RIMS Symposia (open)

Spectral and Scattering Theory and Related Topics

November 29 - December 1, 2023
Room 420, RIMS, Kyoto University, in-person
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Program and Abstracts

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November 29 - December 1, 2023
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Program

- Wednesday, November 29
  - 13:00 - 14:00 Yohei Tanaka (Gakushuin University)
    Half-integer indices for one-dimensional gapless quantum walks
  - 14:20 - 15:20 Vincent Louatron (Ritsumeikan University)
    Semiclassical resonances for matrix Schrödinger operators with vanishing interactions at crossings of classical trajectories
  - 15:40 - 16:40 Atsuhide Ishida (Tokyo University of Science)
    On inverse scattering for time-decaying harmonic oscillators
- Thursday, November 30
  - 10:00 - 11:00 Koichi Kaizuka (Nippon Medical School)
    Some remarks on the Dirac operator on symmetric spaces
  - 11:20 - 12:20 Kazunori Ando (Ehime University)
    Inverse scattering on the metric graph for graphene
  - 14:20 - 15:20 Serge Richard (Nagoya University)
    Scattering theory and an index theorem on the radial part of $SL(2, \mathbb{R})$
  - 15:20 Group Photo,
  - 15:50 - 16:50 Tomoyuki Kakehi (University of Tsukuba)
    Snapshot problem for the wave equation
- Friday, December 1
  - 10:00 - 11:00 Yuta Nakagawa (Kyoto University)
    Asymptotic behaviors of IDS for random Schrödinger operators associated with Gibbs point processes
  - 11:20 - 12:20 Sohei Ashida (Gakushuin University)
    Lower bound of a quadratic form defined on a direct sum of Sobolev spaces of divided regions
  - 14:20 - 15:20 Kenichi Ito (University of Tokyo)
    Stationary scattering theory for C^2 *long-range potentials*

- 15:40-16:40 Free Discussion

- URL `https://hcfio.github.io/events/RIMS2023/`
- Inquiry `hc@trevally.net`
- Organizers Hiroyuki Chihara (University of the Ryukyus), Setsuro Fujiié (Ritsumeikan University)
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HALF-INTEGER INDICES FOR ONE-DIMENSIONAL GAPLESS QUANTUM WALKS

YOHEI TANAKA

§1. Preliminaries

This talk is based mainly on index theory for ***chiral-symmetric unitary operators***. More precisely, we shall focus on an abstract unitary operator U on a Hilbert space $\mathcal{H}$, which satisfies the following algebraic condition;

$$U^* = \varGamma U \varGamma, \tag{1}$$

where $\varGamma$ can be any unitary self-adjoint operator on $\mathcal{H}$. Note that $\varGamma$ allows us to decompose the underlying Hilbert space $\mathcal{H}$ into an orthogonal sum of the form $\mathcal{H} = \ker(\varGamma - 1) \oplus \ker(\varGamma + 1)$ as is well-known, and that the ***chiral-symmetry condition*** (1) implies that the spectrum of U, denoted by $\sigma(U)$, is symmetric about the real axis.

If U is a chiral-symmetric unitary operator satisfying (1) and if $R = (U + U^*)/2$ denotes the real part of U, then it follows from (1) that the self-adjoint operator R can be written as a diagonal block-operator matrix of the form $R = R_1 \oplus R_2$ with respect to $\mathcal{H} = \ker(\varGamma - 1) \oplus \ker(\varGamma + 1)$. We obtain

$$\ker(U \mp 1) = \ker(R \mp 1) = \ker(R_1 \mp 1) \oplus \ker(R_2 \mp 1). \tag{2}$$

This motivates us to introduce $\operatorname{ind}_{\pm}(\varGamma, U) := \dim\ker(R_1 \mp 1) - \dim\ker(R_2 \mp 1)$. Note that this formal index is well-defined, if $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$. We get $|\operatorname{ind}_{\pm}(\varGamma, U)| \leq \dim\ker(U \mp 1)$ by (2).

§2. A concrete example

We consider the following block-operator matrices on the Hilbert space $\ell^2(\mathbb{Z}, \mathbb{C}^2) = \ell^2(\mathbb{Z}, \mathbb{C}) \oplus \ell^2(\mathbb{Z}, \mathbb{C})$ of square-summable $\mathbb{C}^2$-valued sequences on $\mathbb{Z}$:

$$\varGamma := \begin{pmatrix} 1 & 0 \\ 0 & L^* \end{pmatrix} \begin{pmatrix} p & \sqrt{1-p^2} \\ \sqrt{1-p^2} & -p \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & L \end{pmatrix}, \qquad \varGamma' := \begin{pmatrix} a & \sqrt{1-a^2} \\ \sqrt{1-a^2} & -a \end{pmatrix}. \tag{3}$$

where L is the left-shift operator on $\ell^2(\mathbb{Z}, \mathbb{C})$, and where $p = (p(x))_{x\in\mathbb{Z}}$ and $a = (a(x))_{x\in\mathbb{Z}}$ are two arbitrary sequences taking values in $[-1, 1]$. Here, p, a are viewed as the multiplication operators on $\ell^2(\mathbb{Z}, \mathbb{C})$ in the obvious way. Since $\varGamma, \varGamma'$ are unitary self-adjoint by construction, the unitary operator $U := \varGamma\varGamma'$ satisfies the chiral-symmetry condition (1). This unitary operator is often referred to as the time-evolution operator of the so-called ***(one-dimensional) split-step quantum walk***.

