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# The Twisting Trick for Double Well Hamiltonians

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**Abstract.** We show that the use of a twisting trick allows a transparent geometrical analysis of the spectral properties of double well Hamiltonians. In particular one can prove *norm* resolvent convergence of the relevant Hamiltonians whenever one has two centres of force whose separation $R$ diverges to infinity.

## 1. Introduction

Our goal in this paper is to rederive results of Aventini and Seiler [1], Combes and Seiler [2], Morgan and Simon [8], Harrell [5, 6], Harrell and Klaus [7], and many others concerning the spectral properties of double well Hamiltonians, by a method which we hope will be easy to understand. Although our method applies to the whole range of problems above, we spell out all the details only for one simple case, and make some remarks about further developments in Sect. 4.

We consider the Hamiltonian

$$H_R = -\Delta + A(x - Re) + B(x + Re)$$

on $L^2(\mathbb{R}^3)$ as $R \to \infty$, where $e = (0, 0, 1)$ and $A, B$ are potentials satisfying

(i) $A(H_0 + i)^{-1}$ and $B(H_0 + i)^{-1}$ are compact for $H_0 = -\Delta$,

(ii) $\|A\chi_{|x| \geqq R}\| + \|B\chi_{|x| \geqq R}\| \leqq cR^{-1}$ for large enough $R > 0$.

The second condition can certainly be weakened, but the form given already suffices for many problems in quantum chemistry.

It follows from (i) that the essential spectrum of $H_R$ (like that of $H_0$) equals $[0, \infty)$, so that its discrete spectrum consists of isolated negative eigenvalues of finite multiplicity with 0 as the only possible limit point. Our proposal is that one should study the discrete spectrum not of $H_R$ but of the self-adjoint operator

$$K_R = U_R \begin{bmatrix} H_R & 0 \\ 0 & H_0 \end{bmatrix} U_R^* \qquad (1)$$

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