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Semiclassical Analysis of Low Lying Eigenvalues. III. Width of the Ground State Band in Strongly Coupled Solids*

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A smooth periodic potential, V, with one minima per unit cell, is considered. Let $\Delta(\lambda)$ be the width of the ground state band for $-\Delta+\lambda^2 V$. It is rigorously proved that $\lim_{\lambda\to\infty} -\lambda^{-1}\ln\Delta(\lambda)$ is given by the minimum action among all instantons connecting two distinct minima of V. © 1984 Academic Press Inc.

Double well problems appear to be among the easiest tunneling problems to analyze in a rigorous mathematical manner, in part because it is easier to give precise meaning to an eigenvalue splitting than to a lifetime. The first mathematically rigorous treatment of the precise leading order behavior in a tunneling problem is Harrell's analysis [3] of one dimensional double wells. More recently, Simon [8, 9] obtained the leading order in certain multidimensional multiwell tunneling problems, and Helffer and Sjostrand [5] have even gone beyond leading order.

Harrell realized that widths of bands for strongly coupled periodic potentials are essentially a multiwell problem, and he analyzed such problems in one dimension if the potentials were both periodic and reflection invariant [4]. More recently, Keller and Weinstein [6] have analyzed the one dimensional problem without the reflection symmetry restriction. Our main goal in this note is to obtain the leading asymptotics in the multidimensional case. The proofs are an easy extension of those used in [9] to handle double wells; indeed, a special case of the situation in [9, Section 6.3], is a large box whose size is a multiple of the basic periods with periodic boundary conditions (discretizing momentum space). Because of the unbounded nature of R^n and the infinity of minima, there are some technical issues which we must (and will) handle.

We first describe our results and then sketch the proofs drawing heavily on the ideas and results of [9]. We will suppose that the potential V is smooth and has one minimum per unit cell. By adding a constant to V and shifting, we can without loss suppose $V\geqslant 0$ and $V(0)=0$. We will also suppose that the minimum is nondegenerate. Thus, our hypotheses are

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(1) V is C^∞ on R^ν.

(2) There is a linearly independent set $a_1, \ldots, a_\nu$ so that $V(x + a_j) = V(x)$.

(3) $V(x) \geqslant 0$.

(4) Let $L = \{n_j a_j \mid n_j = 0, \pm 1, \ldots\}$. Then $V(x) = 0$ if and only if x lies in L.

(5) $(\partial^2 V/\partial x_i\, \partial x_j)(0) = A_{ij}$ is *strictly* positive definite.

We are interested in the operators

$$H(\lambda) = -\tfrac{1}{2}\Delta + \lambda^2 V \tag{1}$$

We recall (see, e.g., [7, Section XIII.16]) that for each k in the Brillouin zone, B, there is an operator with discrete spectrum, $H(\lambda; k)$, on a space $\mathscr{H}_k$ so that

$$L^2(R^\nu) = \int_B^\oplus \mathscr{H}_k\, d^\nu k, \qquad H(\lambda) = \int_B^\oplus H(\lambda; k)\, d^\nu k \tag{2}$$

(we describe this in more detail later). The eigenvalues $\varepsilon_1(\lambda; k) \leqslant \varepsilon_2(\lambda; k) \leqslant \cdots$ (counting multiplicity) of $H(\lambda; k)$ are continuous and are the band functions. The set $b_n(\lambda) \equiv \bigcup_{k \in B} \varepsilon_n(k; \lambda)$ is the nth band (and $\operatorname{spec}(H(\lambda)) = \bigcup_n b_n(\lambda)$).

Our first result is the analog of the results of [8]:

THEOREM 1. *Let $\alpha_1 \leqslant \alpha_2 \leqslant \cdots$ so the eigenvalues of $-\frac{1}{2}\Delta + \frac{1}{2}\sum_{i,j=1}^{\nu} A_{ij} x_i x_j$. Then $\lim_{\lambda \to \infty} \lambda^{-1} \varepsilon_n(k; \lambda) = \alpha_n$ and the limit (for n fixed) is uniform in k.*

Of course the eigenvalues, α_n, can be written down explicitly in terms of eigenvalues of the $\nu \times \nu$ matrix A. One consequence of Theorem 1 is that if α_j is a simple eigenvalue, then for λ large, $b_j(\lambda)$ is disjoint from the other bands. Moreover, for λ large, it is easy to see that $\operatorname{spec}(H)$ is guaranteed to have an arbitrarily large number of gaps in its spectrum.

As in [8], one can write down asymptotic perturbation series in λ^{-1} for $\varepsilon_n(\lambda, k)$ in case α_n is nondegenerate. The series are k independent, so one sees that $|b_n(\lambda)| = O(\lambda^{-l})$ for all l. In fact

THEOREM 2. $|b_n(\lambda)| \leqslant C_n e^{-d|\lambda|}$.