Theorem 1. *Let us assume the existence of the following limits for each* $\star = -\infty, +\infty$:

$$p(\star) := \lim_{x \to \star} p(x), \qquad a(\star) := \lim_{x \to \star} a(x). \tag{4}$$

Then $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$ *if and only if* $p(\star) \mp a(\star) \neq 0$ *for each* $\star = -\infty, +\infty$. *In this case, we have*

$$\operatorname{ind}_{\pm}(\varGamma, U) = \frac{\operatorname{sign}\,(p(+\infty) \mp a(+\infty)) - \operatorname{sign}\,(p(-\infty) \mp a(-\infty))}{2}, \tag{5}$$

where sign *denotes the sign function, and where we set* $\operatorname{sign} 0 := 0$.

A sketch of proof. It follows from the *half-step decomposition method*[1] that $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$ if and only if $X_{\pm} := (\mp\sqrt{(1+p)(1 \mp a)} + \sqrt{(1 - p(\cdot - 1))(1 \pm a)}L^*)/2$ is a Fredholm operator. In this case, $\operatorname{ind}_{\pm}(\varGamma, U)$ coincides with the Fredholm index of $X_{\pm}$. The remaining part of the claim follows from the fact that $X_{\pm}$ can be identified with the orthogonal sum of two Toeplitz operators constructed from (4), since we have the invariance of the Fredholm index and essential spectum with respect to compact perturbations. □

§3. A generalisation of the index formula

A bounded operator A on $\mathcal{H}$ is called ***trace-compatible***, if $A^*A - AA^*$ is of trace-class. For such A, we define

$$\operatorname{ind}_t(A) := \operatorname{Tr}(e^{-tA^*A} - e^{-tAA^*}), \qquad t \in \mathbb{R}.$$

If the limit $w(A) := \lim_{t \to \infty} \operatorname{ind}_t(A)$ exists, then we call $w(A)$ the ***Witten index*** of A (see [BGGSS87] for details).

Theorem 2. *Let* U *be the time-evolution operator of the split-step quantum walk, and let us assume the existence of limits of the form* (4)*. We also impose the following additional assumption;*

$$\sum_{x=0}^{\infty} |\zeta(-x) - \zeta(-\infty)| + \sum_{x=1}^{\infty} |\zeta(x) - \zeta(+\infty)| < \infty, \qquad \zeta = p, a. \tag{6}$$

Then $X_{\pm}$ *is trace-compatible, and the Witten index* $w(X_{\pm})$ *is given by the right hand side of* (5)*.*

A derivation of this index formula requires some scattering theoretic tools such as the spectral shift function. Note that $\operatorname{ind}_{\pm}(\varGamma, U)$ in (5) takes values from $\{-1, 0, 1\}$, since we assume $p(\star) \mp a(\star) \neq 0$ for each $\star = -\infty, +\infty$ as in Theorem 1. On the other hand we have $w(X_{\pm}) \in \{-1, 0, 1\} \cup \{-1/2, 1/2\}$, since we remove this assumption in Theorem 2.

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[CGWW21] C. Cedzich, T. Geib, A. H. Werner, R. F. Werner, Chiral floquet systems and quantum walks at half-period, Ann. Henri Poincaré **22**(2), 375–413 (2021).

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[1]This highly non-trivial step is one of the main topics of [CGWW21].

Semiclassical resonances for matrix Schrödinger operators with vanishing interactions at crossings of classical trajectories

Vincent LOUATRON (Ritsumeikan University)

1 Framework and assumptions

We investigate spectral properties in the semiclassical limit of the matrix-valued Schrödinger operator

$$P := \begin{pmatrix} P_1 & hU \\ hU^* & P_2 \end{pmatrix} \tag{1}$$

where $P_j := (hD_x)^2 + V_j(x)$, $j \in \{1, 2\}$ are the scalar Schrödinger operators, D_x is $-i\partial_x$ and $h > 0$ denotes the usual semiclassical parameter. Here U is a multiplication operator by a smooth, real-valued function $r(x)$. This model arises in the framework of the Born-Oppenheimer approximation, motivated for example by the study of the molecular predissociation phenomena in quantum chemistry (see [GM14] for an history). In this context, the imaginary part of the resonances of P is proportional to the inverse of the half-life of the particle described by P. The aim of this talk is to give an h-asymptotic expansion of the imaginary part of the resonances.

