A self-adjointness criterion for the Schrödinger operator with infinitely many point interactions and its application to random operators

by

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Abstract

We prove the Schrödinger operator with infinitely many point interactions in $\mathbb{R}^d$ ($d = 1, 2, 3$) is self-adjoint if the support of the interactions is decomposed into uniformly discrete clusters. Using this fact, we prove the self-adjointness of the Schrödinger operator with point interactions on a random perturbation of a lattice or on the Poisson configuration. We also determine the spectrum of the Schrödinger operators with random point interactions of Poisson–Anderson type.

1 Introduction

Let $\Gamma$ be a discrete subset of $\mathbb{R}^d$ ($d = 1, 2, 3$) which is *locally finite*, that is, $\#(\Gamma \cap K) < \infty$ for any compact subset $K$ of $\mathbb{R}^d$, where the symbol $\#S$ is the cardinality of a set $S$. We define the *minimal operator* $H_{\Gamma, \text{min}}$ by

$$H_{\Gamma, \text{min}}u = -\Delta u, \quad D(H_{\Gamma, \text{min}}) = C_0^\infty(\mathbb{R}^d \setminus \Gamma),$$

where $\Delta = \sum_{j=1}^d \partial^2 / \partial x_j^2$ is the Laplace operator. Clearly $H_{\Gamma, \text{min}}$ is a densely defined symmetric operator, and it is well-known that the deficiency indices $n_\pm(H_{\Gamma, \text{min}})$ are given by

$$n_\pm(H_{\Gamma, \text{min}}) := \dim \mathcal{K}_{\Gamma, \pm} = \begin{cases} 2\#\Gamma & (d = 1), \\ \#\Gamma & (d = 2, 3), \end{cases}$$

where $\mathcal{K}_{\Gamma, \pm} := \text{Ker}(H_{\Gamma, \text{min}}^* \mp i)$ are the deficiency subspaces (see e.g. [2]). So $H_{\Gamma, \text{min}}$ is not essentially self-adjoint unless $\Gamma = \emptyset$. A self-adjoint extension of $H_{\Gamma, \text{min}}$ is called the Schrödinger operator with *point interactions*, since the support of the interactions is concentrated on countable number of points in $\mathbb{R}^d$. The Schrödinger operator with point interactions is known as a typical
example of solvable models in quantum mechanics, and numerous works are
devoted to the study of this model or its perturbation by a scalar potential
or a magnetic vector potential. The book [2] contains most of fundamental
facts about this subject and exhaustive list of references up to 2004. The
papers [9, 20] also give us recent development of this subject.

There are mainly three popular methods of defining self-adjoint extensions
$H$ of $H_{\Gamma,\min}$. Here we denote the free Laplacian by $H_0$, that is, $H_0 = -\Delta$
with $D(H_0) = H^2(\mathbb{R}^d)$.

(i) Calculate the deficiency subspaces $K_{\Gamma,\pm}$, and give the difference of the
resolvent operators $(H - z)^{-1} - (H_0 - z)^{-1}$ (Im $z \neq 0$) for the desired
self-adjoint extension $H$ by using von Neumann’s theory and Krein’s
resolvent formula.

(ii) Introduce a scalar potential $V$, choose the renormalization factor $\lambda(\epsilon)$
appropriately, and define the operator $H$ as the norm resolvent limit
$H = \lim_{\epsilon \to 0} H_\epsilon, \quad H_\epsilon = -\Delta + \lambda(\epsilon)\epsilon^{-d}V(\cdot/\epsilon).$ (1)

(iii) Define the operator domain $D(H)$ of the desired self-adjoint extension
$H$ in terms of the boundary conditions at $\gamma \in \Gamma$.

These methods are mutually related with each other, and give the same
operators consequently. Historically, the seminal works by Kronig–Penney
[21] ($d = 1$) and Thomas [27] ($d = 3$) start from the method (ii), and
conclude the limiting operators are described by the method (iii). Bethe–
Peierls [7] also obtain a similar boundary condition for $d = 3$. Berezin–
Faddeev [6] start from the method (ii) for $d = 3$ by using the cut-off in
the momentum space, and show the limiting operator is also defined by
the method (i). After the paper [6], the method (i) becomes probably the
most commonly used one. It is mathematically rigorous and useful in the
analysis of spectral and scattering properties of the system, since various
quantities (e.g. spectrum, scattering amplitude, resonance, etc.) are defined
via the resolvent operator. The characteristic feature in the method (ii) is
the dependence of the renormalization factor $\lambda(\epsilon)$ on the dimension $d$. We
can take $\lambda(\epsilon) = 1$ for $d = 1$, but $\lambda(\epsilon) \to 0$ as $\epsilon \to 0$ for $d = 2, 3$. Recently, the
method (iii) is reformulated in terms of the boundary triplet (see [9, 20] and
references therein). The method (iii) is useful when we cannot calculate the
deficiency subspaces explicitly, e.g. the point interactions on a Riemannian
manifold, etc. In the present paper we adapt the method (iii), as explained
below.
We define the maximal operator $H_{\Gamma,\text{max}}$ by $H_{\Gamma,\text{max}} = H_{\Gamma,\text{min}}^*$, the adjoint operator of $H_{\Gamma,\text{min}}$. The operator $H_{\Gamma,\text{max}}$ is explicitly given by