The ground state band, $\varepsilon_1(\lambda, k)$, can be analyzed in more detail. Let $\Delta(\lambda) \equiv b_1(\lambda)$. Recall the definition of the Agmon metric [1, 2]

$$\rho(x, y) = \inf_\gamma \left(\int_0^1 \sqrt{2V(\gamma(s))}\, |\dot\gamma(s)|\, ds \,\middle|\, \gamma(0) = x, \gamma(1) = y \right) \tag{3}$$

$$= \inf_{T,\gamma} \left(\frac{1}{2} \int_0^T \dot\gamma^2(s)\, ds + \int_0^T V(\gamma(s))\, ds \,\middle|\, \gamma(0) = x, \gamma(T) = y \right) \tag{4}$$

(the equality of the two infs is from [2]). The width, $\Delta(\lambda)$, will have asymptotics determined by the minimum distance between minima in the Agmon metric:

THEOREM 3. $\lim_{\lambda\to\infty} -(1/\lambda)\ln|\Delta(\lambda)| = \min(\rho(a,0)\mid a\in L, a\neq 0)$.

We will sketch the proofs of Theorems 1 and 3. Given our proof of Theorem 3, the proof of Theorem 2 just follows the arguments in Section 6.5 of [9]. We also remark here that eventually we will present a heuristic picture of the form of Block waves associated to the ground state.

To begin our proofs we must describe the decomposition (2) in more detail: By a *fundamental cell*, we mean a measurable subset, C, of R^ν so that for any $a\in L$, $a+C$, the translate of C by a is disjoint from C and so that $R^\nu\backslash\bigcup_{a\in L}(a+C)$ has measure zero. A standard fundamental cell is the Wigner–Seitz cell, $W=\{x\mid x$ is closer to 0 in Euclidean metric than to any other point of $L\}$. W is a polyhedron whose faces are perpendicular bisectors of some of those vectors $a\in L$ with $|a|\leqslant 2\sup(|x|\,|\, x\in W)$.

The dual lattice L^* is defined by $K\in L^*$ if and only if $(1/2\pi)K\cdot a\in Z$, the integers, for all $a\in L$. The *Brillouin zone*, B, is the Wigner–Seitz cell in the dual lattice. For each $k\in B$, we define a Hilbert space, $\mathscr{H}_k$, of functions $f\in L^2_{\text{loc}}$ so that

$$f(x+a)=e^{ik\cdot a}f(x)$$

for all $a\in L$ with inner product

$$\langle f,g\rangle=\int_C \overline{f(x)}\, g(x)\, d^\nu x$$

where C is any fundamental cell. $L^2(R^\nu, d^\nu x)$ is isomorphic to $\int_B^\oplus \mathscr{H}_k\, d^\nu k$ under the isomorphism that associates $g\in L^2$ to $\{f_k\in\mathscr{H}_k\}$ by the relation of Fourier transforms

$$\hat f_k(l)=c\sum_{K\in L^*}\hat g(l)\,\delta(l-k-K)$$

with $c=(2\pi)^{\nu/2}[\text{vol}(C)]^{-1/2}$.

Inside $\mathscr{H}_k$, let D_k denote those $f\in\mathscr{H}_k$ which have a distributional Laplacian in $\mathscr{H}_k$. Define $H(\lambda;k)$ on D_k by

$$(H(\lambda;k)f)(x)=-(\tfrac12\Delta f)(x)+\lambda^2V(x)f(x). \tag{5}$$

Then $H(\lambda;k)$ is selfadjoint on D_k, has compact resolvent, and

$$H(\lambda)=\int_B^\oplus H(\lambda;k)\,d^\nu k.$$

Sketch of the proof of Theorem 1. We assume the reader is familiar with [8]. Let $\varphi_n(\lambda;x)$ be the nth eigenvector of $-\frac12\Delta+\frac12\lambda^2\sum_{i,j=1}^{\nu}A_{ij}x_ix_j$. Let $\psi_n(\lambda;k;x)=$

$\sum_{a\in L} e^{ik\cdot a}\varphi_n(\lambda; x-a)$. Then $\psi_n(\lambda; k)\in\mathscr{H}_k$ and by elementary calculations (with errors uniform in k)

$$\langle\psi_n(\lambda; k), \psi_m(\lambda; k)\rangle = \delta_{nm} + O(e^{-c\lambda})$$
$$\langle H(\lambda, k)\,\psi_n(\lambda; k), \psi_m(\lambda; k) = \alpha_n\lambda\delta_{nm} + O(\lambda^{1/2})$$

and from this and the variational principle, one obtains (as in [8]) that $\overline{\lim}\,\lambda^{-1}\varepsilon_n(k;\lambda)\leqslant\alpha_n$ (uniformly in k).