We consider potentials V_j that are analytic outside of a compact set, and we fix an energy $E_0 \in \mathbb{R}$ for which V_1 has a "simple well" and V_2 is "non-trapping". In the absence of the interaction U, P_2 has an essential spectrum, P_1 has eigenvalues that can be approximated by a Bohr-Sommerfeld quantification condition **(B-S)** and locally around E_0 we have $\sigma(P) = \sigma(P_1) \cup \sigma(P_2)$. However in the presence of the interaction term U, the eigenvalues of P_1 can shift under the real line and become *resonances* for the operator P (Fermi's golden rule). In this talk, we assume that the set $\{x \in \mathbb{R}, V_1(x) = V_2(x)\}$ is reduced to $\{0\}$ and that $V_2 - V_1$ vanish at $x = 0$ at a finite order $m \in \mathbb{N}^*$:

$$(V_2 - V_1)^{(j)}(0) = 0 \text{ for all } j \in \{0, \dots, m-1\}, \quad \text{and} \quad (V_2 - V_1)^{(m)}(0) \neq 0.$$

Moreover, we assume $E_0 > V_1(0) = V_2(0)$.

In this setting, authors in [AFH22] computed an asymptotic expansion of the imaginary part of the resonances for P. However they also assumed an elliptic condition on U, that is to say $r(0) \neq 0$ (independently of h). In this talk, we generalize the results obtained in [AFH22] by relaxing this elliptic condition. More specifically, we assume that the function r can vanish at $x = 0$ at a finite order $k \in \mathbb{N}$ satisfying $k < m$.

2 Main result

Theorem 2.1 ([Lou23]). *Consider a complex box $\mathcal{R}_h := [E_0 - Lh, E_0 + Lh] + i[-Lh, Lh]$ with $L > 0$. We note $\mathfrak{B}_h$ the set of $E \in \mathcal{R}_h$ satisfying **(B-S)**. Then for all small $h > 0$, there exist a* *one-to-one correspondance* $z_h : \mathfrak{B}_h \to \mathrm{Res}(P) \cap \mathcal{R}_h$ *satisfying* $|z_h(E) - E| = O\left(h^{1+2\frac{k+1}{m+1}}\right)$ *and, for all* $E \in \mathfrak{B}_h$,

$$\operatorname{Im} z_h(E) = -h^{1+2\frac{k+1}{m+1}} \frac{2\sqrt{2}|\omega_k|^2}{\sqrt{\mathcal{A}'(E_0)}} \left|\sin\left(\arg(\omega_k) + \frac{\mathcal{B}(E)}{2h}\right)\right|^2 + O\left(h^{1+2\frac{k+1}{m+1}+s}\right). \tag{2}$$

When both k *and* m *are odd and satisfy* $k+1 < m$*, then* $|z_h(E) - E| = O\left(h^{1+2\frac{k+2}{m+1}}\right)$ *and*

$$\operatorname{Im} z_h(E) = -h^{1+2\frac{k+2}{m+1}} \frac{2\sqrt{2}|\omega_{k,odd}|^2}{\sqrt{\mathcal{A}'(E_0)}} \left|\sin\left(\arg(\omega_{k,odd}) + \frac{\mathcal{B}(E)}{2h}\right)\right|^2 + O\left(h^{1+2\frac{k+2}{m+1}+s}\right). \tag{3}$$

Here, $\omega_k, \omega_{k,odd} \in \mathbb{C}$ *are constants independent of* E *and* h*,* $s := \min(1/3, 1/(m+1))$*,* $\mathcal{B}(E) := 2\left(\int_{a(E)}^{0} \sqrt{E - V_1(x)}dx + \int_0^{b(E)} \sqrt{E - V_2(x)}dx\right)$ *and* $\mathcal{A}(E) := 2\int_{a(E)}^{a'(E)} \sqrt{E - V_1(x)}dx$.

3 Difficulties and key ideas

The study revolves around the analysis of the microlocal solutions of $(P - E)u = 0$, called *resonant states*. Ideally, we would construct these microlocal solutions via usual WKB constructions as in the scalar case. It is possible to construct them *away* from crossing points (the construction can be brought to the scalar case). However this is not possible at the crossing points of the two classical trajectories $\Gamma_j(E_0) := \{(x, \xi) \in \mathbb{R}^2,\ \xi^2 + V_j(x) = E_0\}$.

This difficulty can be overcome by proving a **microlocal connection formula**. This formula states that the space of microlocal solutions at crossing points is two dimensional, and it states the existence of a *transfer matrix* (or microlocal scattering matrix) that describes the microlocal behavior of resonant states at the crossing points. We will give an h-asymptotic expansion of this matrix.

One way to prove this is to construct *exact* solutions in a neighborhood of the crossing points (it is possible only locally). Essentially, the h-asymptotic behavior of the transfer matrix is given by the h-asymptotic behavior of those exact solutions. Those solutions are integrals of functions of the form $\sigma(x)e^{\frac{i}{h}\phi(x)}$ whose phase ϕ has a critical point at $x = 0$ corresponding to the $x-$coordinate of the crossing points. In our case, $r(x)$ appears as a multiplicative factor in $\sigma(x)$ and also vanishes at $x = 0$ which is why we need a **stationary phase estimate** for this **degenerate case**.

References

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On inverse scattering for time-decaying harmonic oscillators

Atsuhide Ishida (Tokyo University of Science)

Different from the usual harmonic oscillator, it is known that the time-decaying harmonic oscillator accelerates the particles and constructs the scattering state. We study one of the multidimensional inverse scattering in this two-body quantum system perturbed by the short-range interaction potentials that have the bounded part and locally singular part. In this talk, applying the Enss-Weder time-dependent method, we report that the scattering operator determines interaction potentials uniquely.

