Discrete Schrödinger operators and Finsler metric

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Abstract

In this article, we review the results in [9] on the Agmon estimate for discrete Schrödinger operators. We first discuss the semiclassical analysis for discrete Schrödinger operators with emphasis on the microlocal analysis on the torus. We discretize a semiclassical continuous Schrödinger operator with mesh size proportional to the semiclassical parameter. Under this setting, we show the Agmon estimate for eigenfunctions. The natural Agmon metric for the discrete Schrödinger operator is a Finsler metric rather than a Riemannian metric. It turned out that Klein-Rosenberger (2008) already discussed the semiclassical Agmon estimate in terms of the same Finsler metric by a different argument in the special case of a potential minimum. We also show the Agmon estimate and the optimal anisotropic exponential decay of eigenfunctions for discrete Schrödinger operators in the non-semiclassical standard setting.

1 Introduction

1.1 Discrete Schrödinger operators

In this article, we review the results in [9]. We recall the discrete Schrödinger operator

$$Hu(x) = -\sum_{|x-y|=1} (u(y) - u(x)) + V(x)u(x),$$

where $u \in \ell^2(\mathbb{Z}^d)$.

If the potential $V : \mathbb{Z}^d \to \mathbb{R}$ is bounded, we see that H is a bounded self-adjoint operator. Of course, there are many works on discrete Schrödinger operators. We study a semiclassical setting for discrete Schrödinger operators. We discuss the exponentially small semiclassical estimate of the eigenfunctions in terms of a Finsler metric. We also prove the optimal anisotropic exponential decay of the eigenfunctions for non-semiclassical discrete Schrödinger operators.

1.2 Finsler metric

Finsler metric is a generalization of Riemannian metric. Roughly speaking, a Finsler metric measures the length of tangent vectors by norms, while a Riemannian metric does by inner products. The relation is similar to that between Banach space and Hilbert space in functional analysis. The precise definition of Finsler metric is as follows ([2, Section 1.1]). Suppose that a nonnegative number $L(x, v)$ is given for any point x on a given smooth manifold and any tangent vector v at x. We say that L is a Finsler metric if the following hold.

1. $L(x, v)$ is smooth near any (x, v) with $v \neq 0$.

2. $L(x, \lambda v) = \lambda L(x, v)$ for any (x, v) and $\lambda > 0$.

3. $\partial_v^2 L(x, v)^2$ is positive definite for any (x, v) with $v \neq 0$.

In general, it may not be true that $L(x, v) = L(x, -v)$. The Finsler metric in this article satisfies $L(x, v) = L(x, -v)$.

We discuss a relation between discrete Schrödinger operators and Finsler metric. This relation appears if we study discrete Schrödinger operators from the viewpoint of semiclassical analysis.

2 Semiclassical analysis for discrete Schrödinger operators

2.1 Semiclassical analysis

We recall semiclassical analysis for the continuous Schrödinger operator

$$H^{\mathrm{cont}}(h) = -h^2 \Delta + V(x) \quad \text{on} \quad L^2(\mathbb{R}^d).$$

Semiclassical analysis studies its semiclassical $(h \to 0)$ behavior with emphasis on

$$p^{\mathrm{cont}}(x, \xi) = \xi^2 + V(x) \quad \text{on} \quad T^* \mathbb{R}^d.$$

See for instance [16] for semiclassical analysis. We would like to consider a discrete analogue. Since the discrete Laplacian is a bounded operator, the straightforward generalization does not seem to be so interesting.

2.2 Discretization

If we discretize $H^{\mathrm{cont}}(h)$ with mesh size $\tau > 0$, we obtain a discrete Schrödinger operator $H^{\tau}(h)$ on $\ell^2(\tau \mathbb{Z}^d)$ defined by

$$H^{\tau}(h) u(x) = -\left(\frac{h}{\tau}\right)^2 \sum_{|x-y|=\tau} (u(y) - u(x)) + V(x) u(x),$$

where $x, y \in \tau \mathbb{Z}^d \subset \mathbb{R}^d$ and $u \in \ell^2(\tau \mathbb{Z}^d)$.

