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SEMICLASSICAL ANALYSIS OF SCHRÖDINGER OPERATORS WITH COULOMB-LIKE SINGULAR POTENTIALS

FUMIHIKO NAKANO (中野史彦)

Department of Mathematical Science, University of Tokyo

ABSTRACT. In this paper, we study the behavior of eigenvalues and eigenfunctions of Schrödinger operators whose potentials have finitely many negative singularities. We prove that if potentials behave like $O(|x|^{-\rho})(0<\rho<2)$ near singularities, then eigenvalues behave like $O(h^{-\frac{2\rho}{2-\rho}})$ when the Planck constant h approaches to zero. Then we obtain the asymptotic expansion of the eigenvalues and eigenfunctions in h. We also study the splitting of the lowest eigenvalues and derive that the asymptotic is estimated by a suitable Riemann metric called Agmon distance.

0. INTRODUCTION

We consider Schrödinger operators whose potentials have finitely many negative singularities, and study the behavior of eigenfunctions and eigenvalues when h, the Planck constant, approaches to zero.

The Schrödinger operator we consider is,

$$H(h):=-h^2\triangle+V(x) \text{ on } L^2(\mathbf{R}^d),$$

where h is the Planck constant.

The assumptions on V is,

Assumptions(A).

(1) $V(x)$ has finitely many singular points $p_1,p_2,\cdots,p_n\in\mathbf{R}^d$, and $V(x)$ is bounded below in the complement of the union of neiborhoods of singular points, i.e., for any $\varepsilon>0$, there exists a constant $M_\varepsilon>0$ such that,

$$\text{if } |x-p_i|>\varepsilon \text{ (for any } i=1,\cdots,n), \text{ then } V(x)\geq -M_\varepsilon.$$

(2) $V(x)\in C^\infty(\mathbf{R}^d\setminus\{p_1,\cdots,p_n\})$, and $V(x)$ has asymptotic expansions near each p_i in the following form,

$$V(x)\sim-\frac{1}{|x-p_i|^{\rho+1}}\sum_{|\alpha|=1}^{\infty}a_\alpha^{(i)}(x-p_i)^\alpha \quad \text{as } x\to p_i.$$

(3) If $d=1$, then $0<\rho<1$. Otherwise, $0<\rho<2$.

We assume the Assumptions (A) throughout this paper.

Remark. When (3) is satisfied, $V(x)$ is in the Kato class and hence $H(h)$ has a unique Friedrichs extension and is bounded below (cf.[7]).

At first, we study the behavior of $H(h)$ in the limit: $h \downarrow 0$. Let $E_m(h)$ be the m-th eigenvalue of $H(h)$, counting multiplicities. Let $h_0^{(i)}(h) := -\Delta - \sum_{|\alpha|=1} \frac{a_\alpha^{(i)} x^\alpha}{|x|^{\rho+1}}$ $(i = 1, \cdots, n)$ and let $\{e_m\}_{m=0,1,2,\cdots,}$ be the eigenvalues of $\bigoplus_{i=1}^n h_0^{(i)}$, counting multiplicities.

Theorem 1. *Let $N \in \mathbf{N}$. For sufficiently small h, $H(h)$ has at least N eigenvalues and*

$$\lim_{h\downarrow 0} h^\alpha E_m(h) = e_m, \quad 0 \leq m \leq N, \quad \alpha = \frac{2\rho}{2-\rho}.$$

Secondly, we consider asymptotic expansions of eigenvalues and eigenfunctions in h as h tends to zero. In order that, we need additional assumptions on $V(x)$.

Assumptions(B).

(1) $V(x)$ has at most polynomial growth, i.e., there exist $k > 0$, $M > 0$, $C > 0$, such that if $|x| > M$, then $|V(x)| \leq C(1 + |x|)^k$.

(2) If $d \leq 3$, then $\rho < \frac{d}{2}$.

Theorem 2. *Assume (B).*

(1) *Let e_m be a simple eigenvalue of $\bigoplus_{i=1}^n h_0^{(i)}$. Then the corresponding eigenvalue $E_m(H)$ of $H(h)$ has an asymptotic expansion in the following form,*

$$E_m(h) \sim h^{-\alpha}(e_m + \sum_{j=1}^{\infty} \tilde{\alpha}_j (h^\beta)^j),$$

i.e.,

$$E_m(h) - h^{-\alpha}(e_m + \sum_{j=1}^{k} \tilde{\alpha}_j (h^\beta)^j) = O(h^{-\alpha+(k+1)\beta}),$$

where $\alpha = \frac{2\rho}{2-\rho}$, $\beta = \frac{2}{2-\rho}$.

(2) *Let ψ_m be the eigenfuction of $H(h)$ corresponding to an eigenvalue $E_m(h)$ and φ_m be the eigenfuction of $h_0^{(i)}(h)$ corresponding to e_m (i is taken so that e_m is an eigenvalue of $h_0^{(i)}$). And let $U^{(i)}$ be an operator defined by*

$$(U^{(i)} f)(x) := h^{d\beta/2} f(h^\beta x + p_i) \quad \textit{for } f \in L^2(\mathbf{R}^d).$$

Then, $U^{(i)}\psi_m$ has an asymptotic expansion in the following form in L^2-sense,

$$U^{(i)}\psi_m \sim \varphi_m + \sum_{j=1}^{\infty} (h^\beta)^j \tilde{\varphi}_m^{(i)}.$$

When e_m is degenerate, the situation is slightly different.

Theorem 3. *Assume (B). Let $E_m, \cdots, E_{m+k-1}$ be the eigenvalues such that $h^{-\alpha}E_m$ appoaches to e, which is an eigenvalue of $\bigoplus_{i=1}^n h_0^{(i)}$ with multiplicity k. Then each E_{m+p} has an asymptotic expansion in h,*

$$E_{m+p} \sim h^{-\alpha}(e + \sum_{j=1}^{\infty} \tilde{a}_j^p (h^\beta)^j), \quad p = 0, \cdots, k-1.$$

Theorem 4. *Under the same conditions as Thoreom 3, and if no two asymptotic expansions of $E_m, \cdots, E_{m+k-1}$ are the same, then for each corresponding eigenfunction ψ_j, there exists unique singular point of $V(x)$, $\psi_{n(j)}$, such that for any $N \in \mathbf{N}$,*

$$\|(J_{n(j)} - 1)\psi_j\|_2 = O(h^N)$$

holds and $U^{n(j)}\psi_j$ has an asymptotic expansion in L^2 sense, where $J_{n(j)}$ is a function that takes value one in the neiborhood of $p_{n(j)}$ ($\|\cdot\|_2$ is $L^2(\mathbf{R}^d)$-norm.).

Corollary. *If $E_j(h)$ is simple for $h > 0$, then either of the following two holds,*
(1) There exists a singular point $p_{n(j)} \in \mathbf{R}^d$ such that for any $N \in \mathbf{N}$,

$$\|(J_{n(j)} - 1)\psi_j\|_2 = O(h^N), \quad as \ h \downarrow 0.$$

(2) There exists another eigenvalue $E_j'(h)$ such that for any $N \in \mathbf{N}$,

$$|E_j' - E_j| = O(h^N), \quad as \ h \downarrow 0.$$

Physically, the case (2) of this corollary corresponds to the situation that a particle exists near both of at least two singular points. And the quantity $|E_j' - E_j|$ is related to the tunneling effect between the singularities.

When the number of the singularities is two (*i.e.*, $n = 2$), and E_j is the lowest eigenvalue of $H(h)$, we can estimate $|E_j' - E_j|$ sharply.