Some remarks on the Dirac operator on symmetric spaces

KAIZUKA, Koichi (Nippon Medical School)

Abstract

We develop the spectral analysis for the Dirac operator on symmetric spaces of noncompact type based on harmonic analysis on Lie groups. In harmonic analysis on Lie groups, the Dirac operator have been deeply studied to characterize discrete series representations of Lie groups. In this talk, we compute the continuous spectrum of the Dirac operator on irreducible symmetric spaces of noncompact type. We show that the continuous spectrum has a spectral gap if and only if the symmetric space is isomorphic to a coset space of the special pseudo-unitary group of odd matrix size. Furthermore, we give a uniform weighted resolvent estimate for the Dirac operator under a certain assumption on the symmetric space.

Inverse Scattering on the Metric Graph for Graphene

Kazunori Ando

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We consider an inverse scattering problem on the metric graph associated with the hexagonal lattice. Metric graph consists of differential operators on each edge with suitable boundary conditions at every vertex. Here, we consider one-dimensional Schrödinger operators on the edges. We show that the potential can be determined by the scattering amplitude. In order to do this, we introduce an artificial boundary value problem and prove that the potential can be reconstructed from the Dirichlet-to-Neumann map for this boundary value problem.

Let $\Gamma = (\mathcal{V}, \mathcal{E})$ be the hexagonal lattice where $\mathcal{V}$ is the vertex set and $\mathcal{E}$ is the edge set. Every edge $\boldsymbol{e} \in \mathcal{E}$ is identified with the interval $[0, 1]$. Roughly speaking, the Schrödinger operator on $\mathcal{E}$ is a family of differential operators $-d^2/dx^2 + q_{\boldsymbol{e}}(x)$ defined on $\boldsymbol{e}$, where $q_{\boldsymbol{e}}(x) = \overline{q_{\boldsymbol{e}}(x)} \in L^2(0, 1)$. We also assume that $q_{\boldsymbol{e}}(x)$, i.e. $q_{\boldsymbol{e}}(x) = q_{\boldsymbol{e}}(1 - x)$, for every edge $\boldsymbol{e}$, and $q_{\boldsymbol{e}} = 0$ except for a finite number of edges. Moreover, we impose the Kirchhoff condition on every vertices.

We can define the scattering amplitude $A(\lambda)$ associated with the Schrödinger operator of the metric graph for $\lambda \in (0, \infty) \setminus \mathcal{T}$. Here $\mathcal{T}$ is some discrete set. The scattering amplitude $A(\lambda)$ is defined passing through the singularity expansion of generalized eigenfunctions in the momentum space. This method is used in the study of discrete Schrödinger operators on the periodic lattices.

The main result is the following:

Theorem 1. *Suppose that we know the scattering amplitude $A(\lambda)$ associated the Schrödinger operator for $\lambda \in I$ where I is an open interval in $(0, \infty) \setminus \mathcal{T}$. Then we can determine $q = \{q_{\boldsymbol{e}}\}_{\boldsymbol{e} \in \mathcal{E}}$ uniquely.*

References

[1] Kazunori Ando, Hiroshi Isozaki, Evgeny Korotyaev, and Hisashi Morioka. Inverse Scattering on the Metric Graph for Graphene. preprint

Scattering theory and an index theorem on the radial part of $SL(2, \mathbb{R})$

Serge Richard (Nagoya University)

In this talk, we present the spectral and scattering theory of the Casimir operator acting on the radial part of $SL(2, \mathbb{R})$. After a suitable decomposition, the initial problem consists in studying a family of differential operators acting on the half-line. For these operators, explicit expressions can be found for the resolvent, the spectral density, and the Moeller wave operators, in terms of Gauss hypergeometric functions. Finally, an index theorem is introduced and discussed. This work is a first attempt to connect group theory, special functions, scattering theory, C^*-algebras, and Levinson's theorem. This presentation is based on a joint work with H. Inoue.

Snapshot problem for the wave equation

Tomoyuki Kakehi (University of Tsukuba)

Abstract.

In this talk, we deal with the uniqueness and the existence of the solution to the wave equation $\partial_t^2 u - \Delta u = 0$ on $\mathbb{R}^n$ with several snapshots. More precisely, our problem is formulated as follows. For given times $t_1, \cdots, t_m \in \mathbb{R}$, and for m given smooth functions $f_1, \cdots, f_m$ on $\mathbb{R}^n$, we consider the wave equation

$$\partial_t^2 u(t,x) - \Delta u(t,x) = 0, \qquad (t,x) \in \mathbb{R} \times \mathbb{R}^n,$$

with the condition $u|_{t=t_1} = f_1, \cdots, u|_{t=t_m} = f_m$. It is natural to ask when the above equation has a unique solution. We call the above problem the snapshot problem for the wave equation, and the set of m functions $\{f_1, \cdots, f_m\}$ the snapshot data.

Roughly speaking, our main results are as follows.

(1) If we take two snapshots, namely, $m = 2$, then the uniqueness for the snapshot problem does not hold.

