Comment on "Dominant Photodetachment Channels in H^-"

Harris *et al.*[1] have reported the observation of high-lying $^1P^\circ$ ($N=3$–8) resonances in H^- by direct photoionization. Sadeghpour and Greene[2] (SG) were able to calculate the positions of these resonances approximated as bound states in adiabatic hyperspherical potentials. Despite the number of adiabatic potentials converging to each N threshold only states in the lowest-lying curve are populated in the experiment. Consequently, SG propose as part of a propensity rule for photoabsorption from the ground state the requirement $\Delta v=0$, where v is a semiempirical quantum number introduced to quantify the excitation of the bending mode in analogy to a triatomic molecule.[3] SG attribute the propensity rule to the nodal structure of the states, more precisely to the presence of nodes in the interelectronic angle θ_{12}. In the adiabatic wave functions (Fig. 1) they connect directly the quantum v with excitation along the coordinate θ_{12}: "*... where v is the bending vibrational quantum number..., namely, the number of nodes in* θ_{12}."

We would like to point out that their adiabatic two-electron densities (Fig. 1) show a θ_{12} nodal pattern (which would correspond to straight lines parallel to the α axis) only in the region $\alpha/\pi \approx 1/4$. The overall nodal structure is much better described by nodal lines of spheroidal coordinates (λ,μ) which are visualized in Fig. 1. In these coordinates, for fixed interelectronic distance R, the two-electron motion is separable in $\lambda=(r_1+r_2)/R$ and $\mu=(r_1-r_2)/R$, where r_1,r_2 are the electron-nucleus distances. In the molecular-orbital picture this separability is used to classify doubly excited states with quantum numbers n_λ,n_μ.[4,5] In addition, it is evident from the figure that there are well-defined nodal lines, not identified by SG, which correspond to excitation in the μ coordinate. The electron densities displayed in Fig. 1 follow in *shape* and *number* the (n_λ,n_μ) classification.

We conclude that the bending vibrational quantum v is represented by nodes in λ, i.e., $v\equiv n_\lambda$. The propensity rule for photoabsorption is therefore more precisely given by $\Delta n_\lambda=0$.[5]

In the future it will be interesting to combine the numerical accuracy of the hyperspherical approach in the determination of resonance positions[2] with the information on the quasiseparability of the dominant part of resonant wave functions provided by the molecular approach.

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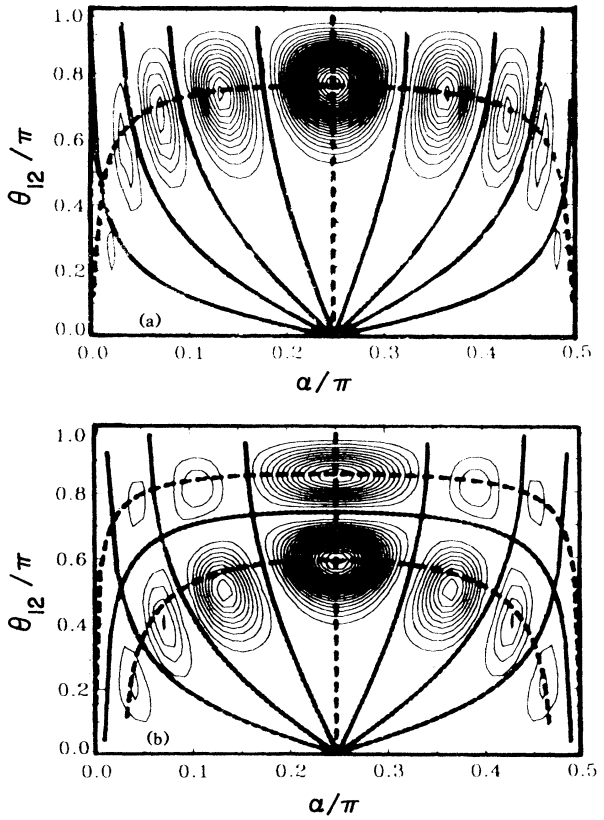

FIG. 1. Contour plot of adiabatic two-electron densities taken from Ref. 2. The nodal (solid) and antinodal (dashed) lines of constant λ and μ are overdrawn for (a) the state with $(n_\lambda n_\mu)=(0,8)$ and (b) the state with $(n_\lambda n_\mu)=(1,6)$.

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[1]P. G. Harris, H. C. Bryant, A. H. Mohagheghi, R. A. Reeder, H. Sharifian, C. Y. Tang, H. Tootoonchi, J. B. Donahue, C. R. Quick, D. C. Rislove, W. W. Smith, and J. E. Stewart, Phys. Rev. Lett. **65**, 309 (1990).

[2]H. R. Sadeghpour and C. H. Greene, Phys. Rev. Lett. **65**, 313 (1990).

[3]D. E. Herrick, Adv. Chem. Phys. **52**, 1 (1983).

[4]J. M. Feagin and J. S. Briggs, Phys. Rev. A **37**, 4599 (1988).

[5]J. M. Rost and J. S. Biggs, J. Phys. B **23**, L339 (1990).