Definition. For $x, y \in \mathbf{R}^d$, the Agmon distance $\rho_h(x, y)$ with respect to the energy $\tilde{E}_o(:= h^{-\alpha}e_0)$ is defined by

$$\rho_h(x, y) := \inf_\gamma \left\{ \int_0^1 \sqrt{\max(V(\gamma(s)) - \tilde{E}_0(h), 0)}|\dot{\gamma}(s)|ds \;\middle|\; \gamma(0) = x, \gamma(1) = y, \gamma \in H^1 \right\}.$$

Theorem 5. *Let $n = 2$, and let a and $b \in \mathbf{R}^d$ be the singular points. Let J_a (resp. J_b) be a function that takes value one in the neiborhood of a (resp. b). Let $E_0(h)$ be the lowest eigenvalue of $H(h)$. And let ψ_0 be the eigenfunction corresponding to the eigenvalue $E_0(h)$.*

Assume that, for any $\varepsilon > 0$, there exist $C_\varepsilon > 0$ such that,

$$\|J_a\psi_0\|_2 \|J_b\psi_0\|_2 \geq C_\varepsilon e^{-\varepsilon/h^\beta}.$$

Then, for any $\varepsilon > 0$, there exist constants $C_{1,\varepsilon} C_{2,\varepsilon}$ such that

$$C_{1,\varepsilon} \exp\left(-\frac{\rho_h(a, b)}{h}(1 + \varepsilon)\right) \leq |E_1 - E_0| \leq C_{2,\varepsilon} \exp\left(-\frac{\rho_h(a, b)}{h}(1 - \varepsilon)\right),$$

where E_1 is the second eigenvalue.

The assumption of Theorem 5, $\|J_a\psi_0\|_2\|J_b\psi_0\|_2 \geq C_\varepsilon e^{-\varepsilon/h^\beta}$ comes from the postulate that particle exists on both a and b. For example, if $V(x)$ has mirror symmetry with respect to one point, this condition is automatically satisfied.

Estimating $\rho_h(a, b)$, we obtain,

Theorem 5'. *Under the same conditions as in Theorem 5, for any $\varepsilon > 0$ there exist constants $C_{1,\varepsilon}$, $C_{2,\varepsilon}$ such that*

$$C_{1,\varepsilon} \exp\left(-\frac{\sqrt{-e_0}|a-b|}{h^\beta}(1+\varepsilon)\right) \le |E_1 - E_0| \le C_{2,\varepsilon} \exp\left(-\frac{\sqrt{-e_0}|a-b|}{h^\beta}(1-\varepsilon)\right).$$

It follows from this theorem that the behavior of $|E_1 - E_0|$ is determined by $|a-b|$, ρ and a_0 only.

As for the known results, similar problems have been studied extensively by many people in the case that $V(x)$ satisfies,

(1) $V(x) \in C^\infty, V(x) \ge 0$,
(2) $\underline{\lim}_{|x|\to\infty} V(x) > 0$,
(3) There exists finitely many points $p_1, \cdots, p_n$ such that $V(p_i) = 0$ $(i = 1, \cdots, n)$ and each minimum is non-degenerate ([1],[2],[4],[5],[6], and in their references).

The aim of this paper is to study the similar results as above hold if $V(x)$ has negative singularities. We use mainly Simon's methods ([1],[2]). We prove Theorem 1 in Section 1, Theorem 2,3,4 in Section 2, and Theorem 5 in Section 4. In the appendix, we show that the similar exponential estimates as Theorem 5 and Theorem 5' can be obtained for the width of the ground state band of Schrödinger operator with periodic potential.

1. Proof of Theorem 1

1.1 Upper Bound

Here, we will show $\overline{\lim}_{h\downarrow 0} h^\alpha E_m(h) \le e_m$.

Take a function $j(x) \in C_0^\infty(\mathbf{R}^d)$ which satisfies,

$$j(x) := \begin{cases} 1, & \text{if } |x| < 1, \\ 0, & \text{if } |x| > 2, \end{cases}$$

and let

$$J_{(i)}^h := j(h^{-\delta}(x - p_i)), \quad i = 1, \cdots, n, \quad 0 < \delta < \frac{\rho}{2-\rho}.$$

We can assume $\mathrm{Supp}J_{(i)} \cap \mathrm{Supp}J_{(j)} = \phi$ by taking h sufficiently small if necessary.

Let e_m be the m-th eigenvalue of $\bigoplus_{i=1}^n h_0^{(i)}$, and φ_m be the corresponding eigenfuction. Then $U^{i(m)^{-1}}\varphi_m$ is an eigenfunction of $H_0^{(i(m))}$, where $H_0^{(i)}(h) := -h^2\Delta - \sum_{|\alpha|=1} \frac{a_\alpha^{(i)} x^\alpha}{|x-p^i|^{\rho+1}}$ ($i(m)$ is defined so that e_m is the eigenvalue of $h_0^{(i(m))}$.).

We take "approximating eigenfunction"

$$\psi_m(h; x) := J_{i(n)}^h U^{i(m)^{-1}} \varphi_m.$$

Then, from the definition of $J_{(i)}^h$ and Assumptions (A), we can see

$$\left(\psi_l, (H - H_0^{(i)})\psi_m\right) = O(h^{\frac{2(1-\rho)}{2-\rho}}), \tag{1.0}$$

where $(\cdot,\cdot)$ is $L^2(\mathbf{R}^d)$-product.

Claim 1.

$$(\psi_l, \psi_m) = \delta_{lm} + O\left(\exp(-ch^{\delta - \frac{2}{2-\rho}})\right). \tag{1.1}$$

Proof of Claim 1. When $i(l) \neq i(m)$, (1.1) is clear. Therefore we assume $i(l) = i(m)$.

$$\begin{aligned}
|(\psi_l, \psi_m) - \delta_{lm}| &= \left| \int (1 - {J^h_{(i)}}^2) {U^{(i)}}^{-1} \varphi_l \, {U^{(i)}}^{-1} \varphi_m dx \right| \\
&= \left| \int_{|x - p_i| \geq ch^\delta} {U^{(i)}}^{-1} \varphi_l \, {U^{(i)}}^{-1} \varphi_m dx \right| \\
&= \int_{|x| \geq ch^\delta} h^{-\frac{2d}{2-\rho}} \varphi_l(h^{-\frac{2}{2-\rho}} x) \varphi_m(h^{-\frac{2}{2-\rho}} x) dx \\
&= O\left(\exp(-ch^{\delta - \frac{2}{2-\rho}})\right).
\end{aligned}$$

□

Claim 2.

$$(\psi_l, H\psi_m) = h^{-\alpha} e_m \delta_{lm} + O(h^{-2\theta}), \tag{1.2}$$

where $\theta := \max\{\delta, \frac{2(1-\rho)}{2-\rho}\}$.

Proof of Claim 2. As in the proof of Claim 1, we can assume $i(l) = i(m)$.

We use the fact that if $H\eta = E\eta$, then

$$(f\tilde{\eta}, Hf\eta) = E(f\eta, f\tilde{\eta}) + (\eta, h^2 (\nabla f)^2 \tilde{\eta}).$$

We substitute $f = J^h_{(i)}$, $H = H_0^{(i)}$, $\eta = {U^{(i)}}^{-1} \varphi_m$, $\tilde{\eta} = {U^{(i)}}^{-1} \varphi_l$ into this. Therefore,

$$(\psi_l, H_0^{(i)} \psi_m) = h^{-\alpha} e_m (\psi_l, \psi_m) + (\psi_l, h^2 (\nabla J^h_{(i)})^2 \psi_m).$$

Estimating $\nabla J^h_{(i)}$, and using (1.0), (1.1), we obtain (1.2). □

Here we use the Min-Max principle. At first, let

$$\mu_m(h) := \sup_{\xi_1, \cdots, \xi_{m-1}} Q(\xi_1, \cdots, \xi_{m-1}; h),$$

$$Q(\xi_1, \cdots, \xi_{m-1}; h) := \inf \left\{ (\psi, H\psi) \,\middle|\, \psi \in \mathcal{D}(H), \|\psi\|_2 = 1, \psi \in \{\xi_1, \cdots, \xi_{m-1}\}^\perp \right\}.$$

Then $\mu_m(h)$ equals to either the m-th eigenvalue of H (counting multiplicities) or $\inf \sigma_{ess}(H)$.

