Scattering of rotating molecules through an aperture: a simple quantum mechanical model

Piroska Dömötör,[1,*] Péter Földi,[1] Mihály G. Benedict,[1] Bruce W. Shore,[2] and Wolfgang P. Schleich[3]

[1]*Department of Theoretical Physics, University of Szeged, H-6720 Szeged, Hungary*
[2]*618 Escondido Circle, Livermore, CA 94550, USA*
[3]*Institut für Quantenphysik Universität Ulm, Albert-Einstein-Allee 11, D-89069 Ulm, Germany*

Scattering of a quantum particle with internal structure is fundamentally different from that of a point particle. We consider a two-dimensional model of a rotating diatomic molecule traveling through a small aperture in a thin but impenetrable screen. The centre-of-mass is constrained to

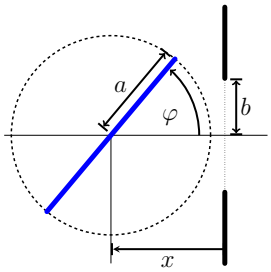

FIG. 1. Geometry of the symmetric rotor.

move along the symmetry axis of the aperture, resulting in entanglement between the position and the orientation angle of the rotating object. We turn this geometrical model into a *two-dimensional stationary scattering problem* by requiring that the energy eigenfunction should vanish for classically forbidden rotor orientations (Figure 2 gray region).

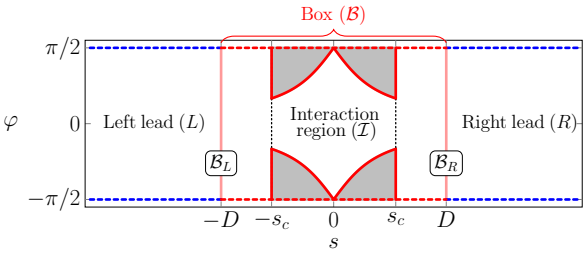

FIG. 2. The two-dimensional Interaction region $\mathcal{I}$ resulting from the constraints. Shape and size is determined by the aperture-to-length ratio and mass distribution of the rotor. The artificial $\mathcal{B}$ box containing $\mathcal{I}$ connects to leads of free traveling modes.

Far away from the Interaction region $\mathcal{I}$ we have well defined ϕ_m rotational mode functions in the leads. The stationary wavefunction for each mode has asymptotic forms:

$$\left\langle s,\phi_m \mid \Psi_\varepsilon^L \right\rangle = c_m e^{ik_m s} + r_m e^{-ik_m s}, \quad \left\langle s,\phi_m \mid \Psi_\varepsilon^R \right\rangle = t_m\, e^{ik_m s}.$$

For non-rotating incident particles of low energy we obtain results by means of analytical approximations [1]. Starting from a suitable ansatz, we decouple the translational and rotational motions thereby obtaining a set of one-dimensional Schrödinger equations for the hindered translation with *effective potentials*. These effective potentials can be further approximated by a fictitious harmonic oscillator, eigenenergies of which provide us with a good qualitative picture of the possible resonances in transmission.

To verify our approximative result and to reach the full scope of the scattering problem, we use a method relying on the *Green's function* that solves the problem in a numerically exact way [2]. We make the problem finite by partitioning the Hilbert space into "Left lead + Box + Right lead" as indicated in Figure 2 and incorporate the effect of the leads in the domain of the Box by a *self-energy* correction $\mathbf{\Sigma}$ [3]:

$$\mathbf{G}^B(\varepsilon) = \left[\varepsilon \mathbf{1} - \mathbf{H}^B - \mathbf{\Sigma}(\varepsilon)\right]^{-1} \tag{1}$$

The S matrix and the wavefunction restricted to the Box can be calculated from $\mathbf{G}^B$. Additional quantities like the *density-of-states* $\mathcal{N}(\varepsilon)$ and the *local density-of-states* help us to determine energies where resonance effects may occur. We show that for incident waves of odd angular symmetry *quasi-bound states* appear for specific values of the parameters describing the geometrical situation. [2]

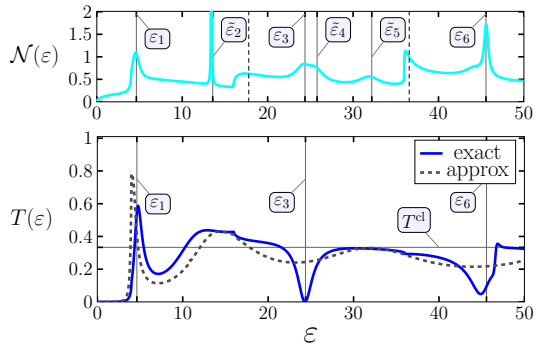

FIG. 3. Transmission as function of energy in case of $e^{ik_0 s}\, 1/\sqrt{\pi}$, "non-rotataing" incident wave compared to the DOS showing the possible resonance energies. The first resonance appears at the ground state energy of the fictitious oscillator.

* dpiri@physx.u-szeged.hu

[1] B. W. Shore, P. Dömötör, G. Süssmann, E. Sadurní, and W. P. Schleich, *New Journal of Physics* **17**, 013046, (2015)
[2] P. Dömötör, P. Földi, M.G. Benedict, B. W. Shore, W. P. Schleich, *New Journal of Physics* **17** 023044 (2015)
[3] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, 1995).