There are several works on "$\lim_{\tau \to 0} H^{\tau}(h) = H^{\mathrm{cont}}(h)$" for fixed $h > 0$. This is the problem of the continuum limit. See [7], [13]. In this article, we set $\tau = h$ and consider the limit $h \to 0$. It will be interesting to study $\tau = h^{\alpha}$ for $1 < \alpha < \infty$. The continuum limit formally corresponds to $\alpha = \infty$.

2.3 Semiclassical discrete Schrödinger operators

We then study

$$H(h)u(x) = -\sum_{|x-y|=h} (u(y) - u(x)) + V(x)u(x)$$

on $\ell^2(h\mathbb{Z}^d)$, where $V : \mathbb{R}^d \to \mathbb{R}$. This is unitarily equivalent to the discrete Schrödinger operator on $\ell^2(\mathbb{Z}^d)$ with the potential $V(hx)$.

When $d = 1$, this was studied by Helffer-Sjöstrand [6] in the context of the Harper operator

$$H_{\theta,h}u(n) = \frac{1}{2}(u(n+1) + u(n-1)) + \cos(hn + \theta)u(n)$$

on $\ell^2(\mathbb{Z})$. This operator is related to the problem of the 2d-electron in a periodic electric potential and a periodic magnetic field. For general d, see the discussions in Subsection 3.5.

2.4 Microlocal analysis on the torus

We set $\mathbb{T}^d = \mathbb{R}^d/2\pi\mathbb{Z}^d$. The coordinate of $\mathbb{T}^d$ is denoted by ξ and the dual variable is denoted by x. We identify functions on $\mathbb{T}^d$ or $T^*\mathbb{T}^d$ with those on $\mathbb{R}^d$ or $T^*\mathbb{R}^d$ which are $2\pi\mathbb{Z}^d$-periodic with respect to ξ.

We define $a(\xi, hD_\xi) : C^\infty(\mathbb{T}^d) \to C^\infty(\mathbb{T}^d)$ by

$$a(\xi, hD_\xi)u(\xi) = (2\pi h)^{-d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} a(\xi, x)e^{i\langle \xi-\eta, x\rangle/h}u(\eta)d\eta dx$$

for $a \in C_b^\infty(T^*\mathbb{T}^d)$ and $u \in C^\infty(\mathbb{T}^d)$. Although this definition is based on the special structure of the torus, we can employ the general theory of pseudodifferential operators on manifolds.

2.5 Quantum-classical correspondence

The semiclassical discrete Fourier transform $\mathcal{F}_h : \ell^2(h\mathbb{Z}^d) \to L^2(\mathbb{T}^d)$ is defined by

$$\mathcal{F}_h u(\xi) = (2\pi)^{-d/2} \sum_{x \in h\mathbb{Z}^d} u(x)e^{i\langle x,\xi\rangle/h}.$$

We then have

$$\begin{aligned} \widetilde{H}(h) \overset{\text{def}}{=} \mathcal{F}_h H(h) \mathcal{F}_h^{-1} &= \sum_{j=1}^d (2 - 2\cos\xi_j) + V(hD_\xi) \\ &= p(\xi, hD_\xi), \end{aligned}$$

where $p(\xi, x) = \sum_{j=1}^d (2 - 2\cos\xi_j) + V(x) \in C^\infty(T^*\mathbb{T}^d)$. Thus our semiclassical setting is natural from the viewpoint of semiclassical analysis and we expect "$\lim_{h\to 0} H(h) = p(\xi, x)$".

