

Double Wells*

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Abstract. Schrödinger operators with interactions symmetric about a plane (double-well potentials) occur in several branches of physics, such as chemistry and quantum field theory. They commonly exhibit asymptotic eigenvalue degeneracy, i.e., pairs of eigenvalues coalesce as the potential wells get farther apart. After a sketch of the theory of double wells, it is shown that the problem of estimating the gap between two such eigenvalues is reducible to finding asymptotics of eigenfunctions. For several examples and classes of potentials the gap is estimated or bounded above and below. The general case is fully n -dimensional.

I. Introduction

It is well known that if a potential $V(\mathbf{x})$ with two minima is symmetric under reflection through a plane (hyperplane, if $N > 3$), then the eigenvalues of the Schrödinger operator

$$-\Delta + V \quad \text{on} \quad L^2(\mathbb{R}^N) \quad (1.1)$$

tend to group in pairs (possibly after restriction to some symmetry subspace). In the simplest case, V has two equivalent, widely separated minima. The physical explanation for the grouping is that the particle evolving according to the Hamiltonian (1.1) could be localized near either well (minimum) in approximately the state it might be in if the second well did not exist. To some degree of accuracy there will be a two-fold degeneracy because of the possibility of being at either well. However, the presence of the second well has two weak effects, a) that the actual eigenstates must be even or odd about the central plane, in chemical language, they must be gerade (g) or ungerade (u); and b) that the degeneracy is split by the perturbation, making the antisymmetric state lie slightly above the

* Much of this work was done with support of an NSF National Needs Fellowship at the Department of Mathematics, M.I.T.