Fix any $\varepsilon > 0$. For each $h \in (0, 1]$, we can find $\xi_1^h, \cdots, \xi_{m-1}^h$ such that,

$$\mu_m(h) \leq Q(\xi_1^h, \cdots, \xi_{m-1}^h; h) + \varepsilon.$$

From (1.1), $\{\psi_1, \cdots, \psi_m\}$ span m-dimensional subspace if h is sufficiently small. Hence there exists $\varphi \in \{\xi_1, \cdots, \xi_{m-1}\}^\perp$ which is a linear combination of $\{\psi_1, \cdots, \psi_m\}$. From (1.2),

$$Q(\xi_1, \cdots, \xi_{m-1}; h) \leq (\varphi, H\varphi) \leq h^{-\alpha} e_m + O(h^{-2\delta}).$$

Since $\varepsilon > 0$ is arbitrary,

$$\mu_m(h) \leq h^{-\alpha} e_m + O(h^{-2\delta}).$$

As $V(x)$ is bounded below outside of a compact set, $\inf \sigma_{ess}(H) > -\infty$. On the other hand, $\lim_{h\downarrow 0} h^{-\alpha} e_m = -\infty$. Hence $\mu_m(h) = E_m(h)$ if h is sufficiently small and thus we obtain the upper bound. □

1.2 Lower bound

We prove $\underline{\lim}_{h\downarrow 0} h^\alpha E_m(h) \geq e_m$ here. When we have finish it, we complete the proof of Theorem 1. Fix arbitrary r such that $e_m \leq r \leq e_{m+1}$. It suffices to show,

$$H \geq r h^{-\alpha} \mathbf{1} + F$$

where $\mathbf{1}$ is an identity operator and $\mathrm{rank} F \leq m$.

We define $J_0^h \in C^\infty(\mathbf{R}^d)$ so that $(J_0^h)^2 := 1 - \sum_{i=1}^n (J_{(i)}^h)^2$. Let $P^{(i)}$ be eigenprojections onto the eigenspaces of $H_0^{(i)}$ whose corresponding eigenvalues are smaller than $h^{-\alpha} r$ (hence,$\sum \mathrm{rank} P^{(i)} = m$), and let $F^{(i)} := H_0^{(i)} P^{(i)}$.

By IMS-localization formula (see [7]), for any $\varepsilon > 0$,

$$H = J_0 H J_0 + (1-\varepsilon) \sum_{i \neq 0} J_i H_0^{(i)} J_i + \sum_{i \neq 0} J_i (\varepsilon H_0^{(i)} + H - H_0^{(i)}) J_i - \sum (\nabla J_i)^2. \tag{1.3}$$

From the definition of $F^{(i)}$,

$$J_{(i)}^h H_0^{(i)} J_{(i)}^h \geq J_{(i)}^h F^{(i)} J_{(i)}^h + h^{-\alpha} r (J_{(i)}^h)^2. \tag{1.4}$$

On the other hand, since $|x - p_i| \geq c h^\delta$ on $\mathrm{Supp} J_0$,

$$J_0 H J_0 \geq (J_0)^2 O(-c h^{-\delta\rho}) \geq r h^{-\alpha} (J_0)^2, \tag{1.5}$$

and

$$\begin{aligned} \varepsilon H_0^{(i)} + H - H_0^{(i)} &\geq \frac{\varepsilon}{2}(-h^2\Delta - \sum_{|\alpha|=1} \frac{2a_\alpha^{(i)} x^\alpha}{|x|^{\rho+1}}) - \frac{\varepsilon}{2} h^2 \Delta - \sum_{|\alpha|=2} \frac{a_\alpha^{(i)} x^\alpha}{|x|^{\rho+1}} - O(h^{2-\rho}) \\ &\geq -c\varepsilon h^{-\alpha} - c_\varepsilon h^{-\alpha'} - O(h^{2-\rho}), \end{aligned} \tag{1.6}$$

where $\alpha' := \frac{2(\rho-1)}{3-\rho}$, and c, c_ε is independent of h .

Substituting (1.4)∼(1.6) into (1.3),

$$H \geq (1 - c\varepsilon) r h^{-\alpha} \mathbf{1} - O(h^{-\rho}) + F, \qquad \gamma := \max(\alpha', 2\delta),$$

($F = \sum J_{(i)} F^{(i)} J_{(i)}$, $\mathrm{rank} F \leq m$). Since $\varepsilon > 0$ is arbitrary, we have done.

1.3 Additional arguement

We shall show here that if e_m is non-degenerate, the "approximating eigenfunction", we used in the proof of Theorem 1, approaches to the "real" eigenfunction in L^2-sense. We will use this result in Section 2,4. At first, for each l, we find ε_l such that for any m, either $e_m = e_l$ or $|e_m - e_l| > \varepsilon_l$ holds.

Proposition 1.1. *Let*

$$P_l^h := \frac{1}{2\pi i}\oint_{|z-h^{-\alpha}|=h^{-\alpha}e_l} (z - H(h))^{-1} dz,$$

then, $\|(1 - P_l^h)\psi_l^h\|_2 \to 0$ $(h \downarrow 0)$.

Proof. We use the inductive arguement. Assume that the proposition is valid for any l for $l < k$.

Claim. *For any l such that $e_l < e_k$, $P_l^h \psi_k^h \to 0$ in L^2.*

Proof of Claim. If the degeneracy of e_l is m, $P_l\psi_{l_j} - \psi_{l_j} \to 0$ in L^2 $(j = 1, \cdots, m)$ (where $\psi_{l_j}(j = 1, \cdots, m)$ are eigenfunctions corresponding to e_l.). From (1.1), we see $\{\psi_{l_j}\}_{j=1,\cdots,m}$ and moreover, $\{P_l\psi_{l_j}\}_{j=1,\cdots,m}$ are linearly independent (for h small). Let $\{u_{l_j}\}_{j=1,\cdots,m}$ be the orthonormal basis of Ran P_l (the range of P_l). Since $\{P_l\psi_{l_j}\}$ is linearly independent and contained in Span$\{u_{l_j}\}(j = 1, \cdots, m)$, we can write each u_j by linear combination of $\{P_l\psi_{l_j}\}_{j=1,\cdots,m}$ and we write $u_j = \sum a_k^j P_l\psi_{l_k}$.

$$\begin{aligned} P_l\psi_k &= \sum_{j=1}^{m}(\psi_k, u_{l_j})u_{l_j} \\ &= \sum_{j=1}^{m}(\psi_k, \sum_{p=1}^{m} a_p^j P_l\psi_{l_p}) \sum_{q=1}^{m} a_q^j P_l\psi_q. \end{aligned}$$

From the assumption of the induction,

$$(\psi_k, \sum_{p=1}^{m} a_p^j P_l\psi_{l_p}) - (\psi_k, \sum_{p=1}^{m} a_p^j \psi_{l_p}) \xrightarrow{h\downarrow 0} 0.$$