2.6 The Weyl law

As an illustration of "$\lim_{h\to 0} H(h) = p(\xi, x)$", we present the following Weyl law. Assume that $V \in C_b^\infty(\mathbb{R}^d; \mathbb{R})$, $\underline{\lim}_{|x|\to\infty} V(x) \geq 0$ and there exists $0 < \theta \leq 1$ such that

$$|\partial^\alpha V(x)| \leq C_\alpha (1 + |x|)^{-\theta|\alpha|} \tag{1}$$

for any $\alpha \in \mathbb{Z}_{\geq 0}^d$. Then for any fixed $a < b < 0$, the number $N_{[a,b]}(h)$ of eigenvalues of $H(h)$ in $[a, b]$ satisfies

$$N_{[a,b]}(h) = (2\pi h)^{-d} \mathrm{Vol}(\{(\xi, x) \in T^*\mathbb{T}^d |\, a \leq p(\xi, x) \leq b\}) + o(h^{-d})$$

when $h \to 0$.

The condition (1) comes from a technical reason. The proof follows the standard strategy.

3 The semiclassical Agmon estimate for discrete Schrödinger operators

3.1 Usual Agmon estimate

The Agmon estimate ([1]) describes the exponential decay of eigenfunctions. We recall the semiclassical Agmon estimate for $H^{\mathrm{cont}}(h) = -h^2\Delta + V(x)$. For $E \in \mathbb{R}$, the Agmon metric is defined by

$$ds_E^{\mathrm{cont}} = \sqrt{(V(x) - E)_+}\, ds,$$

where ds is the length of the standard metric on $\mathbb{R}^d$. Note that this vanishes on the classically allowed region $\mathcal{G}_E = \{x \in \mathbb{R}^d |\, V(x) \leq E\}$. This induces the (pseudo-)distance $d_E^{\mathrm{cont}}(x, y)$. Set $d_E^{\mathrm{cont}}(x) = \inf_{y\in\mathcal{G}_E} d_E^{\mathrm{cont}}(x, y)$.

Then the semiclassical Agmon estimate roughly states that if $(H^{\mathrm{cont}}(h) - E)u = 0$ and $\|u\|_{L^2(\mathbb{R}^d)} = 1$, then $|u(x)| \leq Ce^{-((1-\varepsilon)d_E^{\mathrm{cont}}(x)-\varepsilon)/h}$ for small $h > 0$.

3.2 Strategy of the proof

We recall the strategy of the proof of the semiclassical Agmon estimate (see [12], [16, Chapter 7] for details). We set $H_\rho^{\mathrm{cont}}(h) = e^{\rho(x)/h} H^{\mathrm{cont}}(h) e^{-\rho(x)/h}$. Then

$$H_\rho^{\mathrm{cont}}(h) = (hD_x + i\partial\rho(x))^2 + V(x).$$

Its semiclassical principal symbol is

$$(\xi + i\partial\rho(x))^2 + V(x) = \xi^2 + V(x) - |\partial\rho(x)|^2 + 2i\xi \cdot \partial\rho(x).$$

If $|\partial\rho(x)|^2 \leq V(x) - E$ outside $\mathcal{G}_E$, the elliptic estimate for $H_\rho^{\mathrm{cont}}(h) - E$ proves the Agmon estimate. We can take $\rho(x)$ as a smooth approximation of $(1 - \varepsilon)d_E^{\mathrm{cont}}(x)$.

We employ an analogous argument for $\widetilde{H}(h)$ though we work on the Fourier space.

3.3 Exponentially conjugated operator

We compute $\widetilde{H}_\rho(h) = e^{\rho(hD_\xi)/h}\widetilde{H}(h)e^{-\rho(hD_\xi)/h}$. We have $e^{\rho(hD_\xi)/h}V(hD_\xi)e^{-\rho(hD_\xi)/h} = V(hD_\xi)$. We set $p_0(\xi) = \sum_{j=1}^d (2 - 2\cos\xi_j) = 4\sum_{j=1}^d \sin^2\frac{\xi_j}{2}$.

