Continuum limits of discrete Schrödinger operators on square lattices

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Abstract. We consider two different approaches of continuum limit problems of Schrödinger operators $H = -\Delta + V$ on $\mathbb{R}^d$. The first part of this proceedings deals with asymptotic behavors of discrete Schrödinger operators $H_h = -\Delta_h + V|_{h\mathbb{Z}^d}$ on square lattice $h\mathbb{Z}^d$ with mesh size h, and we study conditions of the potential V and the projection from $L^2(\mathbb{R}^d)$ onto $\ell^2(h\mathbb{Z}^d)$ where H_h converges to the corresponding contiuum operator H the generalized resolvent sense. The sencond one involves Schrödinger operators defined on the edges of $h\mathbb{Z}^d$, then we prove that a similar continuum limit problem holds under weaker assumption of V.

1. Introduction

The aim of this report is to develop continuum limit problems of Schrödinger operators

$$H = H_0 + V(x), \quad H_0 = -\triangle, \quad x \in \mathbb{R}^d.$$

on $\mathcal{H} = L^2(\mathbb{R}^d)$, where $d \geq 1$, with considering the two corresponding discretizations described below.

The first one is onto the vertices of square lattices: Let $h > 0$ be the mesh size, then we set

$$\mathcal{H}_h = \ell^2(h\mathbb{Z}^d), \quad h\mathbb{Z}^d = \big\{(hz_1, \ldots, hz_d) \bigm| z \in \mathbb{Z}^d\big\},$$

equipped with the norm

$$\|v\|_h = \left(h^d \sum_{z \in h\mathbb{Z}^d} |v(z)|^2\right)^{\frac{1}{2}}$$

for $v \in \mathcal{H}_h$. We denote the standard basis of $\mathbb{R}^d$ by $e_j = (\delta_{ik})_{k=1}^d \in \mathbb{R}^d$, $j = 1, \ldots, d$. The corresponding discrete Schrödinger operator is defined by

$$H_h = H_{0,h} + V(z), \quad z \in h\mathbb{Z}^d,$$

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where

$$H_{0,h}v(z) = h^{-2}\sum_{j=1}^{d}(2v(z) - v(z+he_j) - v(z-he_j)), \quad v \in \mathcal{H}_h.$$

The second one is onto the edges of square lattices: Let

$$\mathcal{L} = \{\mathcal{L}_{jn} = [j,n] \mid j,n \in h\mathbb{Z}^d, |j-n| = h\},$$

where $[j,n]$ is the line segment connecting j and n, and

$$\mathcal{H}'_h = L^2(\mathcal{L}) = \bigoplus_{|j-n|=h} L^2(\mathcal{L}_{jn})$$

with the norm

$$\|\varphi\|'_h = \left(\frac{h^{d-1}}{d}\sum_{|j-n|=h}\int_{[j,n]}|\varphi_{jn}(t)|^2 dt\right)^{\frac{1}{2}}$$

for $\varphi = (\varphi_{jn}) \in \mathcal{H}'_h$. We also set

$$H^1(\mathcal{L}) = \{(\varphi_{jn}) \in \mathcal{H}'_h \mid \varphi_{jn} \in H^1([j,n]), \varphi_{jn}(j) = \varphi_{jm}(j) \text{ for } j \in h\mathbb{Z}^d \text{ and } n,m : \text{neiborhood of } j\}$$

Suppose that $V : \mathbb{R}^d \to \mathbb{R}$ is bounded from below, and denote $V_j = V(j)$ for $j \in h\mathbb{Z}^d$. For $\varphi, \psi \in \mathcal{H}'_h$, we define the quadratic form by

$$q(\varphi,\psi) = \langle \varphi', \psi' \rangle + \sum_{j \in h\mathbb{Z}^d} hV_j\varphi_j\overline{\psi_j},$$

where $(\varphi')_{jn}(t) = \frac{d}{dt}\varphi_{jn}(t)$, $\varphi_j = \varphi_{jn}(j)$ and $\langle \cdot,\cdot \rangle$ denotes the innner product of $\mathcal{H}'_h$. Let H'_h be the selfadjoint operator associated to $q(\cdot,\cdot)$, and we call H'_h the Schrödinger operator on the quantum graph $\mathcal{L}$. Note that the boundedness of V from below implies

$$\mathcal{D}(H'_h) \subset \left\{\psi = (\psi_{jn}) \in \oplus H^2(\mathcal{L}_{jn}) \mid \sum_{|j-n|=h}\psi'_{jn}(j) = hV_j\psi_j\right\},$$
$$(H'_h\psi)_{jn}(t) = -\psi''_{jn}(t), \quad |j-n| = h.$$

