = \mp\sigma$, one integrates by parts as in (7.12), and one uses

$$\left| t + \int_0^x k_j^\sigma(y, E)\, dy \right| \;\geq\; c\,(|t| + |x|) \;\geq\; c\,|t|^{\beta'}\,|x|^{1-\beta'},$$

for all $0 < \beta' < 1$, to bound the corresponding $L^2(I\!\!R^{\mp})$ norms by constants times $|t|^{-\beta}$, with $0 < \beta < 1/2$.

Consequently, the statement of Theorem 5.1 should be amended as follows:

A The first equation should read

$$\lim_{t\to-\infty} \|\, \psi(x,t,\epsilon) \;-\; \psi_j^-(x,t,\epsilon,-)\,\|_{L^2(R^-)} \;=\; 0,$$

instead of "$\lim_{t\to-\infty} \|\, \psi(x,t,\epsilon) - \psi_j^-(x,t,\epsilon,-)\,\| = 0$," and it should be followed by the qualification "for negative x's."

B The sentence before equation (5.8) should begin: *Then, there exist $\delta_0 > 0$, $p > 0$ arbitrarily close to 5/2, and a function $\epsilon_0 : (0,\delta_0) \to I\!\!R^+$, such that for all $0 < \beta < 1/2$, $\delta < \delta_0$, and $\epsilon < \epsilon_0(\delta)$, the following asymptotics hold as $t \to \infty$:*

C Finally, each occurrence of $O_\epsilon(1/t)$ should be replaced by $O_\epsilon(1/t^\beta)$.

As indicated in **B**, p is arbitrary close to 5/2 instead of 3, as previously erroneously stated. This comes from a missing square root in the computation of the $L^2(I\!\!R)$ norm of the error terms in the last paragraph of page 987. They should read $O(e^{-\alpha(E^*)}\,\epsilon^{1+3s/2})$ and $O(e^{-\alpha(E^*)}\,\epsilon^{7s/2-1})$ instead of $O(e^{-\alpha(E^*)}\,\epsilon^{1+2s})$ and $O(e^{-\alpha(E^*)}\,\epsilon^{4s-1})$. Keeping track of the consequences of this correction, one sees that p is arbitrarily close to 5/2. This change should also be made in Lemma 5.1 and Lemma 5.2.

Finally, due to a miscalculation, formula (5.10) in Lemma 5.1 must be simplified to

$$\begin{aligned} T(\epsilon,x,t) \;&=\; \epsilon\,\sqrt{2\pi k^*}\; P(E^*,\epsilon)\; e^{-\alpha(E^*)/\epsilon^2} \\ &\qquad\times \frac{\exp\left\{-i\frac{(tE^*+\kappa(E^*)-xk^*)}{\epsilon^2}\right\}}{\left(\frac{d^2}{dk^2}\alpha(E(k))|_{k^*} + i(t+\frac{d^2}{dk^2}\kappa(E(k))|_{k^*})\right)^{1/2}} \\ &\times \exp\left\{-\frac{(x-k^*(t+\kappa'(E^*)))^2}{2\epsilon^2\left(\frac{d^2}{dk^2}\alpha(E(k))|_{k^*} + i(t+\frac{d^2}{dk^2}\kappa(E(k))|_{k^*}\right)}\right\} \;+\; O(e^{-\alpha(E^*)/\epsilon^2}\,\epsilon^p). \end{aligned}$$

This leads to a simplification of Lemma 5.2: Only the second statement should be kept, and the error term $O(\epsilon^{3/2}/|t|)$ should be removed.
This mistake came from the incorrect computation of the Gaussian integral at the end of the proof of Lemma 5.1. It should read, $\int_{-\infty}^{\infty} e^{-(M(k-k^*)^2/2+iN(k-k^*))/\epsilon^2}dk = \epsilon\,\sqrt{\frac{2\pi}{M}}\; e^{-\frac{N^2}{2\epsilon^2 M}}$ (for Re $M > 0$).

References

[1] G.A. Hagedorn and A. Joye, Determination of Non–Adiabatic Scattering Wave Functions in a Born–Oppenheimer Model, *Ann. Henri Poincaré* **6** (2005), 5, 937–990.

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