On the other hand, from (1.1), $(\psi_k, \sum_{p=1}^{m} a_p^j \psi_{l_p}) \xrightarrow{h\downarrow 0} 0$. By combining two, we see $P_l\psi_k \to 0 (h \downarrow 0)$ in L^2. □

Let E_Ω^h be the spectral measure of $h^\alpha H$. From the claim above, for any $\varepsilon > 0$, $E^h_{(-\infty, e_k-\varepsilon)}\psi_k^h \to 0$ as $h \downarrow 0$ in L^2. On the other hand, $(\psi_k, h^\alpha H\psi_k) \to e_k$ (from (1.2)). Then it must be $\|E^h_{(e_k-\varepsilon, e_k+\varepsilon)}\psi_k^h\|_2 \to 1$ $(h \downarrow 0)$. □

2. Asymptotic Expansions of Eigenvalues and Eigenfunctions

2.1 Proof of Theoreom 2

To simplify the notation, we write i instead of $i(m)$. Let

$$K_0 := h^\alpha U^{(i)} H_0^{(i)} {U^{(i)}}^{-1} \quad (= h_0^{(i)});$$

$$K := h^\alpha U^{(i)} H {U^{(i)}}^{-1} = K_0 + h^\alpha V(h^\beta x + p_i) + \sum_{|\alpha|=1} \frac{a_0^{(i)} x^\alpha}{|x|^{\rho+1}}.$$

From the assumption, $K - K_0$ has an asymptotic expansion near the origin in the following form as $h \downarrow 0$,

$$K - K_0 \sim -\frac{1}{|x|^{\rho+1}} \sum_{|\alpha|=2}^{\infty} a_\alpha^{(i)} (h^\beta)^{|\alpha|} x^\alpha. \tag{2.1}$$

Let

$$\tilde{P}(h) := \frac{1}{2\pi i} \oint_{|z-e_m|=\varepsilon} (z-K)^{-1} dz,$$

where we take ε sufficiently small such that $\{z \mid |z - e_m| < \varepsilon\}$ contains no other $e_j (j \neq m)$.

Then, by Theorem 1, $\mathrm{rank}\tilde{P}(h) = 1$ for h sufficiently small, and by Proposition 1.1, $\tilde{P}(h)\varphi_m \to \varphi_m$ $(h \downarrow 0)$. Hence it is enough to obtain L^2-asymptotic expansion of $\tilde{P}(h)\varphi_m$. In fact,

$$h^\alpha E_m = \frac{(K\varphi_m, \tilde{P}\varphi_m)}{(\varphi_m, \tilde{P}\varphi_m)}, \tag{2.2}$$

$$U^{(i)}\psi_m = \frac{1}{(\varphi_m, \tilde{P}\varphi_m)^{1/2}} \tilde{P}\varphi_m, \tag{2.3}$$

hold and $K\varphi_m$ has obviously L^2-asymptotic expansion under Assumptions (B). From the definition of $\tilde{P}(h)$ it suffices to obtain L^2-asymptotic expansion of $(z - K)^{-1}\varphi_m$.

One can expand $(K-z)^{-1}\varphi_m$ as follows.

$$(K-z)^{-1}\varphi_m = \sum_{k=0}^{l} f_k + r_l,$$

where

$$f_k = (-1)^k (K_0 - z)^{-1} [V(K_0 - z)^{-1}]^k \varphi_m,$$

and

$$r_l = (-1)^{-1} (K - z)^{-1} [V(K_0 - z)^{-1}]^{l+1} \varphi_m.$$

We shall estimate the L^2 norm of φ_k and r_l. Write $V = V_1 + V_2$ where $V_1(x) = V\chi_{\mathbf{R}^d \setminus \cup_{j=1}^n B_j^\varepsilon}$, $V_2(x) = V\chi_{\cup_{j=1}^n B_j^\varepsilon}$ (χ_A is the characteristic function of A and $B_j^\varepsilon := \{x \mid |x - p_j| < \varepsilon\}$.).

Claim. $\|f_k\|_2 = O(h^{\beta k})$, $\|r_l\|^2 = O(h^{\beta(l+1)})$.

Proof of Claim. Due to the induction. We assume $\|[V(K_0 - 1)^{-1}]^k \varphi_m\|_2 = O(h^{\beta k})$. At first we consider the contribution of V_2. By the Sobolev's embedding theorem,

(1) When $d \le 3$, $H^2(\mathbf{R}^d) \subsetneq L^\infty(\mathbf{R}^d)$. From (2) of Assumptions (B), $V_2 \in L^2(\mathbf{R}^d)$. Hence $V_2(K_0 - z)^{-1}\psi \in L^2$(for any $\psi \in L^2$).

(2) When $d = 4$, $\chi_K(K_0 - z)^{-1}\psi \in L^r$ for any $r < \infty$ and for any compact set K. And if $\rho < 2$, there exists $\delta > 0$ such that $V_2 \in L^{2+\delta}$. Hence $V_2(K_0 - z)^{-1}\psi \in L^2(\mathbf{R}^d)$ by the Hölder's inequality.

(3) When $d \ge 5$, $H^2(\mathbf{R}^d) \subsetneq L^q(\mathbf{R}^d)$ (where $\frac{1}{q} := \frac{1}{2} - \frac{2}{d}$). Hence if $\rho < 2$, $V_2(K_0 - z)^{-1}\psi \in L^2(\mathbf{R}^d)$ by the Hölder's inequality.

Combining above we obtain,

$$\|V_2(K_0 - z)^{-1}[V(K_0 - z)^{-1}]^k \varphi_m\|_2 = \begin{cases} O(\varepsilon^{(d-2\rho)/2} h^{\beta k}), & \text{if } d \le 3, \\ O(\varepsilon^{(4-(2+\delta)\rho)2/(2+\delta)} h^{\beta k}), & \text{if } d = 4, \\ O(\varepsilon^{d(1-\rho/2)4/d} h^{\beta k}), & \text{if } d \ge 5. \end{cases}$$

If we take a suitable constant $C_d > 0$ (dependent on the dimension d), and put $\varepsilon = h^{\beta C_d(l+1)}$, then we obtain

$$\|V_2(K_0 - z)^{-1}[V(K_0 - z)^{-1}]^k \varphi_m\|_2 = O(h^{\beta(l+1)}). \tag{2.4}$$

If we take ε as above, we can write (from (2.1)) for any $N \in \mathbf{N}$,

$$V_1 = Q_N(h; x) + R_N(h; x) + S(h; x),$$

where $Q_N(h; x)$ is a polynomial of x and h^β of degree at most N, and

$$\begin{aligned} |R_N| &\le C h^{-\rho\beta c_d(l+1)} |h^\beta x|^{N+1}, \\ |Q_N| &\le C h^\beta (1 + |x|)^N, \\ |S| &\le C h^\beta |x|^{-(\rho-1)}. \end{aligned} \tag{2.5}$$

We take N sufficiently large such that

$$\beta(N+1) - \rho\beta c_d(l+1) \ge \beta(l+1). \tag{2.6}$$

Lemma 2.1. *For any $l \in \mathbf{R}$, $(1 + |x|)^l (K_0 - z)^{-1} (1 + |x|)^{-l}$ is a bounded operator.*

For its proof, we refer to [3].