(2) If we take three snapshots, namely, $m = 3$, and if the ratio $(t_3 - t_1)/\pi(t_2 - t_1)$ is irrational, then the uniqueness for the snapshot problem holds.

(3) We assume that $m = 3$ and $(t_3 - t_1)/\pi(t_2 - t_1)$ is irrational and not a Liouville number. In addition, we assume a certain compatibility condition on the snapshot data $\{f_1, f_2, f_3\}$. Then the snapshot problem for the wave equation has a unique solution.

If we have enough time, we would like to mention a generalization to the wave equation on symmetric spaces.

This is a joint work with Jens Christensen, Fulton Gonzalez, and Jue Wang.

- Group Photo (about 15:20 Nov 30)

- Wireless LAN in RIMS
  - ssh connection and website browsing are available.
  - How to get your account using your smartphone
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Asymptotic behaviors of IDS for random Schrödinger operators associated with Gibbs point processes

Yuta Nakagawa*

In this talk, we consider the integrated density of states $N(\lambda)$ of the random Schrödinger operators with nonpositive potentials associated with the Gibbs point processes. For some Gibbs point processes, the leading terms of $N(\lambda)$ as $\lambda \downarrow -\infty$ are determined, which are very different from that for a Poisson point process, which is known. This presentation is based on [2].

1 Introduction

We consider the random Schrödinger operator on $L^2(\mathbb{R}^d, dx)$ defined by

$$H_\omega = -\Delta + V_\omega, \quad V_\omega(x) = \sum_{y \in \Gamma(\omega)} u(x-y),$$

where u, called *single site potential*, is a nonpositive continuous measurable function on $\mathbb{R}^d$ with compact support, and Γ is a point process, i.e. a random variable with values in sets of points in $\mathbb{R}^d$.

When Γ is a stationary Poisson point process, the *integrated density of states (IDS)* $N(\lambda)$ of the Schrödinger operator is formally given by

$$\lim_{L \to \infty} \frac{1}{L^d} \#\{\text{eigenvalues of } H^D_{\omega,L} \text{ less than or equal to } \lambda\},$$

where $H^D_{\omega,L}$ is the operator H_ω restricted to the box $(-L/2, L/2)^d \subset \mathbb{R}^d$ with Dirichlet boundary condition. Then the IDS and the spectrum of H_ω are independent of ω almost surely, and $N(\lambda)$ is a nondecreasing function increasing only on the spectrum (see [4]). It is known that

$$\log N(\lambda) \sim \frac{\lambda \log|\lambda|}{|\min u|} \quad (\lambda \downarrow -\infty), \tag{1}$$

which is proved by Pastur (see [3]).

In this talk, we consider the case where Γ is a *Gibbs point process* i.e. point processes with interaction between the points (see [1]), and investigate the asymptotic behaviors of $N(\lambda)$ as $\lambda \downarrow -\infty$.

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2 Main result

If the interaction is sufficiently weak, the asymptotic behavior of the IDS is identical to (1). However, when the interaction is *pairwise interaction*, the behavior can be different.

Theorem 1. *In the case of the pairwise interaction: the energy of the points* $\{x_j\}$ *is*

$$a \sum_{i<j} 1_{[0,R]}(|x_i - x_j|) \quad (a, R > 0),$$

we have

$$\log N(\lambda) \sim -\frac{a}{2\|u\|_R^2}\lambda^2 \quad (\lambda \downarrow -\infty),$$

where

$$\|u\|_R^2 = \sup\{\sum_{j=1}^{\infty} u(x_j)^2 \mid |x_i - x_j| > R \ (i \neq j)\}$$

This implies that the IDS decays much faster than that for a Poisson point process.

References

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[3] L. A. Pastur, The behavior of some Wiener integrals as $t \to \infty$ and the density of states of Schrödinger equations with random potential, *Teor. Mat. Fiz.* **32**, 88–95 (1977) (in Russian).

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LOWER BOUND OF A QUADRATIC FORM DEFINED ON A DIRECT SUM OF SOBOLEV SPACES OF DIVIDED REGIONS

SOHEI ASHIDA

Gakushuin University

1. Introduction

1.1. **Connection of locally constructed solutions.** We consider the Schrödinger equation

$$(-\Delta + V)u = Eu, \tag{1.1}$$

in $\mathbb{R}^n$, where Δ is the Laplacian, V is a real valued function in $\mathbb{R}^n$, u is the eigenfunction and E is the eigenvalue. When the space dimension n is 1, exceptionally detailed information of the eigenfunctions and the eigenvalues is obtained by connecting solutions constructed on intervals at the end points of the intervals. Since the structures of the solutions of (1.1) are strongly affected by the local behavior of the potential V (in particular, the structure of an eigenfunction of an electron in neighborhoods of nuclei is very different from that in the interstitial region), it is desirable to develop methods that construct local solutions in several regions $\Omega_1, \ldots, \Omega_N$ and connect the solutions at the boundaries $\Omega_\alpha \cap \Omega_\beta,\ \alpha \neq \beta$ also in the case of $n \geq 2$.