We can obtain the lower bound exactly as in [8] if we note first that any periodic, C^∞, function j maps $\mathscr{H}_k$ to itself and that if $j_1,\ldots, j_l$ are periodic and C^∞ with $\sum_1^l j_a^2 = 1$, then $H(\lambda; k) = \sum_1^l j_a H(\lambda; k) j_a - \sum_1^l(\nabla j_a)^2$. We need only take $l = 2$ and choose $j_1(x;\lambda) = \sum_{b\in L}\varphi(\lambda^{2/5}(x-b))$ where $\varphi\in C_0^\infty$ with $\varphi(x) = 1$ for $|x|$ small. ∎

Now let $\Omega_1(\lambda; x)$ denote the lowest eigenvector in $\mathscr{H}_0$ of $H(\lambda; k=0)$. As in [9], we prove the tunneling result, Theorem 3, by first controlling Ω_1:

THEOREM 4. $\lim_{\lambda\to\infty}\lambda^{-1}\ln\Omega_1(\lambda; x) = -\min_{a\in L}\rho(x, a)$ *with a limit uniform in* x.

Proof. Let $e^{-tH(\lambda)}(x, y)$ be the integral kernel of $e^{-tH(\lambda)}$ and define $P_t(x, y;\lambda)\equiv \sum_{a\in L} e^{-tH(\lambda)}(x, y+a)$. P_t is the integral kernel of $H(\lambda, k=0)$ in the sense that

$$(e^{-tH(\lambda; k=0)}\varphi)(x) = \int_C P_t(x, y;\lambda)\,\varphi(y)\,d^\nu y \tag{6}$$

for any $\varphi\in\mathscr{H}_0$.

Since P_t is an integral kernel, it is not hard to show that with Ω_j the jth eigenvector for $H(\lambda; k=0)$, we have

$$P_t(x, y;\lambda) = \sum_{j=1}^\infty e^{-t\varepsilon_j(\lambda; k=0)}\Omega_j(\lambda; x)\,\Omega_j(\lambda; y)$$

and in particular

$$|\Omega_1(\lambda; x)|^2\leqslant e^{t\varepsilon_1(\lambda, k=0)}P_t(x, x;\lambda). \tag{7}$$

We claim that

$$\lim_{\lambda\to\infty}\lambda^{-1}\ln P_{T/\lambda}(x, y;\lambda) = -\tilde{a}(x, y; T)$$

with

$$\tilde{a}(x, y; T) = \min_{\gamma; a\in L}\left[\frac{1}{2}\int_0^T\dot{\gamma}^2(s)\,ds + \int_0^T V(\gamma(s)\,ds \mid \gamma(0) = x, \gamma(T) = y + a\right]. \tag{8}$$

This can be proven either by applying large deviations [10] for conventional Brownian motion to each term in the sum defining P_t and controlling the infinite sum by suitable estimates or (even better) writing P_t directly in terms of Brownim motion on a torus and using large deviations for that motion.

Given (6)–(8), the proof of Theorem 4 just follows the proof in Section 3 of [9] of Theorem 2.3 of that paper. Uniformity is easy by the periodicity in x. ∎

Remarks. (1) As in [9], Theorem 4 has a PDE proof using Agmon's methods.

(2) $\sum_{a\in L} e^{-ik\cdot a}\, e^{-tH(\lambda)}(x, y+a)$ is the integral kernel of $e^{-tH(\lambda;k)}$ in just the same way that $P_t(x, y; \lambda)$ is an integral kernel for $e^{-tH(\lambda;k=0)}$.

As a final preparation for Theorem 3, we need

THEOREM 5. *Let $\varphi \in \mathscr{H}_k$. Then*

$$(\varphi, [H(\lambda; k) - \varepsilon_1(\lambda; k=0)]\varphi) = \frac{1}{2}\int_C |\nabla(\varphi\Omega_1^{-1})|^2 \Omega_1^2\, d^\nu x. \tag{9}$$

Proof (*analog of the proof of Proposition* 2.2 *in* [9]). Let f be a bounded function in $\mathscr{H}_k$. Then M_f, the operator of multiplication by f maps $\mathscr{H}_0 \to \mathscr{H}_k$ and

$$H(\lambda, k)M_f - M_f H(\lambda, 0) = -\tfrac{1}{2}G_k \cdot M_{\nabla_f} - \tfrac{1}{2}M_{\nabla_f} \cdot G_0$$

where G_k is the operator on $\mathscr{H}_k$ given by $\vec{G}_k g = \vec{\nabla} g$. Similarly $M_{\bar{f}}: \mathscr{H}_k \to \mathscr{H}_0$ and $M_{\bar{f}} G_k - G_0 M_{\bar{f}} = -M_{\nabla\bar{f}}$. Thus (the analog of $[\bar{f}, [f, -\tfrac{1}{2}\Delta]] = -|\nabla f|^2$ on L^2)

$$M_{\bar{f}} M_f H(\lambda, 0) + H(\lambda, 0)\, M_{\bar{f}} M_f - 2M_{\bar{f}} H(\lambda, k) M_f = -M_{|\nabla f|^2}.$$