In this report we develop continuum limit problems of Schrödinger operators H in the above two different settings. It is clear that the first discretized operator H_h formally converges to H, e.g. for any $u \in \mathcal{S}(\mathbb{R}^d)$

$$\sup_{z \in h\mathbb{Z}^d} |H_h\left(u|_{h\mathbb{Z}^d}\right)(z) - Hu(z)| \to 0, \quad h \to 0.$$

In order to treat the problems strictly in the terminology of operator theory, we easily find the following obstructions:

- Since H, H'_h, and possibly H_h, are not bounded, it is not allowed to formally write $H_h \to H$ or $H'_h \to H$.
- Continuum and discretized operators are defined on different functional spaces with each other.

The first obstruction is easy to avoid, since we only have to consider their resolvents $(H-\mu)^{-1}$, $(H_h-\mu)^{-1}$ and $(H'_h-\mu)^{-1}$. In order to get over the second one, we need to give appropriate identifications between continuum and discretized functional spaces.

The first half of this report, Sections 2 and 3, conserns a continuum limit from H_h to H, and we consider generalized strong/norm resolvent convergences. More precisely, we determine conditions of the potential V and identification operator

$$P_h : \mathcal{H} \to \mathcal{H}_h$$

to satisfy the convergence

$$P_h^*(H_h - \mu)^{-1}P_h \to (h - \mu)^{-1}, \quad h \to 0 \tag{1}$$

in the strong/operator norm sense.

The second half is devoted to comparison between asymptotic behavors of H_h and H_h'. In this case we set concrete identifications between $\mathcal{H}_h$ and $\mathcal{H}_h'$, and then we prove the generalized norm resolvent convergence for the pair of H_h and H_h'.

Similar convergence problems in the norm resolvent sense are studied by, e.g., [**3**], [**7**] and [**11**]. Note that [**13**] considers a continuum limit of scattering states of discrete Schrödinger operators, and that [**7**] is a generalization to fractional Laplacians. For studies of continuum limits of NLS equations, see [**2**], [**12**] and references therein.

2. Continuum limit of H_h in generalized strong resolvent sense

In this section, we first consider what the identification $P_h : \mathcal{H} \to \mathcal{H}_h$ should satisfy, and we introduce the definition of P_h in our case. Then we study the characterization of the condition that the generalized strong resolvent convergence (1) holds when V is absent.

If we assume the translation and scaling invariance, P_h should be of the form

$$P_h u(z) = h^{-d} \int_{\mathbb{R}^d} \overline{\varphi_{h,z}(x)} u(x) dx, \quad h > 0,\ z \in h\mathbb{Z}^d, \tag{2}$$

where $\varphi : \mathbb{R}^d \to \mathbb{C}$ and

$$\varphi_{h,z}(x) = \varphi(h^{-1}(x - z)), \quad x \in \mathbb{R}^d.$$

Note that, if $\varphi \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ then (2) is bounded uniformly in h, and that

$$P_h^* v(x) = \sum_{z \in h\mathbb{Z}^d} \varphi_{h,z}(x) v(z), \quad h > 0,\ v \in \mathcal{H}_h.$$

In addition, it is natural to expect that $\mathcal{H}_h$ is regarded as a subspace of $\mathcal{H}$ via P_h^*, that is, P_h^* is an isometry. It is easy to observe that P_h^* is an isometry and hence P_h is a partial isometry, if and only if $\{\varphi_{1,z} \mid z \in \mathbb{Z}^d\}$ is an orthonormal system. This condition is also equivalent to the condition:

$$\sum_{n \in \mathbb{Z}^d} \left|\hat{\varphi}(\xi + n)\right|^2 = 1 \quad \text{for } \xi \in \mathbb{R}^d, \tag{3}$$

where $\hat{\varphi}$ is the Fourier transform

$$\hat{\varphi}(\xi) = \mathcal{F}\varphi(\xi) = \int_{\mathbb{R}^d} e^{-2\pi i x \cdot \xi} \varphi(x) dx, \quad \xi \in \mathbb{R}^d.$$