Put $A := (1 + |x|)$. We can write $V_1(K_0 - z)^{-1}[V(K_0 - z)^{-1}]^k \varphi_m = (A^{-b}V_1)A^b(K_0 - z)^{-1}A^{-b}(A^{-b}V)A^{2b}(K_0 - z)^{-1}A^{-2b} \cdots A^{(k+1)b}\psi_m$. By lemma 2.1, $A^{pb}(K_0 - z)^{-1}A^{-pb}$ is a bounded operator. On the other hand, by (2.5), $\|A^{-b}(Q_N + R_N)\| = O(h^\beta)$ for suitable b. Hence

$$\|V_1(K_0 - z)^{-1}[V(K_0 - z)^{-1}]^k \varphi_m\|_2 = O(h^{\beta(k+1)}).$$

Combining this with (2.4), we obtain $\|f_{k+1}\|_2 = O(h^{\beta(k+1)})$.

The estimate for r_l is similar. This proves the Claim. □

We set $f'_k := (-1)^k (K_0 - z)^{-1}[Q_N(K_0 - z)^{-1}]^k \varphi_m$. Hence, by (2.4),(2.5), and (2.6), and as the above arguement, we obtain

$$\|f'_k - f_k\|_2 = O(h^{\beta(l+1)}).$$

Noting that f'_k is a polynomial of h^β, we obtain the asymptotic expansion of $(K - z)^{-1}\varphi_m$. □

2.2 Proof of Theorem 3

Lemma 2.2. *Let $C(h)$ be a $k \times k$ Hermitian matrix whose entries have asymptotic expansions of h. Then the eigenvalues of $C(h)$ also have asymptotic expansions of h.*

For the proof, we can refer to [1].

Let P_h be the projection onto the subspace which is spanned by the eigenfuctions of H corresponding to the eigenvalues $E_m, \cdots, E_{m+k-1}$. Hence, by using the eigenfunctions of $H_0^{(i)}$ corresponding to the eigenvalue $h^{-\alpha}e$, it follows that ,

$$(\psi_i, P_h\psi_j) \to \delta_{ij} \tag{2.7}$$

as h tends to 0 (by Proposition 1.1).

Thanks to the same arguement as the proof of theorem 2, one can prove that

$$\triangle_{ij} := (\psi_i, P_h\psi_j), \quad H_{ij} := (\psi_i, HP\psi_j),$$

have asymptotic expansion of h^β. And from (2.7), $\triangle_{ij} = \delta_{ij} + o(h^\beta)$. Hence $C := \triangle^{-1/2}H\triangle^{-1/2}$ has asymptotic expansion of h^β. Therefore, by Lemma.2.2, $E_m, \cdots, E_{m+k-1}$ also have asymptotic expansion of h^β. □

Theorem 4 and its corollary follows easily from the proof of Theorem 3.

3. Exponential decay of eigenfunctions

In order to prove Theorem 5 and Theorem 5', we obtain the exponential decay of the eigenfunction corresponding to the lowest eigenvalue of H. From now on, we assume the number of the singular points is two ($n = 2$): $a, b \in \mathbf{R}^d$.

Proposition 3.1. *There exist $R_0 > 0, C > 0$, and $D > 0$ such that if $|x| > R_0$ and h is sufficiently small,*

$$|\psi_0(h; x)| \leq Ce^{-D|x|/h^\beta}.$$

Proof. Take $R_0 > 0$, $\delta > 0$ such that, if $|x| > R_0/4$ and h is sufficiently small,

$$V(x) - \frac{\delta^2}{h^\alpha} - E_0(h) \leq 1, \tag{3.1}$$

(That is possible since $V(x)$ is bounded below far away from the origin and $E_0(h) = O(h^{-\alpha})$.).

Let φ be a function which satisfies,

$$(1)\ \varphi \in L^\infty, \quad 0 \leq \varphi'(s) \leq 1,$$
$$(2)\ \varphi(x) = x, \quad if \quad |x| \leq R_1,$$
$$(3)\ \varphi(x) = 0, \quad if \quad |x| \geq 2R_1,$$

for a constant $R_1 > 0$.

We set $\rho(x) := \delta\varphi(|x|)/h^{\rho/(2-\rho)}$ $(x \in \mathbf{R}^d)$. Then it follows that $|\nabla\rho(x)|^2 \leq \delta^2/h^\alpha$, $\rho(x)$ is bounded, and is smooth in the complement of the neiborhood of the origin. Let ψ be a R-valued fuction such that its support is contained in $\{x|\ |x| \geq R_0/4\}$. From (3.1), for sufficiently small h, we obtain

$$\begin{aligned}(e^{\rho/h}\psi,(H-E_0)e^{-\rho/h}\psi) &\geq (\psi,(V-(\nabla\rho)^2-E_0)\psi)\\ &\geq \|\psi\|_2^2.\end{aligned} \tag{3.2}$$

Therefore, if we define a function η on $\mathbf{R}^d$ such that,

$$\begin{aligned}&(1)\ 1-\eta \in C_0^\infty,\\ &(2)\ \eta = 0, \quad if \quad |x| < R_0/4,\\ &(3)\ \eta = 1, \quad if \quad |x| > R_0/2,\end{aligned}$$

and if we set $\psi := e^{\rho/h}\eta\psi_0$, it follows that

$$(e^{\rho/h}\psi,(H-E_0)e^{-\rho/h}\psi) = h^2\big(e^{2\rho/h}\eta\psi_0, -2(\nabla\eta)(\nabla\psi_0)-(\Delta\eta)\psi_0\big). \tag{3.3}$$

Since the RHS of (3.3) is independent of R_1, we can take R_1 go to infinity and let $\rho = \delta|x|/h^{\rho/(2-\rho)}$. On the other hand, if we note that $\|\psi_0\|_2 = 1$ and $\|\nabla\psi_0\|_2 = O(h^{-1})$, we obtain (from (3.2),(3.3)),

$$\int_{|x|>R_0/2} e^{2\delta|x|/h^\beta}|\psi_0|^2 dx \leq Che^{\delta R_0/h^\beta}.$$

Hence

$$\int_{|x|>R_0} e^{\delta|x|/h^\beta}|\psi_0|^2 dx \leq Ch.$$

Since ψ_0 is subharmonic on $\{x|\ |x| > R_0\}$, the value of ψ_0 on x is bounded by the integral of itself over the unit ball around x. Therefore we obtain the conclusion. □

Proposition 3.2. *For any $\varepsilon > 0$, $R_0 > 0$, and $\kappa > 0$, there exists a constant $C_{\varepsilon,R_0,\kappa} > 0$, such that if $|x| < R_0$, $|x-a| > \kappa$, $|x-b| > \kappa$ and h is sufficiently small,*

$$|\psi_0(h;x)| \leq C_{\varepsilon,R_0,\kappa}\exp\left(-\frac{\min(\rho(x,a),\rho(x,b))(1-\varepsilon)}{h}\right).$$