Lemma 3.1. *For $\rho \in C_b^\infty(\mathbb{R}^d;\mathbb{R})$,*

$$e^{\rho(hD_\xi)/h}p_0(\xi)e^{-\rho(hD_\xi)/h} = a_\rho(\xi, hD_\xi; h),$$

where $a_\rho \sim \sum_{k=0}^\infty h^k a_{\rho,k}(\xi,x)$ with $a_{\rho,k} \in C_b^\infty(T^*\mathbb{T}^d)$ and

$$a_{\rho,0}(\xi,x) = p_0(\xi - i\partial\rho(x), x).$$

If moreover

$$|\partial_x^\alpha \rho(x)| \leq C_\alpha \langle x\rangle^{1-|\alpha|} \text{ for any } \alpha \in \mathbb{Z}_{\geq 0}^d, \tag{2}$$

then $a_\rho \in S^0$ and $a_{\rho,k} \in S^{-k}$.

Here

$$S^m = \{a(\cdot;h) \in C^\infty(T^*\mathbb{T}^d) \,|\, |\partial_\xi^\alpha\partial_x^\beta a(\xi,x;h)| \leq C_{\alpha,\beta}\langle x\rangle^{m-|\beta|}\},$$

where α and β range over $\mathbb{Z}_{\geq 0}^d$ and $\langle x\rangle = (1+x^2)^{1/2}$. The second part of this lemma is used in the proof of the theorem presented in Section 4.

3.4 The Agmon-Finsler metric

We recall $\mathcal{G}_E = \{x \in \mathbb{R}^d \,|\, V(x) \leq E\}$. We want to find a nontrivial ρ such that $\rho = 0$ on $\mathcal{G}_E$ and

$$\operatorname{Re}\big(p_0(\xi - i\partial\rho(x)) + V(x) - E\big) \geq 0$$

outside $\mathcal{G}_E$. We note that

$$\operatorname{Re} p_0(\xi - i\partial\rho(x)) \geq -4\sum_{j=1}^d \sinh^2\frac{\partial_j\rho(x)}{2}.$$

We set

$$K_x = \Big\{\xi \in \mathbb{R}^d \;\Big|\; 4\sum_{j=1}^d \sinh^2\frac{\xi_j}{2} \leq (V(x)-E)_+\Big\}.$$

Thus we want to find $\rho(x)$ such that $\partial\rho(x) \in K_x \subset T_x^*\mathbb{R}^d$.

We define the Agmon-Finsler metric as the supporting functions of convex sets K_x;

$$L(x,v) = \sup_{\xi\in K_x}\langle\xi, v\rangle \quad \text{for } v \in T_x\mathbb{R}^d = \mathbb{R}^d,$$

which gives the length of $v \in T_x\mathbb{R}^d = \mathbb{R}^d$ in this metric. This induces a (pseudo-)distance $d_E(x,y)$. We set $d_E(x) = d_E(x, \mathcal{G}_E)$. We easily see that $|\langle v, \partial d_E(x)\rangle| \leq L(x,v)$ by the triangle inequality. Recall that the compact convex set K_x is determined by its supporting function as

$$K_x = \{\xi \in \mathbb{R}^d \,|\, \langle\xi, v\rangle \leq L(x,v) \text{ for any } v \in \mathbb{R}^d\}$$

([4, Section 4.3]). Thus $\partial d_E(x) \in K_x$. Then we can take $\rho(x)$ as a smooth approximation of $(1-\varepsilon)d_E(x)$.

3.5 Discrete Agmon estimate

Assume $V \in C_b^\infty(\mathbb{R}^d;\mathbb{R})$ and $\inf_{x\in\mathcal{G}_{E,\delta}^c} V(x) > E$ for any $\delta > 0$, where $\mathcal{G}_{E,\delta}$ is the δ-neighborhood of $\mathcal{G}_E$ in the Euclidean distance.