In the following, we assume $\varphi \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ and (3). Then, for $u \in \mathcal{H}$,

$$\begin{aligned}
&\|(P_h^*(H_h-\mu)^{-1}P_h-(H-\mu)^{-1})u\|^2\\
=&\|(P_h^*(H_h-\mu)^{-1}P_h-(P_h^*P_h+(1-P_h^*P_h))(H-\mu)^{-1})u\|^2\\
=&\|P_h^*((H_h-\mu)^{-1}P_h-P_h(H-\mu)^{-1})u-(1-P_h^*P_h)(H-\mu)^{-1}u\|^2\\
=&\|P_h^*((H_h-\mu)^{-1}P_h-P_h(H-\mu)^{-1})u\|^2+\|(1-P_h^*P_h)(H-\mu)^{-1}u\|^2.
\end{aligned}$$

Thus, if we set

$$\begin{aligned}
R_1(h) :=&P_h^*(H_h-\mu)^{-1}P_h-P_h^*P_h(H-\mu)^{-1},\\
R_2(h) :=&(1-P_h^*P_h)(H-\mu)^{-1},
\end{aligned}$$

we learn

$$\begin{aligned}
\max(\|R_1(h)\|,\|R_2(h)\|) &\le \|P_h^*(H_h-\mu)^{-1}P_h-(H-\mu)^{-1}\|\\
&\le \left(\|R_1(h)\|^2+\|R_2(h)\|^2\right)^{\frac{1}{2}}.
\end{aligned}$$

Hence we have

LEMMA 2.1. *Assume* $\varphi \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ *and* (3). *Then*
(i) (1) *holds in the strong sense if and only if*

$$R_1(h),\ R_2(h) \to 0 \text{ strongly as } h \to 0.$$

(ii) (1) *holds in the operator norm sense if and only if*

$$\|R_1(h)\|,\ \|R_2(h)\| \to 0 \text{ as } h \to 0.$$

The aim of this section is to prove the following proposition.

PROPOSITION 2.2. *Assume* $\varphi \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$, (3) *and* $V \equiv 0$. *Then* (1) *holds in the strong sense if and only if*

$$|\hat{\varphi}(0)| = 1. \tag{4}$$

Before the proof, we introduce the discrete Fourier transform

$$F_h\ :\ \mathcal{H}_h \to \hat{\mathcal{H}}_h = L^2(h^{-1}\mathbb{T}^d), \quad \mathbb{T} = \mathbb{R}/\mathbb{Z},$$

by

$$F_h v(\zeta) = h^d \sum_{z \in h\mathbb{Z}^d} e^{-2\pi i z\cdot\zeta} v(z), \quad \zeta \in h^{-1}\mathbb{T}^d,\ v \in \mathcal{H}_h. \tag{5}$$

F_h is unitary, and its adjoint is given by

$$F_h^* g(z) = \int_{h^{-1}\mathbb{T}^d} e^{2\pi i z\cdot\zeta} g(\zeta) d\zeta, \quad z \in h\mathbb{Z}^d,\ g \in \hat{\mathcal{H}}_h.$$

If we set

$$H_0(\xi) = |2\pi\xi|^2,$$

it is well-known that $H_0 = \mathcal{F}^* H_0(\cdot)\mathcal{F}$ on $\mathcal{H}$. Similarly, if we set

$$H_{0,h}(\zeta) = 2h^{-2}\sum_{j=1}^d (1-\cos(2\pi h\zeta_j)), \quad \zeta \in h^{-1}\mathbb{T}^d,$$

then $H_{0,h} = F_h^* H_{0,h}(\cdot) F_h$. We denote

$$Q_h := F_h P_h \mathcal{F}^* : \hat{\mathcal{H}} = L^2(\mathbb{R}^d) \to \hat{\mathcal{H}}_h.$$

Then we have

LEMMA 2.3. *For $f \in \mathcal{S}(\mathbb{R}^d)$,*

$$Q_h f(\zeta) = \sum_{n\in\mathbb{Z}^d} \overline{\hat{\varphi}(h\zeta+n)} f(\zeta+h^{-1}n), \quad \zeta \in h^{-1}\mathbb{T}. \tag{6}$$

For $g \in \hat{\mathcal{H}}_h$,

$$Q_h^* g(\xi) = \hat{\varphi}(h\xi)\tilde{g}(\xi), \quad \xi \in \mathbb{R}^d, \tag{7}$$

where $\tilde{g}$ is the periodic extension of g on $\mathbb{R}^d$.