Let $f = \varphi\Omega_1^{-1}$ and apply this expression to Ω_1 to get (9). ∎

Sketch of the proof of Theorem 3. Let $a_0 \in L$ be chosen the nearest point to 0 in $L\setminus\{0\}$ in the Agmon metric. Let $d = \rho(a_0, 0)$. It suffices to prove that for any $\varepsilon > 0$, there is C_ε with

$$\varepsilon_1(\lambda, k) - \varepsilon_1(\lambda, 0) \leqslant C_\varepsilon e^{-(d-\varepsilon)\lambda} \tag{10}$$

for λ large and all $k \in B$; and to prove that for any ε and any compact $K \subset B$ disjoint from $\{k \mid (2\pi)^{-1} k \cdot a_0 \in Z\}$, we have a $\tilde{C}_{\varepsilon,k}$ with

$$\varepsilon_1(\lambda, k) - \varepsilon_1(\lambda, 0) \geqslant \tilde{C}_{\varepsilon,k}\, e^{-(d+\varepsilon)\lambda} \tag{11}$$

for λ large.

It will be convenient to deal with a different choice of the fundamental cell from the usual one. Define

$$A = \{x \mid x \text{ is nearer to 0 in the Agmon metric than any other point of } L\}.$$

Thus A is like the Wigner–Seitz cell but with the Agmon metric chosen rather than the Euclidean metric. If $V(-x) = V(x)$, it is not hard to see that bisectors of $0, a \in L$ in the Agmon metric are hyperplanes, so $A = W$, but in general $A \neq W$.

To get (10), choose $j \in C_0^\infty$ so that (i) $\operatorname{supp} j \in A$ (ii) $\operatorname{supp}(1-j) \subset \{x \mid \rho(x, 0) > \frac{1}{2}d - \frac{1}{4}\varepsilon\}$. Let $\varphi(\lambda; k, x) = \sum_{a \in L} e^{ik \cdot a} j(x-a)\, \Omega_1(\lambda; x) \in \mathscr{H}_k$. Then

$$\varepsilon_1(\lambda, k) - \varepsilon_1(\lambda, 0) \leqslant \frac{1}{2} \int_A |\nabla \varphi \Omega_1^{-1}|^2 \Omega_1^2 \, d^\nu x \Big/ \int_A |\varphi|^2 \, d^\nu x$$

$$\leqslant \frac{1}{2} \int_A |\nabla j|^2 \Omega_1^2 \, d^\nu x \Big/ \int_A |j|^2 \Omega_1^2 \, d^\nu x$$

which, by Theorem 4, is $O(e^{-(d-\varepsilon)\lambda})$.

To get (11), let $\{\gamma(s)\}_{0 \leqslant s \leqslant 1}$ be a geodesic from 0 to a_0 with geodesic paraterization (i.e., $\rho(0, \gamma(s)) = sd$). We will consider the cell $\gamma(\frac{1}{2}) + A$ which contains 0 and a_0 in its closure. If $\Omega_1(\lambda; k; x)$ is the lowest eigenvector of $H(\lambda, k)$ normalized so $\Omega_1(\lambda; k; x=0) > 0$, as in [9], we see that $\Omega_1(\lambda; k, x)\, \Omega_1(\lambda, x)^{-1} \to 1$ in a shrinking neighborhood of 0 and then to $e^{ik \cdot a_0}$ in a neighborhood of a_0. So long as $k \cdot a_0 \notin 2\pi Z$, the contribution of a small tube about γ contributes enough to $\frac{1}{2}\int |\nabla \Omega_1(\lambda, k)\, \Omega_1(\lambda)^{-1}|^2 \, |\Omega_1(\lambda)|^2 \, d^\nu x$ to obtain (11) as in the proof of Theorem 1.5 (lower bound) in [9, Sect. 2]. ∎

Let $N = \{x \mid \rho(x, a) = \rho(x, b)$ for some distant $a, b \in L\}$. The above arguments suggest strongly that for λ large, $\Omega_1(\lambda; k; x)\, \Omega_1(\lambda; x)^{-1}$ is very close to a constant in each component of $R^\nu \backslash N$ except for a small neighborhood of N (if the component contains b, the constant is $e^{ik \cdot b}$).

Note added in proof. Outassourt (University of Nantes preprint) has used the methods of Ref. [5] to recover the results of the present paper, and to go beyond leading asymptotics in situations where there is a unique geodesic minimizing the Agmon metric between points on the period lattice.

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