Actually, exact local solution itself is difficult to obtain when $n \geq 2$ in general. Nevertheless, in physical situations we can speculate local basis functions that approximate the local true solutions by their linear combinations. Thus it is expected to obtain approximations of the true eigenfunctions by the linear combinations of the basis functions $u_\alpha^i,\ i = 1, 2, \ldots$ in different regions $\Omega_\alpha,\ \alpha = 1, \ldots, N$. However, these linear combinations can not be connected exactly on the boundaries $\Omega_\alpha \cap \Omega_\beta,\ \alpha \neq \beta$ as stated above. Instead, in practical calculations a feasible method would be to construct linear combinations $u^i,\ i = 1, \ldots M$ that have only small discontinuity on the boundaries $\Omega_\alpha \cap \Omega_\beta$ first, and then solve the secular equation by these functions u^i as in the Rayleigh-Ritz method.

The problem of this method is that the relation between the true eigenvalues and the approximations of the eigenvalues obtained by solving the secular equation are not clear as in the Rayleigh-Ritz method because of the discontinuity of the functions u^i on the boundaries $\Omega_\alpha \cap \Omega_\beta$, that is, the eigenvalues $\tilde{E}_i(u^1, \ldots, u^M),\ i = 1, \ldots, M$ obtained by the secular equation are not upper bounds of the true eigenvalues, and $\inf_{\{u^1, \ldots, u^M\}} \tilde{E}_i(u^1, \ldots, u^M),\ i = 1, \ldots, M$ do not coincide with the true eigenvalues in contrast to the Rayleigh-Ritz method.

1.2. **Augmented plane wave (APW) method.** The augmented plane wave (APW) method is one of the methods of band structure calculations in solid state physics and an example in which the problem as above arises. The purpose of the APW method is to obtain eigenvalues of the Bloch functions. The Bloch function is a generalized eigenfunction in a periodic lattice with the primitive translation vectors $a_1, \ldots, a_n$. The Bloch function restricted to the unit cell $D := \{x = \sum_{i=1}^n c_i a_i : \forall i, 0 < c_i < 1\}$ is an eigenfunction of the selfadjoint operator $-\Delta + V$ in $L^2(D)$ (the selfadjointness can be proved under a mild assumption on the potential) with the domain

$$\{u \in H^2(D) : \forall j, u(x + a_j) = e^{ik\cdot a_j} u(x),\ (G_j \cdot \nabla)u(x + a_j) = e^{ik\cdot a_j}(G_i \cdot \nabla)u(x),\ x = \sum_{l \neq j} c_l a_l,\ 0 < c_l < 1\}, \tag{1.2}$$

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for some $k \in \mathbb{R}^n$, where $G_i \in \mathbb{R}^n$ is the reciprocal lattice vector such that $G_i \cdot a_j = 2\pi\delta_{ij}$. We can also prove that the spectrum of the operator is discrete, the eigenvalue E_m (labeled in ascending order) depend analytically on k if it is simple, and $E_m \to \infty$ $(m \to \infty)$. We divide D into regions as $D = \Omega_1 \cup \left(\bigcup_{\alpha=2}^N \overline{\Omega}_\alpha\right)$,

$$\Omega_\alpha := \{x : |x - \bar{x}_\alpha| < R_\alpha\},\ \alpha = 2, \dots, N,$$
$$\Omega_1 := D \setminus \left(\bigcup_{\alpha=2}^N \overline{\Omega}_\alpha\right),$$

where $\bar{x}_\alpha,\ \alpha = 2, \dots, N$ are atomic sites and $R_\alpha > 0$. We assume that the potential has the form

$$V(x) = \begin{cases} V(|x - \bar{x}_\alpha|), & x \in \Omega_\alpha,\ \alpha = 2, \dots, N \\ 0 & x \in \Omega_1 \end{cases},$$

which is called Muffin-Tin potential. In Ω_1 the eigenfunction u is given by the linear combination of the plane waves $v_G(x) = e^{i(k+G)\cdot x}$, where G is a reciprocal lattice vector i.e. $\forall i,\ G \cdot a_i/(2\pi) \in \mathbb{Z}$. On the other hand, in $\Omega_\alpha,\ \alpha \geq 2$, we consider the linear combination

$$v_G(x) = e^{i(k+G)\cdot \bar{x}_\alpha} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{lm}^{\alpha,k+G} \chi_l^\alpha(r_\alpha, E) Y_{lm}(\theta_\alpha, \varphi_\alpha),$$

where $(r_\alpha, \theta_\alpha, \varphi_\alpha)$ is the polar coordinates of $x - \bar{x}_\alpha$, $\chi_l^\alpha(r_\alpha, E)$ is a radial function depending on the energy E, and coefficients $A_{lm}^{\alpha,k+G}$ are determined so that the right-hand side coincides with $e^{i(k+G)\cdot x}$ on the boundaries $\partial\Omega_\alpha$. We consider the secular equation of such waves $u^i = v_{G_i}$ for different G_i and the eigenvalue E is determined from the condition that the equation has a solution. However, in practice the infinitely many coefficients $A_{lm}^{\alpha,k+G}$ can not be calculated and we need to cut off the expansion at some finite number of coefficients. Thus u^i are discontinuous on the boundaries $\partial\Omega_\alpha$ and the problem stated above arises.