PROOF OF PROPOSITION 2.2. Let

$$\hat{R}_j(h) := \mathcal{F}R_j(h)\mathcal{F}^*, \quad j = 1, 2. \tag{8}$$

A direct computation implies

$$\begin{aligned}\hat{R}_2(h)f(\xi) =&(1 - Q_h^* Q_h)\left((H_0(\xi)-\mu)^{-1}f(\xi)\right)\\ =&(1-|\hat{\varphi}(h\xi)|^2)g(\xi) - \hat{\varphi}(h\xi)\sum_{n\neq 0}\overline{\hat{\varphi}(h\xi+n)}g(\xi+h^{-1}n),\end{aligned}$$

where

$$g(\xi) := (H_0(\xi)-\mu)^{-1}f(\xi).$$

We fix $R > 0$ and let $f \in C_c^\infty((-R,R)^d)$. Then we have for $h > 0$ small enough

$$\begin{aligned}\|\hat{R}_2(h)f(\xi)\|^2 =& \int_{[-R,R]^d} |(1-|\hat{\varphi}(h\xi)|^2)g(\xi)|^2 d\xi\\ &+ \sum_{n\neq 0}\int_{[-R,R]^d} |\hat{\varphi}(h\xi-n)\overline{\hat{\varphi}(h\xi)}g(\xi)|^2 d\xi.\end{aligned}$$

Since the first term tends to

$$|1-|\hat{\varphi}(0)|^2|^2 \int_{[-R,R]^d} |g(\xi)|^2 d\xi$$

as $h \to 0$, the condition $|\hat{\varphi}(0)| = 1$ is necessary. Note that, $|\hat{\varphi}(0)| = 1$ and (3) imply the convergence of the other terms:

$$\begin{aligned}&\sum_{n\neq 0}\int_{[-R,R]^d} |\hat{\varphi}(h\xi-n)\overline{\hat{\varphi}(h\xi)}g(\xi)|^2 d\xi\\ =&\int_{[-R,R]^d}\sum_{n\neq 0}|\hat{\varphi}(h\xi-n)|^2|\overline{\hat{\varphi}(h\xi)}g(\xi)|^2 d\xi\\ =&\int_{[-R,R]^d}(1-|\hat{\varphi}(h\xi)|^2)|\overline{\hat{\varphi}(h\xi)}|^2|g(\xi)|^2 d\xi\\ \to&(1-|\hat{\varphi}(0)|^2)|\overline{\hat{\varphi}(0)}|^2\int_{[-R,R]^d}|g(\xi)|^2 d\xi = 0, \quad h \to 0.\end{aligned}$$

We omit the proof of sufficienty since we will show that (4) implies $\|\hat{R}_2(h)\| \to 0$ as $h \to 0$ in Proposition 3.1.

□

3. Continuum limit of H_h in generalized norm resolvent sense

In this section, we consider sufficient conditions where (1) holds in the norm sense. We first show

PROPOSITION 3.1. *Assume* $\varphi \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$, (3) *and* $V \equiv 0$. *Then* (1) *holds in the operator norm sense if and only if* (4) *holds.*

Combining Propositions 2.2 and 3.1, we see that the generalized strong/norm resolvent convergence $H_{0,h} \to H_0$ is characterized by $|\hat{\varphi}(0)| = 1$.

