Comment on "Full Ambiguity-Free Quantum Treatment of $D^+ + H(1s)$ Charge Transfer Reactions at Low Energies"

Recently, Igarashi and Lin [1] proposed the two-state hyperradial-adiabatic (HA) approximation to calculate $D^+ + H(1s)$ charge transfer reactions at low energies. Here we demonstrate that the authors had overestimated the power of their approach if compared even with the already existing two-state Born-Oppenheimer (BO) adiabatic calculations [2,3] of the same reactions. Some conclusions from [1] are erroneous and some of them are misleading. Here are two examples from the abstract: (a) "The method is free from all the inherent ambiguities associated with the conventional BO approach, such as ... spurious couplings." That is wrong; the residual nonphysical couplings in the HA approach were pictured in our recent paper [4]. (b) "However, like the BO approach, we show that hyperspherical potential curves and coupling terms have to be calculated only once to obtain results for all partial waves." This conclusion is misleading, as we demonstrate below.

As in [1], we choose the Jacobi coordinates (masses) to be $\mathbf{R}$ and $\mathbf{r}$; and define the hyperradius $\rho = [R^2 + (m/M)r^2]^{1/2}$.

The two lowest HA potential curves used in [1] have a strong unphysical attraction in the $\rho \to \infty$ limit {$\hbar = m = e = 1$ units are introduced}:

$$\epsilon^{\mathrm{HA}}_{1\{2\}} = -\frac{1}{2}\,\mu_{\mathrm{D\{H\}}} - \frac{9}{4M}\,\frac{1}{\rho^2} + \ldots . \qquad (1)$$

This behavior disappears when we form the effective potentials with diagonal nonadiabatic corrections [5]

$$v^{\mathrm{HA}}_i = \epsilon^{\mathrm{HA}}_i - \frac{w_{ii}(\rho)}{2M} - \frac{15}{8M\rho^2}\,, \qquad (2)$$

where $w_{ij}(\rho) = \langle i|d^2/d\rho^2|\,j\rangle$. Though Igarashi and Lin [1] are explicitly discussing only the nonadiabatic coupling term $\langle i|d/d\rho|\,j\rangle$, the full close coupling scheme providing (2) has been used [6].

Similarly with (2), on utilizing the two-state BO approximation [2,3] for the same reaction and matching the boundary conditions we get instead of (2) for the asymptotics of the effective potentials {$\kappa = (m_{\mathrm{D}^+} - m_{\mathrm{H}^+})/(m_{\mathrm{D}^+} + m_{\mathrm{H}^+})$ and $\alpha = 1/(4M)$}

$$v^{\mathrm{BO}}_{1\{2\}}(R) = -[1 - \alpha(1 \mp \kappa)^2]/2 + O(1/R^4)\,. \qquad (3)$$

This expression provides for the energy splitting $v^{\mathrm{BO}}_2(\infty) - v^{\mathrm{BO}}_1(\infty) = 3.702$ meV. That is, no "great deal of effort is needed in order to obtain the energy difference 3.7 meV between the $D^+ + H(1s)$ limit and $H^+ + D(1s)$ limit" for both the approaches.

Starting with (b) we note though that Igarashi and Lin [1] are trying to validate the "rotor model," i.e., using the $J = 0$ coupling for all total angular momenta J, "as one would do in the BO approach." But this door is open: Matveenko and Abe [7] have shown that a BO-like total three-body Hamiltonian can be exactly transformed into its HA-like counterpart by the operator that commutes with the Coriolis coupling operator so that the structure of the neglected angular coupling terms is identical in the two approaches. The adiabaticity m/M factor itself is regulating the accuracy.

Recently [8], we have introduced symmetry adapted hyperspherical adiabatic formalism and were able to resolve analytically the Coriolis couplings neglected in [1–3]. Here we just note the very direct by-product of that analytic procedure: the centrifugal effective potential turns to be governed by a $J(J + 4)$ factor, in contrast with the factor $J(J + 1)$ common to [1–3].

In summary, both the HA (1) and (2) and BO (3) adiabatic schemes include spurious couplings which are getting more reasonable when nonadiabatic corrections are taken into account (Matveenko and Fukuda [4]). For extreme adiabatic problems, like the reactions $D^+ + H(1s) \to H^+ + D(1s)$ at low energies, similar approximation should provide roughly the same reasonable accuracy for both cases [1–3], as the neglected terms are governed by a rather small parameter $m/M \sim 10^{-3}$. Thus, for example, using the two-state BO approximation [2] Matveenko was able to calculate and explain the oscillatory structure of the total transfer cross sections reproduced later [1] in the two-state HA approximation.

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