Energy Dependence of
the Scattering Operator II

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Abstract. We study the energy dependence of the scattering operator for a two-body model of electron scattering from a neutral molecule. We show that the methods of the first paper can be applied even though the dipole moment of the molecule is non-zero, and prove continuity of the scattering operator $S(E)$ as $E$ varies, in a very strong sense.

1. Introduction

We study the elastic scattering of an electron from a neutral molecule in the two-body approximation. That is, we study the scattering between $H = -\Delta$ and $K = H + V$ on $\mathcal{H} = L^2(\mathbb{R}^3)$, where

$$V(x) = \int \frac{1}{|x-y|} \mu(dy).$$

We assume that the charge distribution $\mu$ is a signed measure of finite total mass and zero net charge, that is

$$\int \mu(dy) = 0.$$

We also assume that the dipole moment $a$ of $\mu$, given by

$$a = \int y \mu(dy)$$

is non-zero, so that the potential $V$ has the asymptotic form

$$V(x) = \frac{a \cdot x}{r^3} + O(r^{-3})$$

at infinity, where $r = |x|$. To ensure that $a$ is finite we assume $\mu$ has support within $\{x: |x| \leq R\}$ for some $R < \infty$. Our methods could, however, easily cope with a charge distribution with exponential tails at infinity.

The potential $V$ is fairly well-behaved, and there are a variety of techniques [1, 7] which ensure that the wave operators between $H$ and $K$ exist and are complete. We are interested in studying the energy dependence of the scattering operator
in the following sense. We let \( \sim \) denote the unitary isomorphism of \( L^2(\mathbb{R}^3) \) with \( L^2((0, \infty), \mathcal{H}) \) defined by

\[
f'(E)(\omega) = 2^{-1/2} E^{1/4} f(E^{1/2} \omega),
\]

where \( \mathcal{H} = L^2(S^2), E \in (0, \infty), \omega \in S^2 \), and \( \hat{\cdot} \) denotes the Fourier transform. Since the scattering operator \( S \) commutes with \( H \), we have

\[
(Sf)\sim(E) = S(E)\hat{f}(E)
\]

for all \( f \in L^2(\mathbb{R}^3) \), where \( S(E) \) are unitary operators on \( \mathcal{H} \). We wish to determine the form of the operators \( S(E) \) and to show that they depend continuously on \( E \). Our main result is given in Theorem 10.

We start we reviewing some recent literature. There have been some papers \([2, 5, 6]\) proving finiteness of the total cross-section for similar problems. However since our potential \( V(x) = O(r^{-2}) \) at infinity, one does not expect the total cross-section to be finite for our problem. (This appears to be an open problem even for a pure dipole potential.) Even if the methods of \([2, 5]\) could be adapted to the present problem, they would not provide information about sharp energies, but only about the average behaviour of \( S(E) \) over small energy intervals.

Apart from \([4]\), the only method we know which provides pointwise information about the scattering operators \( S(E) \) is that of eigenfunction expansions. We refer to \([3]\), which includes the class of potentials we study here, and to \([1, p.421]\) and \([7, p.107]\) which do not apply to our class of potentials unless the dipole moment vanishes. All of these approaches have the disadvantage of involving a possible exceptional null set in \((0, \infty)\), because of the use of the Fredholm alternative, and do not yield results as sharp as those of Theorem 10. It is noteworthy that we do not have any exceptional set of energies in our approach, in spite of the fact that we do not eliminate the possibility of positive point spectrum, and make no use of the non-existence of singular continuous spectrum \([7]\).

The main limitation of our method is that we have to assume that the charge distribution has a non-trivial symmetry group. This implies that the quadrupole moment of the potential at infinity vanishes, which is absolutely essential for the application of trace-class methods. It would be very interesting to see analogous results without this condition.

The obvious way of dealing with our problem, and one which was in our minds throughout, would be to take

\[
H' = -\Delta + \frac{x \cdot a}{r^3}
\]

as the free Hamiltonian instead of \( H \). Note that \( H' \) is formally of degree \(-2\) under scaling, and the use of the scaling group is absolutely essential to our analysis, as in \([4]\). If the dipole moment is small enough, namely \(|a| < \frac{1}{4} \), then \( H' \) can be defined as a form sum and this approach can probably be carried out. However for larger values \(|a|\), \( H' \) is not even bounded below on \( C_\infty^\omega(\mathbb{R}^3 \setminus 0) \), so there is no possibility of developing a scattering theory between \( K \) and any self-adjoint extension of \( H' \). Interestingly, the approach we adopt does not have any obvious discontinuities as \(|a|\) increases.