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INSTANTONS, DOUBLE WELLS AND LARGE DEVIATIONS

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ABSTRACT. We find the leading asymptotics of the exponentially small splitting of the two lowest eigenvalues of $-\frac{1}{2}\Delta + \lambda^2 V$ in the limit as $\lambda \to \infty$ where V is a nonnegative potential with two zeros.

In this note, we consider eigenvalues of a Schrödinger operator $-\frac{1}{2}\Delta + \lambda^2 V$ in the limit $\lambda \to \infty$ (which is quasiclassical since up to a factor of $\hbar^2$, $-\hbar^2\Delta + V$ has this form with $\hbar = \lambda^{-1}$ going to zero). The method can deal with eigenvalues other than the lowest, with multiple minima (even manifolds of minima) or degenerate minima. In this note, for simplicity we discuss only the two lowest eigenvalues, $E_0(\lambda)$ and $E_1(\lambda)$, with corresponding normalized eigenvectors $\Omega_0(\lambda)$, $\Omega_1(\lambda)$. More general situations and detailed proofs will appear elsewhere [**13**]. We will suppose the following about V. (i) V is C^∞, (ii) $V(x) \geq 0$ for all x and $\underline{\lim}_{|x|\to\infty} V(x) > 0$, (iii) V vanishes at exactly two points a and b and at these points $\partial^2 V/\partial x_i \partial x_j$ is strictly positive definite.

Under these circumstances, one can prove (see e.g. [**12**]) that ψ_0 is concentrated as $\lambda \to \infty$ near the points a, b and that $E_i(\lambda)/\lambda$ has a finite nonzero limit. We want also to suppose that for all ϵ small and for $y = a\, and$ for $y = b$

$$\underline{\lim}_{\lambda\to\infty} \int_{|x-y|\leq\epsilon} |\psi_0(\lambda, x)|^2 dx > 0. \tag{1}$$

One case where (1) holds is when there is a symmetry of order 2 (such as reflection) which leaves V and $-\Delta$ invariant, so that the limit is $\frac{1}{2}$ for $y = a$ or b.

Under these circumstances, one expects that the splitting of E_1 and E_0 will be governed by tunneling and one goal here is to obtain multidimensional

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tunneling results. A basic geometric object which will enter is the *Agmon metric* defined by

$$\rho(x,y)=\inf_{\gamma}\left(\int_0^1\sqrt{2V(\gamma(s))}|\mathring{\gamma}(s)|ds\,\middle|\,\gamma(0)=x,\gamma(1)=y\right) \tag{2}$$

that is the geodesic distance in the metric $2V(x)|dx|^2$. It is an elementary fact (see e.g. [**3**]) that

$$\rho(x,y)=\inf_{\gamma,T}\left(\frac{1}{2}\int_0^T\mathring{\gamma}(s)^2ds+\int_0^T V(\gamma(s))ds\,\middle|\,\gamma(0)=x,\gamma(T)=y\right). \tag{3}$$

One basic result is

THEOREM 1. *Under the above hypotheses on V (including (1))*

$$\lim_{\lambda\to\infty}\left\{-\frac{1}{\lambda}\ln|E_1(\lambda)-E_0(\lambda)|\right\}=\rho(a,b). \tag{4}$$

For the special case of one dimension (and for some slightly different multidimensional problems where the geodesic is a straight line), Harrell [**7**, **8**] has proven (4); indeed, he has obtained even more than the leading asymptotics. Combes et al. [**5**] has announced further results on the one-dimensional case. Our result here is the first rigorous result on leading asymptotics in intrinsically multidimensional double wells.

The geodesic from a to b parameterized to minimize (3) (the path must go from a at $t=-\infty$ to b at $t=\infty$) is called *an instanton* and that the instanton should control the splitting has been discussed in the theoretical physics literature for several years; see e.g. [**4**, **6**].

