# A SEMICLASSICAL DIRECT POTENTIAL FITTING SCHEME FOR DIATOMICS

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For decades the standard procedure for obtaining diatomic potential curves from spectroscopic data involved fitting the data to expressions for the vibrational energy $G_v$ and rotational constant $B_v$ as functions of the vibrational quantum number $v$, and then employing the RKR method to compute potential curves from these. Within the first-order semiclassical formalism of RKR, this "inversion" procedure is exact. However, the resulting potentials are limited in their quantum mechanical reliability, as has been demonstrated frequently by using the numerical Numerov method to compute the quantal properties of the potentials and comparing these with the starting spectroscopic information. A particularly troubling region is the repulsive wall of the potential near dissociation, where RKR curves often show unphysical wiggles and flares. Such behavior has generally been attributed to limitations inherent in the $G_v/B_v$-to-potential construct; by extension, such limitations are similarly responsible for some of the RKR-quantal disparities in other regions of the potential.

In recent years this procedure has begun to be replaced by methods in which the potential curves are the directly fitted quantities in the least-squares analysis of the data, and the so-derived potentials often match the precision of the input data. The question naturally arises, how good might semiclassical methods be in a similar approach? Since the semiclassical calculations are two orders of magnitude faster than the quantal, they might be better than RKR for obtaining approximate potentials and could aid in deciding matters such as best functional forms and appropriate numbers of adjustable parameters. In this paper I will discuss tests of a semiclassical direct potential fitting method.