Proof. Let $\tilde\varphi(x) := \min(\rho(x,a),\rho(x,b))$. Then,

$$|\tilde\varphi(x)-\tilde\varphi(y)| \leq \int_0^1 d\theta\sqrt{V(\theta x+(1-\theta)y)}\,|x-y|,$$

for $x, y \in \{x|\ V(x) - \tilde{E}_0 \geq 0\}$. Hence for any $\varepsilon > 0$, $R > 0$, we can find $\delta > 0$ and $\varphi(x)$ (by convolution and cutoff), such that if $|x| < R$,

$$(1-\varepsilon)\tilde\varphi(x) \leq \varphi(x) \leq (1+\varepsilon)\tilde\varphi(x),$$

$$|\nabla\varphi(x)| \le (1-\delta)\sqrt{V(x)-\tilde{E_0}}.$$

Hence, for any $\kappa > 0$, and if $|x-a| > \kappa, |x-b| > \kappa$, we see that

$$\begin{aligned} V(x) - E_0 - (\nabla\varphi)^2 &\ge (2\delta-\delta^2)(V(x)-\tilde{E_0}) + \tilde{E_0} - E_0 \\ &\ge c_{\delta,\kappa}, \end{aligned}$$

for h sufficiently small. Where the second inequality follows from the fact that by Theorem 1, $-\tilde{E_0} = O(h^{-\alpha})$ and $\tilde{E_0} - E_0 = o(h^{-\alpha})$. Therefore, if we take ψ so that its support is contained in $\{x|\ |x-a| > \kappa, |x-b| > \kappa\}$, we have, by following the same arguement as (3.2),

$$(e^{\rho/h}\psi, (H-E_0)e^{-\rho/h}\psi) \ge c_{\delta,\kappa}\|\psi\|_2^2.$$

On the other hand, there exists κ_0 determined by κ such that, if $|y-a| \le \kappa_0$ or $|y-b| \le \kappa_0$, then $\varphi(y) < \varepsilon\varphi(x)$. By the method used in the proof of the Proposition 3.1, we can obtain

$$|\psi_0(h;x)| \le C\exp\left(-\frac{(1-\varepsilon)^2\tilde{\varphi}}{h}\right) \quad \text{on} \quad |x| < R, |x-a| > \kappa, |x-b| > \kappa.$$

□

Secondly, we consider the lower bound of ψ_0.

Lemma 3.3. *Let $\bar{e_0}$ be the lowest eigenvalue of $-\Delta$ on the $(d-1)$-demensional unit ball with Dirichlet boundary condition and let η be the corresponding eigenfunction (η is normalized so that $\|\eta\|_\infty = 1$). And let $d := \min_{|y|\le 1/2}\eta(y)$. Let D_0 be a cylinder in $\mathbf{R}^d$ such that,*

$$D_0 := \{x = (x_1, x_\perp)|\quad 0 \le x_1 \le a(1+\delta),\ |x_\perp| \le R\}.$$

Let $\Omega(x)$ be such that which satisfies $\Delta\Omega(x) = W(x)\Omega(x)$ on D_0 and $W \ge 0$, $\Omega \ge 0$ there. Let $\alpha^2 := \sup_{x\in D_0}\{\bar{e_0}R^{-2} + W(x)\}$. Then the following estimate holds.

$$\min\{\Omega(x)|\ x_1 = a,\ |x_\perp| \le \frac{R}{2}\} \ge de^{-\alpha a}(1-e^{-2\delta\alpha a})\min\{\Omega(x)|\ x_1 = 0,\ |x_\perp| \le R\}.$$

For its proof we can refer to [2].

Proposition 3.4. *Assume that any $\varepsilon > 0$, $\|J_a\psi_0\|_2\|J_b\psi_0\|_2 \ge C_\varepsilon e^{-\varepsilon/h^\beta}$ for a constant $C_\varepsilon > 0$. Then for any $\varepsilon > 0$, any compact set $K(\subset \mathbf{R}^d)$, there exists a constant $C_{\kappa,\varepsilon} > 0$ such that if $x \in K$,*

$$|\psi_0(h;x)| \ge C_{\kappa,\varepsilon}\exp\left(-\frac{\sqrt{-e_0}\min(|x-a|,|x-b|)(1+\varepsilon)}{h^\beta}\right).$$

By estimating $\rho_h(x,a)$ from below, we immediately obtain,

Corollary. *Under the same conditions as Proposition 3.4,*

$$|\psi_0(h;x)| \geq C_{\kappa,\varepsilon} \exp\left(-\frac{\min(\rho_h(x,a),\rho_h(x,b))(1+\varepsilon)}{h}\right).$$

Proof of Proposition. There is a constant $C > 0$ such that $V(x) - E_0 \geq 0$ if $|x-a| \geq Ch^\beta$. Moreover, from the proof of Lemma 4.3 (in Section 4), for any $C_1 > 0$, we can find a constant $C_2 > 0$ such that if $|x-a| \leq C_1 h^\beta$, then $|\psi_0| \geq C_2$. Hence, we take a cylinder D so that its bottom starts at the position whose distance to a is Ch^β and its top is at x, and its radius is Rh^β. Then, there exists a constant C' (determined by C and R) such that on the bottom of D, $|\psi_0| \geq C'$. Thus we can apply Lemma 3.3 to D and ψ_0. The conclusion is that, for any $\varepsilon > 0$, there exists a sufficiently small $\delta > 0$ such that for sufficiently small h,

$$|\psi_0(h;x)| \geq de^{-\alpha(x-a-\varepsilon)}\left(1-e^{-2\delta\alpha a}\right)C',$$

where $\alpha^2 := e_0R^{-2}h^{-2\beta} + \sup_{x\in D} h^{-2}(V(x)-E_0)$. By taking h sufficiently small, we can let $e^{-2\delta\alpha a} < 1/2$. Moreover, by taking R sufficiently large, we can take $e_0R^{-2} < \varepsilon^2$. Using that $-E_0 = O(h^{-\alpha})$ and the result of Theorem 1, we conclude,

$$|\psi_0(h;x)| \geq C\exp\left(-\sqrt{-e_0}h^{-\beta}|x-a|(1+\varepsilon)\right).$$

The uniformity with respect to x is obvious. □

4. The proof of Theorem 5.

The Upper Bound

Lemma 4.1. *Let f be a C^1 function which is uniformly bounded. Then*

$$(f\psi_0,(H-E_0)f\psi_0) = h^2((\nabla f)\psi_0,(\nabla f)\psi_0).$$

For its proof, we can refer to [2].

We set,

$$d_h(x) := \frac{\rho_h(x,a)-\rho_h(x,b)}{\rho_h(a,b)}.$$

Fix any $\delta > 0$. By convolution, we can find a function $d_\delta(x)$ which satisfies,

$$d_\delta(x) \in C^\infty, \quad |d_h - d_\delta| \leq \delta \quad \text{(uniformly in } h).$$

Fix any $\alpha > 0$, and take a smooth function $h(x)$ on $\mathbf{R}$ so that,

$$h(x) = \begin{cases} -1, & \text{on } (-\infty,-\alpha), \\ 1, & \text{on } (\alpha,\infty). \end{cases}$$

We set $g(x) := h(d_\delta(x))$. Then $g(x) \in C^\infty(\mathbf{R}^d)$, and $\mathrm{Supp}\nabla g$ is contained in a neiborhood of the geodesic bisector of a,b (*i.e.*, is contained in $\{x|\ d(x)=0\} =:$

$B_h\cdot$). Since $\min_{x\in B_h}\{\min(\rho_h(x,a),\ \rho_h(x,b)\} = \frac{1}{2}\rho_h(a,b)$, we can see that, for any $\varepsilon > 0$, and sufficiently small $\alpha, \delta > 0$,

$$\min_{x\in \mathrm{Supp}\nabla g}\{\min(\rho_h(x,a),\rho_h(x,b))\} \geq \frac{1}{2}\rho_h(a,b)(1-\varepsilon). \tag{4.1}$$

Now, let

$$< g >_h := \int g\psi_0^2 dx, \quad f(x) := g(x) - < g >_h .$$

Then $(f\psi_0, \psi_0) = 0$. Therefore, by Lemma 4.1, we obtain

$$E_1 - E_0 \leq \frac{h^2((\nabla f)\psi_0, (\nabla f)\psi_0)}{(f\psi_0, f\psi_0)}. \tag{4.2}$$

Claim. *For any* $\varepsilon > 0$,

$$(f\psi_0, f\psi_0) \geq C_\varepsilon e^{-\varepsilon/h^\beta}. \tag{4.3}$$

Proof of Claim. Suppose that there is a constant $C > 0$ such that $(f\psi_0, f\psi_0) \leq Ce^{-c/h^\beta}$. Assume that there is a sequence $\{h_n\}, h_n \downarrow 0$ such that $< g >_{h_n} \geq 0$. Then $|f(x)| \geq 1$ near the neiborhood of b. Hence $\|J_b\psi_0\|_2 \leq Ce^{-c/2h_n^\beta}$. On the other hand, if $< g >_{h_n} \leq 0$, then $\|J_a\psi_0\|_2 \leq Ce^{-c/2h^\beta}$. But this breaks the assumption of Theorem 5. □

Claim. *If* $x \in K$ *(a compact set of* $\mathbf{R}^d$*),* $|\nabla d_\delta| \leq C_K$ *for a constant* $C_K > 0$.