2. Main result

Set $Q_k := \{u = (\tilde{u}_1, \dots, \tilde{u}_N) \in \bigoplus_{\alpha=1}^N H^1(\Omega_\alpha); \forall j,\ \tilde{u}_1(x + a_j) = e^{ik\cdot a_j}\tilde{u}_1(x),\ x = \sum_{l\neq j} c_l a_l,\ 0 < c_l < 1\}$. We assume relative boundedness of V and that there exist $0 \leq a < 1,\ b \geq 0$ such that

$$\langle \tilde{u}_\alpha, |V| \tilde{u}_\alpha \rangle_{\Omega_\alpha} \leq a \|\nabla \tilde{u}_\alpha\|_{L^2(\Omega_\alpha)} + b \|\tilde{u}_\alpha\|_{L^2(\Omega_\alpha)}, \quad \alpha = 1, \dots N,$$

and that there exists $d \geq 0$ such that $E_m \leq d,\ m = 1, \dots, M$. Let $u^i = (\tilde{u}_1^i, \dots, \tilde{u}_N^i) \in Q_k \cap (\bigoplus_{\alpha=1}^N H^2(\Omega_\alpha)),\ i = 1, \dots, M,\ \ \langle u^i, u^j \rangle = \delta_{ij}$ and set $h_{ij} := \langle \nabla u^i, \nabla u^j \rangle + \langle u^i, V u^j \rangle$, where $\langle u, v \rangle := \sum_{\alpha=1}^N \langle \tilde{u}_\alpha, \tilde{v}_\alpha \rangle_{\Omega_\alpha}$ and $\nabla u^i := (\nabla \tilde{u}_1^i, \dots, \nabla \tilde{u}_N^i)$. We denote by $\tilde{E}_m$ the mth eigenvalue of (h_{ij}). The following is the main result.

Theorem 2.1. *There exist constants $C, \delta > 0$ depending only on $\{\Omega_\alpha\}$, a, b and d such that if*

$$\sum_{i=1}^M \sum_{\alpha\neq\beta} \|\tilde{u}_\alpha^i|_{\partial\Omega_\alpha} - \tilde{u}_\beta^i|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha\cap\partial\Omega_\beta)} + \sqrt{M} \max_{1\leq i\leq M} \sum_{\alpha\neq\beta} \|\tilde{u}_\alpha^i|_{\partial\Omega_\alpha} - \tilde{u}_\beta^i|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha\cap\partial\Omega_\beta)} < \delta,$$

we have for any $1 \leq m \leq M$,

$$\tilde{E}_m \geq E_m - CM^2 \sum_{i=1}^M \sum_{\alpha\neq\beta} \|\tilde{u}_\alpha^i|_{\partial\Omega_\alpha} - \tilde{u}_\beta^i|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha\cap\partial\Omega_\beta)}.$$

Thus the difference between E_m and the infimum of $\tilde{E}_m$ with respect to $\{u^i\}$ is estimated by the discontinuity of u^i on the boundaries. We also have a similar result for nonperiodic case in $\mathbb{R}^n$.

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Stationary scattering theory for C^2 long-range potentials

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1. Setting

In this talk, based on a joint work with Erik Skibsted (Aarhus University), we discuss the stationary scattering theory for the Schrödinger operator

$$H = \frac{1}{2}p^2 + V + q \quad \text{on } \mathcal{H} = L^2(\mathbb{R}^d) \text{ with } d \geq 2.$$

Assumption. Let $V \in C^2(\mathbb{R}^d;\mathbb{R})$, $q \in L^\infty(\mathbb{R}^d;\mathbb{R})$, and assume there exists $\sigma \in (0,1)$ and $C > 0$ such that for any $|\alpha| \leq 2$

$$|\partial^\alpha V| \leq C\langle x\rangle^{-\sigma-|\alpha|}, \quad |q(x)| \leq C\langle x\rangle^{-1-\sigma}.$$

Remark. Ikebe–Isozaki '82 and Gâtel–Yafaev '99 discussed the stationary theory for C^4 and C^3 potentials, respectively. Hörmander called $V+q$ a *2-admissible potential*, and constructed the time-dependent theory for it.

2. Eikonal equation

Theorem. *Let $\lambda_0 > 0$. Then there exist $R > 0$ and*

$$S = (2\lambda)^{1/2}|x|(1+s) \in C^2\big((\lambda_0,\infty) \times \{|x| > R\}\big)$$

such that:

1. *S solves*
$$\frac{1}{2}|\nabla_x S(\lambda,x)|^2 + V(x) = \lambda;$$
2. *$S(\lambda,\cdot)$ is the distance from $\{|x| = R\}$ w.r.t. $g = 2(\lambda - V)\,\mathrm{d}x^2$;*
3. *There exists $C > 0$ such that for any $k + |\alpha| \leq 2$*
$$\big|\partial_\lambda^k \partial_x^\alpha s(\lambda,x)\big| \leq C\lambda^{-1-k}\langle x\rangle^{-\sigma-|\alpha|}.$$

3. Stationary scattering matrix

Let $\mathcal{B}$, $\mathcal{B}^*$ and $\mathcal{B}^*_0$ be the Agmon–Hörmander spaces. Set for any $\xi \in \mathcal{G} := L^2(\mathbb{S}^{d-1})$

$$\phi^S_\pm[\xi](\lambda,x) = \frac{(2\pi)^{1/2}}{(2\lambda)^{1/4}}\chi(|x|/R)|x|^{-(d-1)/2}\mathrm{e}^{\pm\mathrm{i}S(\lambda,x)}\xi(x/|x|),$$

respectively, where $\chi \in C^\infty(\mathbb{R})$ with $\chi(t) = 0$ for $t \geq 1$ and $\chi(t) = 1$ for $t \geq 2$.