Theorem 1 ([9]). *For any $C_0 > 0$, $\delta_0 > 0$ and $\varepsilon > 0$, there exist $C > 0$, $h_0 > 0$, $0 < \delta < \delta_0$, χ, $\tilde{\chi} \in C_b^\infty(\mathbb{R}^d;[0,1])$ with*

$$\operatorname{supp}(1-\chi) \subset \mathcal{G}_{E,\delta},\ \ \operatorname{supp}\tilde{\chi} \subset \mathcal{G}_{E,\delta} \setminus \mathcal{G}_{E,\delta/2}$$

and $\rho \in C^\infty(\mathbb{R}^d;\mathbb{R}_{\geq 0})$ with $|(1-\varepsilon)d_E(x) - \rho(x)| \leq \varepsilon$ such that for $0 < h < h_0$,

$$\|\chi e^{\rho(x)/h} u\|_{\ell^2} \leq C\|\tilde{\chi}u\|_{\ell^2} + C\|\chi e^{\rho(x)/h}(H(h)-z)u\|_{\ell^2}$$

for any $u \in \ell^2(h\mathbb{Z}^d)$ and $z \in [E-C_0, E+C_0 h]+i[-C_0,C_0]$. In particular, if $(H(h)-E)u = 0$, $\|u\|_{\ell^2(h\mathbb{Z}^d)} = 1$, then $|u(x)| \leq Ce^{-((1-\varepsilon)d_E(x)-\varepsilon)/h}$ for small $h > 0$.

After preparing the manuscript [9], we learned that Klein-Rosenberger [10] already introduced the same Finsler metric and proved the Agmon estimate in the case of a potential minimum. The strategy of their proof is similar to that in Dimassi-Sjöstrand [3, Section 6] while our proof is similar to that in Nakamura [12] and is more microlocal. Rabinovich [14] also studied the same semiclassical setting for general d and proved the Agmon estimate though he did not discuss the relation with Finsler metric.

3.6 WKB solutions near a potential minimum

We next discuss WKB solutions for the eigenfunction problem near a potential minimum. Assume the potential $V \in C^\infty(\mathbb{R}^d;\mathbb{R})$ satisfies

$$V(0) = 0,\ \ \partial V(0) = 0 \text{ and } \partial^2 V(0) > 0.$$

Take $E_0 > 0$ such that there exists a unique $\alpha \in \mathbb{Z}_{\geq 0}^d$ with $E_0 = \sum_{j=1}^d \lambda_j(\alpha_j + 1/2)$, where $\lambda_1, \dots, \lambda_d$ are positive square roots of eigenvalues of $\frac{1}{2}\partial^2 V(0)$. Let $d(x) = d_0(x,0)$ be the Agmon-Finsler distance to $0 \in \mathbb{R}^d$ at energy 0 for this potential. Then there exist $E_j \in \mathbb{R}$, $j \geq 1$, and $a_j(x) \in C^\infty(\mathbb{R}^d)$, $j \geq 0$, such that if $E(h) \sim \sum_{j=0}^\infty h^j E_j$ and $a \sim \sum_{j=0}^\infty h^j a_j$ then

$$(H(h) - hE(h))(a(x)e^{-d(x)/h}) = r(x)e^{-d(x)/h},\ \ r(x) = \mathcal{O}(h^\infty)$$

near $0 \in \mathbb{R}^d$.

This suggests that the Agmon-Finsler metric is the natural notion for estimating the tunneling effect for semiclassical discrete Schrödinger operators. The continuous case of this was proved by Helffer-Sjöstrand [5]. The proof for the discrete case follows the arguments in [3, Section 3] with modifications for treating a Finsler metric. After preparing the manuscript [9], we learned that this was already done by Klein-Rosenberger [11].