Proof of Claim. Let ρ_δ be a convolution of $\rho_h(x,a)$. We can write,

$$\nabla d_\delta(x) = \frac{\nabla\rho_\delta(x,a) - \nabla\rho_\delta(x,b)}{\rho_h(a,b)}. \tag{4.4}$$

Since $x \in K$, we can find $M > 0$ such that

$$|\nabla\rho_\delta(x,a) - \nabla\rho_\delta(x,b)| \leq 2\sqrt{M - \tilde{E}_0}. \tag{4.5}$$

For a suitable $\varepsilon > 0$, $V(x) \geq m$, on $|x-a| > \varepsilon$ and $|x-b| > \varepsilon$. Therefore,

$$\rho(a,b) \geq |a-b|\sqrt{m - \tilde{E}_0}. \tag{4.6}$$

Combining (4.4) ~ (4.6), we obtain the conclusion. □

We estimate $E_1 - E_0$ using (4.2), (4.3), the claim above, Proposion 3.1 (to estimate it in the area far from the oirigin) and Proposition 3.2. We have, for a constant $C > 0$,

$$E_1 - E_0 \leq C\exp\left(-\frac{2\min_{x\in \mathrm{Supp}\nabla g}\{\min(\rho(x,a),\rho(x,b))\}}{h}(1-\varepsilon)\right)$$

$$\text{from (4.1),} \qquad \leq C\exp\left(-\frac{\rho(a,b)(1-\varepsilon)^2}{h}\right).$$

This proves the upper bound in Theorem 5.

4.2 LOWER BOUND

Lemma 4.2. *Let $\{W_n\}_{n=1,2,\cdots}$ be a sequence of functions such that they and their derivatives converge to that of a function W_∞ locally uniformlly, and satisfy*

$$(-\Delta + W_n)\varphi_n = E_n\varphi_n, \quad (-\Delta + W_\infty)\varphi_\infty = E_\infty\varphi_\infty.$$

Assume that $E_n \to E_\infty$ and $\varphi_n \to \varphi_\infty$ in L^2_{loc}. Then, $\varphi_n \to \varphi_\infty$ locally uniformly.

For its proof, we can refer to [2].

Lemma 4.3. *Let $\psi_1(h;x)$ be the normalized eigenfunction associated to the eigenvalue E_1, and set $g_h(x) := \dfrac{\psi_1(x)}{\psi_0(x)}$. Then there exists a constant $C > 0$ such that for sufficiently small h,*

$$\textit{If} \quad |x-a| \le h^\beta, \quad g_h \ge C.$$

$$\textit{If} \quad |x-b| \le h^\beta, \quad g_h \le -C.$$

Proof of Lemma 4.3. Let ξ_a, ξ_b be the eigenstates associated to the lowest eigenvalues of the Hamiltonians whose potentials are the first term of the asymptotic expansions of V arround a, b respectively. Then ξ_a, ξ_b are written as follows,

$$\xi_a(h;x) = h^{-2d/\beta}\kappa_a(h^{-\beta}(x-a)),$$

$$\xi_b(h;x) = h^{-2d/\beta}\kappa_b(h^{-\beta}(x-b)),$$

where κ_a, κ_b are the eigenstates corresponding to the lowest eigenvalues of $h_0^{(a)}, h_0^{(b)}$ respectively. Let P_h be a projection to the subspace spanned by ξ_a, ξ_b. It is easy to see $\|(1-P_h)\psi_j\|_2 \to 0$ $(j = 1,2)$ as h tends to zero. (due to a similar arguement to Proposition 1.1) Therefore, there exist $\alpha(h) > 0, \beta(h) > 0$, such that

$$\alpha^2 + \beta^2 = 1, \quad \|\psi_0 - \alpha\xi_a - \beta\xi_b\|_2 \to 0 \quad (h \downarrow 0). \tag{4.7}$$

Since ψ_1 is orthogonal to ψ_0,

$$\|\psi_1 - \beta\xi_a + \alpha\xi_b\|_2 \to 0 \quad (h \downarrow 0). \tag{4.8}$$

By the assumption of Theorem 5, $\alpha \cdot \beta$ is bounded below. Hence α and β is bounded from above and below. If we set

$$\varphi_h := h^{d\beta/2}\alpha(h)^{-1}\psi_0(h^\beta x + a),$$

$$\tilde{\varphi_h} := h^{d\beta/2}\beta(h)^{-1}\psi_1(h^\beta x + a).$$

Then from (4.7) and (4.8), $\varphi_h, \tilde{\varphi_h}$ converge to κ_a in L^2_{loc}. Furthermore, it is easy to see that $K\varphi_h = h^\alpha E_0\varphi_h$, and $K\tilde{\varphi_h} = h^\alpha E_1\tilde{\varphi_h}$. Thus we can apply Lemma 4.2. Then $\varphi_h \to \kappa_a, \tilde{\varphi_h} \to \kappa_a$ as h tends to zero. Thus we see that $|g_h - \frac{\beta}{\alpha}| \to 0$ uniformly on $\{x \mid |x-a| \le h^\beta\}$ and similarly $|g_h + \frac{\alpha}{\beta}| \to 0$ on $\{x \mid |x-b| \le h^\beta\}$. □

Now, we are ready to prove the lower bound part of Theorem 5. Estimating $\rho_h(a,b)$ from below, we see that it is enough to show that for any $\varepsilon > 0$, there exists a constant $C > 0$ such that

$$E_1 - E_0 \geq C\exp(-\sqrt{-e_0}h^{-\beta}|a-b|(1+\varepsilon)).$$

Let γ be a straight line from a to b. Then, $\max_{x\in\gamma}\{\min\{|x-a|,|x-b|\}\} = \frac{|a-b|}{2}$. Thus for any $\varepsilon > 0$, there exists a positive constant δ such that

$$\max\{\min\{|x-a|,|x-b|\}|\operatorname{dist}(x,\gamma)\leq\delta\} \leq \frac{|a-b|}{2}(1+\varepsilon). \tag{4.9}$$

Here we use Proposition 3.4. It follows that

$$|\psi_0|^2 \geq C\exp(-\sqrt{-e_0}h^{-\beta}|a-b|(1+\varepsilon)), \tag{4.10}$$

for $x \in T_\varepsilon := \{x|\operatorname{dist}(x,\gamma)\leq\delta\}$. Taking T_ε sufficiently small if necessary, we can find smooth coordinates $y = (y_1, y_\perp)$ so that

$$T_\varepsilon = \{y|\,|y_\perp|\leq 1\},$$
$$\gamma \subset \{y|\,y_\perp = 0\},$$

and $a = (0,0)$, $b = (1,0)$. Since these coordinates are smooth and γ is a straight line from a to b, we can find $C > 0$ such that for suffciently small h,

$$\{y|\,y_1 = 0, |y_\perp| \leq Ch^\beta\} \subset \{x|\,|x-a| \leq h^\beta\},$$
$$\{y|\,y_1 = 1, |y_\perp| \leq Ch^\beta\} \subset \{x|\,|x-b| \leq h^\beta\}.$$