PROOF. A direct computation implies

$$\hat{R}_1(h)f(\xi) = \sum_{n\in\mathbb{Z}^d} \hat{\varphi}(h\xi)\overline{\hat{\varphi}(h\xi+n)}B_h(\xi+h^{-1}n)f(\xi+h^{-1}n),$$

where

$$B_h(\xi) := (H_{0,h}(\xi)-\mu)^{-1} - (H_0(\xi)-\mu)^{-1}.$$

We see that $|\hat{\varphi}(h\xi)|B_h(\xi) \to 0$ in $L^\infty(\mathbb{R}^d)$, which implies the $n = 0$ term tends to zero. For the other terms, it follows from (3) that

$$\begin{aligned}
&\int_{\mathbb{R}^d} |\hat{\varphi}(h\xi)|^2 \left| \sum_{n\neq 0} \overline{\hat{\varphi}(h\xi+n)} B_h(\xi+h^{-1}n)f(\xi+h^{-1}n) \right|^2 d\xi \\
&\leq \int_{\mathbb{R}^d} |\hat{\varphi}(h\xi)|^2 \sum_{n\neq 0} |\overline{\hat{\varphi}(h\xi+n)}|^2 \sum_{n\neq 0} |B_h(\xi+h^{-1}n)f(\xi+h^{-1}n)|^2 \, d\xi \\
&= \int_{\mathbb{R}^d} |\hat{\varphi}(h\xi)|^2 (1-|\hat{\varphi}(h\xi)|^2) \sum_{n\neq 0} |B_h(\xi+h^{-1}n)f(\xi+h^{-1}n)|^2 \, d\xi \\
&= \int_{\mathbb{R}^d} \sum_{n\neq 0} (|\hat{\varphi}(h\xi-n)|^2 - |\hat{\varphi}(h\xi-n)|^4)|B_h(\xi)f(\xi)|^2 \, d\xi \\
&= \int_{\mathbb{R}^d} (1-|\hat{\varphi}(h\xi)|^2 - \sum_{n\neq 0} |\hat{\varphi}(h\xi-n)|^4)|B_h(\xi)f(\xi)|^2 \, d\xi.
\end{aligned}$$

Note that using the properties (3) and (4) we have

$$\hat{\varphi}(n) = 0, \quad n \in \mathbb{Z}^d \setminus \{0\},$$

which implies the function

$$(1-|\hat{\varphi}(h\xi)|^2 - \sum_{n\neq 0} |\hat{\varphi}(h\xi-n)|^4)|B_h(\xi)|^2$$

converges to zero in $L^\infty(\mathbb{R}^d)$ and hence the reminding terms tend to zero.

We recall that for $f \in \mathcal{S}(\mathbb{R}^d)$

$$\hat{R}_2(h)f(\xi) = (1-|\hat{\varphi}(h\xi)|^2)g(\xi) - \hat{\varphi}(h\xi)\sum_{n\neq 0} \overline{\hat{\varphi}(h\xi+n)}g(\xi+h^{-1}n),$$

where $g(\xi) = (H_0(\xi)-\mu)^{-1}f(\xi)$. The first term tends to zero in norm since $(1-|\hat{\varphi}(h\xi)|^2)(H(\xi)-\mu)^{-1}$ converges to zero in $L^\infty(\mathbb{R}^d)$. For the remaining terms, we learn

$$\begin{aligned}
&\int |\hat\varphi(h\xi)\sum_{n\neq 0}\overline{\hat\varphi(h\xi+n)}g(\xi+h^{-1}n)|^2 d\xi \\
&\leq \int |\hat\varphi(h\xi)|^2 \sum_{n\neq 0}|\hat\varphi(h\xi+n)|^2 \sum_{n\neq 0}|g(\xi+h^{-1}n)|^2 d\xi \\
&= \int |\hat\varphi(h\xi)|^2(1-|\hat\varphi(h\xi)|^2)\sum_{n\neq 0}|g(\xi+h^{-1}n)|^2 d\xi \\
&= \int \sum_{n\neq 0}|\hat\varphi(h\xi-n)|^2(1-|\hat\varphi(h\xi-n)|^2)|g(\xi)|^2 d\xi \\
&= \int (1-|\hat\varphi(h\xi)|^2-\sum_{n\neq 0}|\hat\varphi(h\xi-n)|^4)|g(\xi)|^2 d\xi.
\end{aligned}$$

The similar computation as in $\hat{R}_1(h)$ implies that the function

$$(1-|\hat\varphi(h\xi)|^2-\sum_{n\neq 0}|\hat\varphi(h\xi-n)|^4)|H(\xi)-\mu|^{-2}$$

tends to zero with respect to the L^∞ norm. Thus the remaining terms converge to zero as $h\to 0$. $\square$