4 The non-semiclassical Agmon estimate for discrete Schrödinger operators

4.1 Exponential decay of discrete eigenfunctions

Set

$$Hu(x) = -\sum_{|x-y|=1} (u(y) - u(x)) + V(x)u(x),$$

where $x, y \in \mathbb{Z}^d$. Namely, we set $H = H(1)$. We also take $E < 0$. Assume that the potential $V : \mathbb{Z}^d \to \mathbb{R}$ extends to $\widetilde{V} : \mathbb{R}^d \to \mathbb{R}$ such that

$$|\partial^\alpha \widetilde{V}(x)| \le C_\alpha (1 + |x|)^{-\theta|\alpha|}, \ 0 < \theta \le 1, \tag{3}$$

and $\underline{\lim}_{|x|\to\infty} \widetilde{V}(x) \ge 0$. We set $K^E = \{\xi \in \mathbb{R}^d | \, 4\sum_{j=1}^d \sinh^2 \frac{\xi_j}{2} \le |E|\}$ and

$$\rho_E(x) = \sup_{\xi \in K^E} \langle x, \xi \rangle.$$

Theorem 2 ([9])**.** *Under the above setting, for any $C_0 > 0$ and $\varepsilon > 0$ there exist $C > 0$ and $1 - \chi$, $\tilde{\chi} \in \ell^\infty_{\mathrm{comp}}(\mathbb{Z}^d)$ such that*

$$\|\chi e^{(1-\varepsilon)\rho_E(x)} u\|_{\ell^2} \le C\|\tilde{\chi} u\|_{\ell^2} + C\|\chi e^{(1-\varepsilon)\rho_E(x)} (H - z)u\|_{\ell^2}$$

for any $u \in \ell^2(\mathbb{Z}^d)$ and any $z \in [E - C_0, E] + i[-C_0, C_0]$.

In particular, if $(H - E)u = 0$ and $u \in \ell^2(\mathbb{Z}^d)$, then for any $\varepsilon > 0$ there exists $C_\varepsilon > 0$ such that

$$|u(x)| \le C_\varepsilon e^{-(1-\varepsilon)\rho_E(x)}$$

for any $x \in \mathbb{Z}^d$.

The proof is similar to that of Theorem 1. Rabinovich-Roch [15] proved the exponential decay of eigenfunctions for the discrete Schrödinger operator with a slowly oscillating potential. In our notation, their exponential decay corresponds to $|u(x)| \le C_\varepsilon e^{-(1-\varepsilon)\rho(x)}$ with a condition on $\sup_j |\partial_{x_j} \rho(x)|$. Our condition $\partial\rho(x) \in K^E$ is more precise and is optimal as seen in the next subsection.

4.2 Optimality of the exponential decay

Fix any $E < 0$ and define $u_E \in \ell^2(\mathbb{Z}^d)$ by

$$u_E(x) = (2\pi)^{-d} \int_{\mathbb{T}^d} \big(4\sum_{j=1}^d \sin^2 \frac{\xi_j}{2} + |E|\big)^{-1} e^{-i\langle x, \xi \rangle} d\xi.$$

Then we have $Hu_E(x) = Eu_E(x)$ if we set $V(x) = -u_E(0)^{-1}\delta_0(x)$. Take a bounded domain $0 \in \Omega \subset \mathbb{R}^d$ and set

$$\rho_\Omega(x) = \sup_{\xi \in \Omega} \langle x, \xi \rangle.$$

Assume that

$$|u_E(x)| \le Ce^{-\rho_\Omega(x)}$$

for some $C > 0$ and any $x \in \mathbb{Z}^d$. Then $\Omega \subset K^E$, which shows the optimality of Theorem 2. This is easily seen in view of the relation between the exponential decay of a function and the analytic continuation of its Fourier transform.

We note that Ito-Jensen [7] discussed explicit forms of $u_E(x)$ in terms of generalized hypergeometric functions.

Acknowledgement

The author is grateful to Shu Nakamura and Kenichi Ito for discussions and encouragement. The author is also grateful to Kouichi Taira for informing him of the article [14]. The author was supported by the FMSP program at the University of Tokyo and is supported by JSPS KAKENHI Grant Number JP21J10860. This article is based on a talk at a conference supported by the Research Institute for Mathematical Sciences, an International Joint Usage/Research Center located in Kyoto University.

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