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On the Born-Oppenheimer Approximation of Wave Operators in Molecular Scattering Theory

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Abstract. In this paper we study the diatomic molecular scattering by reducing the number of particles through Born-Oppenheimer approximation. Under a non-trapping assumption on the effective potential of the molecular Hamiltonian we use semiclassical resolvent estimates to show that non-adiabatic corrections to the adiabatic (or Born-Oppenheimer) wave operators are small. Furthermore we study the classical limit of the adiabatic wave operators by computing its action on quantum observables microlocalized by use of coherent states.

1. Introduction

In this work, we are concerned with a mathematical study of the scattering process that a diatomic molecule dissociates into two ions. A direct mathematical study of this problem may be rather difficult, since the number of particles can be arbitrarily large. However, there is a folk-theorem in molecular scattering theory (see e.g. [Ch, De, WO]) that the contribution of electrons can be taken care of by effective potentials and the motion of nuclei can be well approximated by classical dynamics. This indicates that one can reduce the number of particles and thus considerably simplify the problem. This beautiful physical intuition dates back to Born-Oppenheimer [BO] and is based on the existence of a natural small parameter in molecular Schrödinger operators: the ratio of the mass of the electron to the mass of the nucleus. It is surprising to us that until now, there is no rigorous mathematical work on Born-Oppenheimer approximation in scattering theory, unless the attempt made in [Ra] where no quantitative result was given. Concerning mathematical works on Born-Oppenheimer approximation in spectral theory, the reader can track back from the reference quoted in [KMSW].

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