

Rotational structure of weakly bound molecular ions

Mikhail Lemeshko* and Bretislav Friedrich*

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

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Abstract. Relying on the quantization rule of Raab and Friedrich [Phys. Rev. A 80 (2009) 052705], we derive simple and accurate formulae for the number of rotational states supported by a weakly bound vibrational level of a diatomic molecular ion. We also provide analytic estimates of the rotational constants of any such levels up to threshold for dissociation and obtain a criterion for determining whether a given weakly bound vibrational level is rotationless. The results depend solely on the long-range part of the molecular potential.

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1 Introduction

Molecular systems bound by a potential which varies asymptotically with the inverse power of the distance, r , between their constituents

$$V(r) \stackrel{r \rightarrow \infty}{\sim} -\frac{C_n}{r^n} \quad \text{with } n > 2 \quad (1)$$

are amenable to an accurate analytic semiclassical (WKB) treatment, as long as the system's states are sufficiently ensconced within the potential energy well. However, for states near threshold for dissociation, the WKB approximation fails, as the system's classical action, proportional to momentum, no longer exceeds Planck's constant. And yet, it is the near-threshold states that have come to the fore recently, through the work in cold-atom physics where such states arise in photo- and magneto-association [1–3] or

*Corresponding author. *Email address:* lemeshko@fhi-berlin.mpg.de (M. Lemeshko); brich@fhi-berlin.mpg.de (B. Friedrich)

other types of “assisted” collisions of (ultra) cold atoms [4] or atomic ions [5–8]. Therefore, a considerable effort has been expended at amending the WKB approximation to also allow for tackling near-threshold states analytically. A leading approach is that of H. Friedrich *et al.*, who showed that, firstly, the bound-state eigenenergies, E_b , can be expressed in terms of the quantization function, $F(E_b)$ [9], which relates the state’s integral quantum number v to the generally non-intergral quantum number, v_{th} , of a state exactly at threshold, via

$$F(E_b) = v_{th} - v. \quad (2)$$

Secondly, they were able to find an explicit analytic form of the quantization function for attractive inverse-power potentials with $n = 6$ [10, 11], and, most recently, with $n = 4$ [12]. Note that the binding energy, $E_b = D - E_v$, with D the dissociation energy and E_v the energy of the vibrational level v , is thus positive, $E_b > 0$.

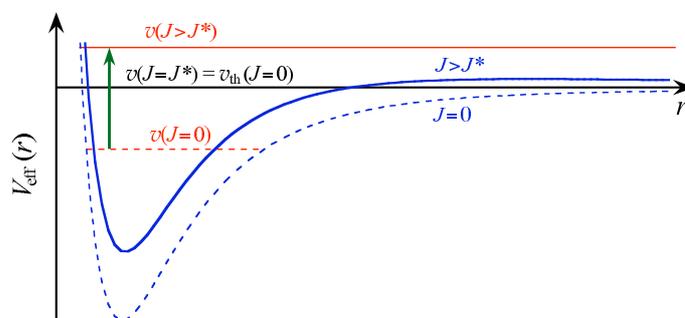


Figure 1: (Color online) A schematic illustrating the role of the centrifugal term in the effective potential, $V_{\text{eff}}(r) = -\frac{C_4}{r^4} + \frac{\hbar^2}{2m} \frac{J(J+1)}{r^2}$. The energy splittings have been exaggerated for clarity. Shown is the position of a rotationless vibrational level, $v(J=0)$ (dashed line), as well as the position of the same level when pushed up by the centrifugal term to threshold, $v(J=J^*) = v_{th}(J=0)$ (full line, at threshold). When the rotational angular momentum J exceeds the critical value J^* , the centrifugal term pushes the vibrational level above threshold, $v(J > J^*)$ (full line, above threshold), thus leading to dissociation.

In our previous work [13], we have shown that for each vibrational level, v , the rotational angular momentum, J , can take a critical value, J^* , such that the vibrational level is pushed up to threshold, thereby causing the level’s binding energy to vanish. Hence the angular momentum J in excess of J^* , $J > J^*$, dissociates the molecule, cf. Figure 1. Furthermore, we have shown that the critical angular momentum is related to the quantization function by

$$J^* = F(E_b)(n-2). \quad (3)$$

The corollary of Eq. (3) is that the number of rotational states supported by a weakly bound vibrational level of a dimer is given by the integer part of the critical angular momentum, $J_{max} = \text{Int}[J^*]$. By making use of the explicit form of the quantization function of refs. [10, 11] for $n = 6$, we were able to evaluate J^* and estimate the rotational constant B for near-threshold states of $^{85}\text{Rb}_2$.