Let $T^{(h)} := \{y|\,|y_\perp| \leq Ch^\beta\}$. From Lemma 4.1 and the definition of g_h,

$$\begin{aligned} E_1 - E_0 &= h^2\int|\nabla g_h|^2|\psi_0|^2dx \\ &\geq h^2\int_{T^{(h)}}|\nabla g_h|^2|\psi_0|^2dx. \end{aligned}$$

We substitute (4.10) into this and change the variables from x to y. Since Jacobian is bounded above and below, $|\frac{\partial g_h}{\partial x}|$ is bounded below by $C|\frac{\partial g_h}{\partial y}|$. Therefore,

$$E_1 - E_0 \geq C\exp(-\sqrt{-e_0}h^{-\beta}|a-b|(1+\varepsilon))\int_{|y_\perp|\leq Ch^\beta}dy_\perp\int_0^1 dy_1\left|\frac{\partial g_h}{\partial y}\right|^2. \tag{4.11}$$

On the other hand,

$$\begin{aligned} |g_h(0,y_\perp) - g_h(1,y_\perp)|^2 &= \left|\int_0^1 dy_1(\frac{\partial g_h}{\partial y_1})(y_1,y_\perp)\right|^2 \\ &\leq \int_0^1 dy_1\left|\frac{\partial g_h}{\partial y}\right|^2. \end{aligned} \tag{4.12}$$

The last inequality is due to the Schwarz inequality. By Lemma 4.3, if $|y_\perp| \leq Ch^\beta$, the LHS of (4.12) is bounded below by $(2C)^2$. Therefore, we get

$$E_1 - E_0 \geq Ch^{\beta(d-1)}exp(-\sqrt{-e_0}h^{-\beta}|a-b|(1+\varepsilon)).$$

□

5. Appendix. The periodic potential

It is known that if the periodic potential have negative singularities, the spectrum of the Schrödinger operator have the band structure. We will see that the width of the lowest band have an asymptotic similar to that of Theorem 5'. The strategy is due to [8].

Assumptions of $V(x)$.

(1) There are $a_1, a_2, \cdots, a_d \in \mathbf{R}^d$, mutually independent, such that $V(x+a_j) = V(x)$ $(j = 1, \cdots, d)$.

(2) $V(x)$ has an asymptotic expansion around $a \in L := \{n_j a_j; n_j = 0, \pm 1, \cdots\}$ in the following form,

$$V(x) \sim -\frac{1}{|x-a|^{\rho+1}} \sum_{|\alpha|=1}^{\infty} a_\alpha (x-a)^\alpha.$$

(3) $V(x) \in C^\infty(\mathbf{R}^d \setminus L)$

(4) If $d \leq 3$, $\rho < d/2$. If $d \geq 4$, $\rho < 2$.

Now we shall decompose $H(h) := -h^2\Delta + V(x)$ on $L^2(\mathbf{R}^d)$ into the direct integral.

Definition.

(1) We say a mesurable set $C \subset \mathbf{R}^d$ is a fundamental cell if and only if, (a) For any $a \in L$, $C + a$ and C are disjoint. (b) $\mathbf{R}^d \setminus \cup_{a \in L}(a + C)$ has measure zero.

(2) A fundamental cell W is a Wigner-Seitz cell if and only if,
$W = \{x | \ x$ is the nearest point to the origin among all $a \in L$ with respect to the Euclidian metric$\}$.

(3) We define the dual lattice of L (denoted by L^*) if and only if,

$$k \in L^* \Leftrightarrow \frac{1}{2\pi} k \cdot a \in \mathbf{Z} \quad \text{for } any\ a \in L.$$

(4) The Brillouin zone B is defined as the Wigner Seitz cell of L^*.

We take any fundamental cell: C. For each $k \in B$, we define Hilbert space $\mathcal{H}_k$ as follows,

$$\mathcal{H}_k := \{f \in L^2_{loc} \mid f(x+a) = e^{ik\cdot a} f(x), \quad \text{for all } a \in L\}.$$

For $f, g \in \mathcal{H}_k$, we define the inner product,

$$< f, g >:= \int_C \overline{f(x)} g(x) dx.$$

For $g \in L^2(\mathbf{R}^d)$, we define $f_k \in \mathcal{H}_k$ using the Fourier transform,

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

where $c = (2\pi)^{d/2}[vol\ C]^{-1/2}$. This gives an isomorphism between $L^2(\mathbf{R}^d)$ and $\int_B^{\oplus} \mathcal{H}_k dk$. The fiber of H is,

$D_k := \{f \in \mathcal{H}_k |$ the Laplacian of f (in the sense of distribution) belongs to $\mathcal{H}_k\}$.

And for $f \in D_k$, we define

$$(H(h;k)f)(x) := -h^2(\Delta f)(x) + V(x)f(x).$$

From the Assumption, $H(h;k)$ is self-adjoint on D_k, and has compact resolvent, and

$$H(h) = \int_B^{\oplus} H(h;k)dk.$$

Let $\varepsilon_0(h;k) \le \varepsilon_1(h;k) \le \cdots$ denote the spectrum of $H(h;k)$. Hence, $b_n(h) := \cup_{k\in B} \varepsilon_n(h;k)$ is the n-th band of H. The similar arguement as Theorem 1 proves (for detail, see [8]),

Theorem A.1. *Let* $e_0 \le e_1 \le \cdots$ *be the eigenvalues of* $h_0 := -\Delta - \frac{1}{|x|^{\rho+1}} \sum_{|\alpha|=1} a_\alpha x^\alpha$. *It follows that*

$$\lim_{h\downarrow 0} h^\alpha \varepsilon_n(h;k) = e_n, \quad \alpha = \frac{2\rho}{2-\rho},$$

and the convergence is uniform with respect to k.

We see from Theorem A.1, that the width of each band behaves $|b_n(h)| \to 0$ as h tends to zero. We shall estimate $|b_0(h)|$ in more detail.

Theorem A.2. *For any* $\varepsilon > 0$, *there exist constants* $C_{1,\varepsilon}, C_{2,\varepsilon}$ *such that*

$$C_{1,\varepsilon} \exp\left(-\frac{\sqrt{-e_0}}{h^\beta} \min_{a\in L} |a|(1+\varepsilon)\right) \le |b_0(h)| \le C_{2,\varepsilon} \exp\left(-\frac{\sqrt{-e_0}}{h^\beta} \min_{a\in L} |a|(1-\varepsilon)\right),$$

where $\beta = \frac{2}{2-\rho}$.

The method of its proof is basically the same as [8]. To prove Theorem A.2, we need the exponential decay of the eigenfunction ψ_0 associated to the lowest eigenvalue of $H(h;0)$.

Theorem A.3. *For any* $\varepsilon > 0$, $\kappa > 0$, *there exists constants* $C_{\varepsilon,\kappa}, C_\varepsilon$ *such that*

$$\psi_0 \le C_{\varepsilon,\kappa} \exp\left(-\frac{\sqrt{-e_0}}{h^\beta} \min_{a\in L} |x-a|(1-\varepsilon)\right) \quad on \ \min_{a\in L} |x-a| > \kappa,$$

and

$$\psi_0 \ge C_\varepsilon \exp\left(-\frac{\sqrt{-e_0}}{h^\beta} \min_{a\in L} |x-a|(1+\varepsilon)\right).$$

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