The rest of this section is devoted to the case $V\neq 0$. We assume

Assumption A. V is a real-valued continuous function on $\mathbb{R}^d$, and bounded from below. $(V(x)+M)^{-1}$ is uniformly continuous with some $M>0$, and there is $c_1>0$ such that

$$c_1^{-1}(V(x)+M)\leq V(y)+M\leq c_1(V(x)+M),\quad \text{if } |x-y|\leq 1. \tag{9}$$

The above assumption implies V is slowly varying in some sense, and uniformly continuous relative to the size of $V(x)$. Note that (9) is essentially equivalent to

$$\left|\partial_x^\alpha V(x)\right|\leq C_\alpha V(x),\quad x\in\mathbb{R}^d.$$

The assumption is satisfied if V is bounded and uniformly continuous. $V(x)=a\langle x\rangle^\mu$ with $a,\mu>0$, also satisfies the assumption.

The following theorem and corollaries are due to [**17**], while the assumption of φ is relaxed silightly.

Theorem 3.2. *Suppose Assumptions A and $\varphi\in L^1(\mathbb{R}^d)\cap L^2(\mathbb{R}^d)$ satisfies* (3), (4) *and $\sum_{n\in\mathbb{Z}^d}\varphi(\cdot+n)\in L^\infty(\mathbb{R}^d)$. Then, for any $\mu\in\mathbb{C}\backslash\mathbb{R}$,*

$$\|P_h^*(H_h-\mu)^{-1}P_h-(H-\mu)^{-1}\|_{\mathcal{B}(\mathcal{H})}\to 0\quad \text{as } h\to 0,$$

where $\mathcal{B}(\mathcal{H})$ denotes the Banach space of the operators on $\mathcal{H}$

$$\begin{array}{ccc}
\mathcal{H}_h & \xrightarrow{(H_h-\mu)^{-1}} & \mathcal{H}_h \\
{\scriptstyle P_h}\uparrow & & \downarrow{\scriptstyle P_h^*} \\
\mathcal{H} & \xrightarrow[(H-\mu)^{-1}]{} & \mathcal{H}
\end{array}$$

Combining this with the argument of Theorem VIII.23 (b) in [**21**], we obtain

Corollary 3.3. *Under the same assumption as Theorem 3.2, let $a, b \in \mathbb{R}$, $a < b$, be not in $\sigma(H)$. Then $a, b \notin \sigma(H_h)$ for sufficiently small $h > 0$ and*

$$\|P_h^* E_{H_h}((a,b))P_h - E_H((a,b))\|_{\mathcal{B}(\mathcal{H})} \to 0 \quad \text{as } h \to 0,$$

where $\sigma(A)$ denotes the spectrum of a self-adjoint operator A, and $E_A(\Omega)$ denotes the spectral projection for $\Omega \subset \mathbb{R}$.

Corollary 3.4. *Suppose Assumptions A. Then for $M > -\inf \sigma(H)$,*

$$d_H\left(\sigma((H_h + M)^{-1}), \sigma((H + M)^{-1})\right) \to 0 \quad \text{as } h \to 0,$$

where

$$d_H(X, Y) = \max\left\{\sup_{x\in X} d(x, Y), \sup_{y \in Y} d(y, X)\right\}$$

is the Hausdorff distance between sets $X, Y \subset \mathbb{C}$.

For the proof of Theorem 3.2, we need in addition to the argument in Proposition 3.1 the norm convergence of potentials

$$(V - \mu)^{-1} P_h - P_h(V - \mu)^{-1} \to 0, \quad h \to 0$$

and relative boundedness

$$\begin{aligned} &H_0(H - \mu)^{-1},\ V(H - \mu)^{-1} \in \mathcal{B}(\mathcal{H}),\\ &\sup_{h\in(0,1]} \|H_{0,h}(H_h - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H}_h)} < \infty,\\ &\sup_{h\in(0,1]} \|V(H_h - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H}_h)} < \infty. \end{aligned}$$

4. Continuum limit of H_h' and comparison to H_h

The last section aims to connect discrete Schrödinger operators H_h on $h\mathbb{Z}^d$ and quantum graph Hamiltonians H_h' through the continuum limit. First we introduce a set of operators $\mathcal{H}_h \to \mathcal{H}_h'$ and $\mathcal{H}_h' \to \mathcal{H}_h$. Then we prove the norm resolvent convergence for the pair of H_h and H_h'.