Theorem. *There exist continuous mappings $F^\pm\colon (\lambda_0,\infty) \times \mathcal{B} \to \mathcal{G}$ such that for any $(\lambda,\psi) \in (\lambda_0,\infty) \times \mathcal{B}$*

$$R(\lambda \pm \mathrm{i}0)\psi - \phi^S_\pm\big[F^\pm(\lambda)\psi\big](\lambda,\cdot) \in \mathcal{B}^*_0,$$

respectively. Moreover, they satisfy for any $\lambda > \lambda_0$:

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1. *One has*
$$(H-\lambda)F^{\pm}(\lambda)^*=0,\quad F^{\pm}(\lambda)^*F^{\pm}(\lambda)=\delta(H-\lambda),$$
respectively, where $\delta(H-\lambda)=\pi^{-1}\operatorname{Im}R(\lambda+\mathrm{i}0)\in\mathcal{L}(\mathcal{B},\mathcal{B}^*)$*.*

2. *For any* $\lambda>\lambda_0$*,* $F^{\pm}(\lambda)\colon\mathcal{B}\to\mathcal{G}$ *are surjective.*

Definition. 1. $F^{\pm}(\lambda)\colon\mathcal{B}\to\mathcal{G}$ are the *stationary wave operators*, and they are *complete* if they are surjective.

2. $F^{\pm}(\lambda)^*\colon\mathcal{G}\to\mathcal{B}^*$ are the *stationary wave matrices*.
3. The *stationary scattering matrix* $\mathsf{S}(\lambda)$ is a unitary operator on $\mathcal{G}$ obeying
$$F^{+}(\lambda)=\mathsf{S}(\lambda)F^{-}(\lambda).$$

Corollary. *The stationary scattering matrix* $\mathsf{S}(\lambda)$ *uniquely exists. Moreover, it is strongly continuous in* λ*.*

4. Asymptotics of generalized eigenfuctions

Set
$$\mathcal{E}_\lambda=\bigl\{\phi\in\mathcal{B}^*;\ (H-\lambda)\phi=0\text{ in the distributional sense}\bigr\}.$$

Theorem. *1. For any one component of* $(\xi_-,\xi_+,\phi)\in\mathcal{G}\times\mathcal{G}\times\mathcal{E}_\lambda$ *the other two components uniquely exist such that*
$$\phi-\phi_+^S[\xi_+](\lambda,\cdot)+\phi_-^S[\xi_-](\lambda,\cdot)\in\mathcal{B}_0^*.$$

2. *The above correspondence is given by the formulas*
$$\phi=2\pi\mathrm{i}F^{\pm}(\lambda)^*\xi_{\pm},\quad \xi_+=\mathsf{S}(\lambda)\xi_-.$$

3. $F^{\pm}(\lambda)^*\colon\mathcal{G}\to\mathcal{E}_\lambda\subseteq\mathcal{B}^*$ *are topological linear isomorphisms.*

4. $\delta(H-\lambda)\colon\mathcal{B}\to\mathcal{E}_\lambda$ *is surjective.*

5. Generalized Fourier transforms

Set $I=(\lambda_0,\infty)$, and we let
$$\mathcal{H}_I=P_H(I)\mathcal{H},\quad H_I=H_{|\mathcal{H}_I},\quad \widetilde{\mathcal{H}}_I=L^2(I,\mathrm{d}\lambda;\mathcal{G}).$$

Thanks to the continuity of $F^{\pm}$, we have
$$\mathcal{F}_0^{\pm}:=\int_I^{\oplus}F^{\pm}(\lambda)\,\mathrm{d}\lambda\colon\mathcal{B}\to C(I;\mathcal{G}).$$

Theorem. *The above* $\mathcal{F}_0^{\pm}$ *induce unitary operators* $\mathcal{F}^{\pm}\colon\mathcal{H}_I\to\widetilde{\mathcal{H}}_I$*, respectively. Moreover, they satisfy*
$$\mathcal{F}^{\pm}H_I(\mathcal{F}^{\pm})^*=M_\lambda,$$
respectively.

We will also discuss the time-dependent scattering theory, and present stationary representation of the time-dependent wave operators. Key ingredients of the proofs are (1) Hörmander's regularization of V, (2) Estimates for a solution to the eikonal equation, cf. Cruz–Skibsted '13, (3) The strong radiation bounds, and (4) The WKB approximation for $R(\lambda\pm\mathrm{i}0)$. We will mainly focus on (3) in the rest of the talk.