The Agmon metric was introduced by Agmon [**1**] (see also [**2** and **3**]) to discuss decay of eigenfunctions as $x\to\infty$ and it enters here also through decay of eigenfunctions. Indeed, Theorem 1 is proven using

THEOREM 2.

$$\lim_{\lambda\to\infty}\left\{-\frac{1}{\lambda}\ln\Omega_0(\lambda,x)\right\}=\min(\rho(x,a),\rho(x,b)) \tag{5}$$

where the limit is uniform on compact subsets of x. Moreover, for some R and $d>0$,

$$|\Omega_0(\lambda,x)|\le Ce^{-d\lambda|x|} \tag{6}$$

if $|x|>R$.

To prove Theorem 1, given Theorem 2, one uses

$$E_1-E_0=\inf\left(\int(\nabla f)^2\Omega_0^2\,dx\Big/\int f^2\Omega_0^2\,dx\right) \tag{7}$$

the inf being over all f with $\int f\Omega_0^2dx=0$. To get the upper bound in (4), we pick an f obeying this condition and $\int f^2\Omega_0^2=1$ (f is bounded by (1)), so that ∇f is concentrated in a neighborhood of the geodesic bisector (points with $\rho(x,a)=\rho(x,b)$) and then use Theorem 2 and the fact that $\rho(x,a)\ge\frac{1}{2}\rho(a,b)$

for any such x. We get the lower bound by looking at the contribution to (7) of a small tube about the geodesic from a to b using the fact that for any x on the geodesic, $\min(\rho(x,a),\rho(x,b)) \leq \frac{1}{2}\rho(a,b)$.

One can prove Theorem 2 by using the differential equation methods of Agmon [**2**] (see [**13**]). We prefer an alternative proof, which was our original one, which depends on *the method of large deviations*, a procedure of estimating asymptotics of path integrals [**14**]. Let $e^{-tH(\lambda)}(x,y)$ denote the integral kernel of the semigroup generated by $H(\lambda) \equiv -\Delta + \lambda^2 V$. Using the Feynman-Kac formula (see e.g. [**11**]) and thinking of Brownian motion as *formally* $\int d^\infty b\delta(b(0))e^{-\int \mathring{b}^2/2}$, we find after scaling that *formally*

$$\exp(-TH(\lambda)/\lambda)(x,y) \equiv \int d^\infty b\delta(b(0)-x)\delta(b(T)-y)\exp\left[-\frac{\lambda}{2}\int_0^T \mathring{b}^2(s)ds - \lambda\int_0^T V(b(s))ds\right].$$

This suggests the following result, which can be proven by the methods of Schilder [**10**] and Pincus [**9**].

THEOREM 3.

$$\lim_{\lambda\to\infty} -\lambda^{-1}\ln[\exp(-TH(\lambda)/\lambda)(x,y)] \equiv A(x,y;T)$$

where the limit is uniform on compact sets of x,y,T *and where*

$$A(x,y;T) \equiv \inf\left(\frac{1}{2}\int_0^T \mathring{\gamma}(s)^2 ds + \int_0^T V(\gamma(s))ds \,\middle|\, \gamma(0)=x, \gamma(T)=y\right).$$

The lower bound in (5) now follows by noting that

$$\Omega_0(\lambda,x) \geq \left[\min_{|y-a|\leq\epsilon} e^{-TH(\lambda)/\lambda}(x,y)\right]\int_{|y-a|\leq\epsilon}\Omega_0(\lambda,y)dy + \left[\min_{|y-b|\leq\epsilon} e^{-TH(\lambda)/\lambda}(x,y)\right]\int_{|y-b|\leq\epsilon}\Omega_0(\lambda,y)dy$$

and that $\lim_{T\to\infty} A(x,a;T) = \rho(x,a)$ (and similarly for b). The upper bound in (5) comes from

$$|\Omega_0(\lambda,x)|^2 \leq e^{TE_0(\lambda)/\lambda}e^{-TH(\lambda)/\lambda}(x,x)$$

and the interesting fact that

LEMMA.

$$\lim_{T\to\infty} A(x,x;T) \equiv \min(2\rho(x,a), 2\rho(x,b)).$$

SKETCH OF PROOF. When T is large, to prevent the potential term in the action from diverging, the path must go to a or b and sit near there for intermediate times and then return to x. □

The last statement in Theorem 2 also has a path integral proof.

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