Let $I : \mathcal{H}_h \to \mathcal{H}_h'$, $\varphi = (\varphi_j) \mapsto I\varphi = (\varphi_{jn})$, be the linear interpolation, i.e.

$$\varphi_{jn}(x(t)) = (1 - t)\varphi_j + t\varphi_n, \quad t \in [0, 1],$$

where $x(t) = (1 - t)j + tn$. Since $3^{\frac{1}{2}}\|\varphi\|_{\mathcal{H}_h} \le \|I\varphi\|_{\mathcal{H}_h'} \le \|\varphi\|_{\mathcal{H}_h}$,

$$\operatorname{Ran} I \subset \mathcal{H}_h'$$

is a closed subspace and there is a bounded inverse of I:

$$J = I^{-1} : \operatorname{Ran} I \to \mathcal{H}_h.$$

Let $P : \mathcal{H}_h' \to \operatorname{Ran} I$ be the orthogonal projection. Then, we use the operators

$$\begin{aligned} I &: \mathcal{H}_h \to \mathcal{H}_h',\\ JP &: \mathcal{H}_h' \to \mathcal{H}_h \end{aligned}$$

to identify $\mathcal{H}_h'$ with $\mathcal{H}_h$. The following is the main result of this section.

THEOREM 4.1 (Exner-Nakamura-T., in prepararion). *Assume that*
(1) V is bounded from below.
(2) V is slowly varying, i.e.

$$\sup_{|x-y|<1} \frac{V(x)-M}{V(y)-M} < \infty,$$

where $M := \inf_{x\in\mathbb{R}^d} V(x) - 1$. Then, for any $\mu \in \mathbb{C}\backslash\mathbb{R}$,

$$\|(\frac{1}{d}H_h - \mu)^{-1} - JP(H_h' - \mu)^{-1} I\|_{\mathcal{B}(\mathcal{H}_h)} \to 0,$$
$$\|(H_h' - \mu)^{-1} - I(\frac{1}{d}H_h - \mu)^{-1} JP\|_{\mathcal{B}(\mathcal{H}_h')} \to 0.$$

$$\begin{array}{ccc} \mathcal{H}_h & \xrightarrow{(\frac{1}{d}H_h-\mu)^{-1}} & \mathcal{H}_h \\ {\scriptstyle JP}\uparrow & & \downarrow{\scriptstyle I} \\ \mathcal{H}_h' & \xrightarrow[(H_h'-\mu)^{-1}]{} & \mathcal{H}_h' \end{array}$$

REMARK 4.1. (1) The coefficient $\frac{1}{d}$ comes from the degree $2d$ of each vertex, the number of edges incident to the vertex.
(2) Compared to Theorem 3.2, the continuity condition of $(V(x) - M)^{-1}$ is removed, since we need only H_h-boundedness of $H_{0,h}$ with uniform bound in h.
(3) We also obtain the asymptotics of spectral projection and spectra, i.e.

$$\|E_{H_h}((a,b)) - JPE_{H_h'}((a,b))I\|_{\mathcal{B}(\mathcal{H})} \to 0,$$
$$d_{\mathrm{H}}\left(\sigma((H_h - M)^{-1}), \sigma((H_h' - M)^{-1})\right) \to 0,$$

if $a, b \notin \sigma(H_h) \cup \sigma(H_h')$ for sufficiently small h.

Combining the above theorem with Theorem 3.2, we obtain the following continuum limit.

$$\begin{array}{ccc} \mathcal{H}_h' & \xrightarrow{(dH_h'-\mu)^{-1}} & \mathcal{H}_h' \\ {\scriptstyle I}\uparrow & & \downarrow{\scriptstyle JP} \\ \mathcal{H}_h & \xrightarrow{(H_h-\mu)^{-1}} & \mathcal{H}_h \\ {\scriptstyle P_h}\uparrow & & \downarrow{\scriptstyle P_h^*} \\ \mathcal{H} & \xrightarrow[(H-\mu)^{-1}]{} & \mathcal{H} \end{array}$$

The idea of proof is analogous to [**10**], which uses the boundiary condition of quantum graph Hamiltonians.

We set the trace operator $K : H^1(\mathcal{L}) \to \mathcal{H}_h$ by

$$K : \varphi = (\varphi_{jn}) \mapsto (K\varphi)_j = \varphi_{jn}(j)$$

We will show the explicit formula for $K(H_h' - k^2)^{-1} I$.

For $\varphi = (\varphi_j) \in \mathcal{H}_h$, we consider the equation

$$(H_h' - k^2)\psi = I\varphi, \quad \psi \in \mathcal{D}(H_h').$$

Then for each jn

$$-\psi_{jn}'' - k^2\psi_{jn} = \varphi_{jn} \quad \text{on } \mathcal{L}_{jn},$$

where

$$\varphi_{jn}(x) = (1-\frac{x}{h})\varphi_j + \frac{x}{h}\varphi_n = \varphi_j + \frac{x}{h}(\varphi_n - \varphi_j), \quad x \in [0,h] \cong \mathcal{L}_{jn}.$$

Adding the boundary condition $\psi_{jn}(0) = \psi_j$ and $\psi_{jn}(h) = \psi_n$, we solve the equation and we have

$$\begin{aligned}\psi_{jn}(x) =& \frac{\sin(kx)}{\sin(kh)}\psi_n + \frac{\sin(k(h-x))}{\sin(kh)}\psi_j \\ &+ \frac{1}{k^2}(\frac{\sin(kx)}{\sin(kh)} - \frac{x}{h})\varphi_n + \frac{1}{k^2}(\frac{\sin(k(h-x))}{\sin(kh)} - 1 + \frac{x}{h})\varphi_j.\end{aligned}$$

In particular,

$$\begin{aligned}\psi_{jn}'(j) =& \psi_{jn}'(0) \\ =& \frac{k}{\sin(kh)}(\psi_n - \psi_j) + \frac{k(1-\cos(kh)))}{\sin(kh)}\psi_j \\ &+ \frac{1}{k^2}(\frac{k}{\sin(kh)} - \frac{1}{h})(\varphi_n - \varphi_j) + \frac{1-\cos(kh)}{k\sin(kh)}\varphi_j.\end{aligned}$$

Substituting this to the boundary condition

$$\sum_{|j-n|=h} \psi_{jn}'(j) = hV_j\psi_j,$$

we have for any j,

$$\begin{aligned}&-\frac{1}{h^2}\sum_{|n-j|=h}(\psi_n - \psi_j) + \frac{\sin(kh)}{kh}V_j\psi_j - k^2 d\frac{1-\cos(kh)}{(kh)^2/2}\psi_j \\ =& -\frac{\sin(kh)-kh}{(kh)^3}\sum_{|n-j|=h}(\varphi_n - \varphi_j) + d\frac{1-\cos(kh)}{(kh)^2/2}\varphi_j.\end{aligned}$$

Let

$$\begin{aligned}(M_1\psi)_j &= d^{-1}(\frac{\sin(kh)}{kh} - 1)V_j\psi_j - k^2(\frac{1-\cos(kh)}{(kh)^2/2} - 1)\psi_j, \\ (M_2\varphi)_j &= -d^{-1}\frac{\sin(kh)-kh}{(kh)^3}\sum_{|n-j|=h}(\varphi_n - \varphi_j) + (\frac{1-\cos(kh)}{(kh)^2/2} - 1)\varphi_j.\end{aligned}$$

Then we have

$$(H_h - k^2 + M_1)K\psi = (1 + M_2)\varphi.$$

Taking into account the Taylor series expansion of $\frac{\sin(kh)}{kh}$, $\frac{1-\cos(kh)}{(kh)^2/2}$ and $\frac{\sin(kh)-kh}{(kh)^3}$ (all of them are $1 + O(h^2)$), we see that

$$(H_h - k^2)^{-1}M_m = O(h^2), \quad m = 1, 2.$$

Thus we have

$$K(H_h' - k^2)^{-1}I = (H_h - k^2 + M_1)^{-1}(1 + M_2),$$

which implies

$$K(H_h' - k^2)^{-1}I - (H_h - k^2)^{-1} = O(h^2).$$

Using the fact that $\|K - JP\|_{\mathcal{B}(H^1(\mathcal{L}),\mathcal{H}_h)} \leq Ch$, we obtain

$$JP(H_h' - k^2)^{-1}I - (H_h - k^2)^{-1} = O(h)$$

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