$$H_{\Gamma,\text{max}}u = -\Delta u, \quad D(H_{\Gamma,\text{max}}) = \{u \in L^2(\mathbb{R}^d); \Delta u \in L^2(\mathbb{R}^d)\},$$

where the Laplacian $\Delta$ is regarded as a linear operator on the space of Schwartz distributions $D'(\mathbb{R}^d \setminus \Gamma)$ on $\mathbb{R}^d \setminus \Gamma$ (see [2] or Proposition 8 below; we interpret $\Delta$ in this sense in the sequel). When $d = 1$, an element $u \in D(H_{\Gamma,\text{max}})$ has boundary values $u(\gamma \pm 0) := \lim_{x \to \gamma \pm 0} u(x)$ and $u'(\gamma \pm 0)$ for any $\gamma \in \Gamma$. When $d = 2, 3$, it is known that any element $u \in D(H_{\Gamma,\text{max}})$ has asymptotics

$$u(x) = u_{\gamma,0} \log |x - \gamma| + u_{\gamma,1} + o(1) \quad \text{as } x \to \gamma \quad (d = 2),$$

$$u(x) = u_{\gamma,0} |x - \gamma|^{-1} + u_{\gamma,1} + o(1) \quad \text{as } x \to \gamma \quad (d = 3)$$

for every $\gamma \in \Gamma$, where $u_{\gamma,0}$ and $u_{\gamma,1}$ are constants (see [2, 9] or Proposition 9 below).

Let $\alpha = (\alpha_\gamma)_{\gamma \in \Gamma}$ be a sequence of real numbers. We define a closed linear operator $H_{\Gamma,\alpha}$ in $L^2(\mathbb{R}^d)$ by

$$H_{\Gamma,\alpha}u = -\Delta u, \quad D(H_{\Gamma,\alpha}) = \{u \in D(H_{\Gamma,\text{max}}); u \text{ satisfies } (BC)_\gamma \text{ for every } \gamma \in \Gamma\}.$$  

The boundary condition $(BC)_\gamma$ at the point $\gamma \in \Gamma$ is defined as follows.

$$\begin{cases}  
u(\gamma + 0) = u(\gamma - 0) = u(\gamma), & (d = 1), \\ u'(\gamma + 0) - u'(\gamma - 0) = \alpha_\gamma u(\gamma) & (d = 2), \\ 2\pi \alpha_\gamma u_{\gamma,0} + u_{\gamma,1} = 0 & (d = 2), \\ -4\pi \alpha_\gamma u_{\gamma,0} + u_{\gamma,1} = 0 & (d = 3), \end{cases}$$

where $u_{\gamma,0}$ and $u_{\gamma,1}$ are the constants in (2). The constants $2\pi$ and $-4\pi$ before coupling constants are chosen so that the results in [2] can be used without modification, though our $H_{\Gamma,\alpha}$ is denoted by $-\Delta_{\alpha,Y}$ in [2]. When $d = 1$, the case $\alpha_\gamma = 0$ for all $\gamma$ corresponds to the free Laplacian $H_0$, and the formal expression $H_{\Gamma,\alpha} = -\Delta + \sum_{\gamma \in \Gamma} \alpha_\gamma \delta_\gamma$ is justified in the sense of quadratic form, where $\delta_\gamma$ is the Dirac delta function supported on the point $\gamma$ (see (3)). However, when $d = 2, 3$, the case $\alpha_\gamma = \infty$ for all $\gamma$ corresponds to $H_0$, and the coupling constant $\alpha_\gamma$ is not the coefficient before the delta function, but the parameter appearing in the second term of the expansion of the renormalization factor $\lambda(\epsilon)$ in (1) (see [2] for the detail).
It is well-known that $H_{\Gamma,\alpha}$ is self-adjoint when $\#\Gamma < \infty$. When $\#\Gamma = \infty$, the self-adjointness of $H_{\Gamma,\alpha}$ is proved under the uniform discreteness condition

$$d_* := \inf_{\gamma,\gamma \in \Gamma, \gamma \neq \gamma'} |\gamma - \gamma'| > 0$$

in the book [2] and many other references (e.g. [16, 10, 15]). There are only a few results in the case $d_* = 0$. Minami [23] studies the self-adjointness and the spectrum of the random Schrödinger operator $H_\omega = -\frac{d^2}{dt^2} + Q'_t(\omega)$ on $\mathbb{R}$, where $\{Q_t(\omega)\}_{t \in \mathbb{R}}$ is a temporally homogeneous Lévy process. If we take

$$Q_t(\omega) = \int_0^t \sum_{\gamma \in \Gamma} \alpha_{\omega,\gamma} \delta(s - \gamma) ds$$

for the Poisson configuration (the support of the Poisson point process; see Definition 14 below) $\Gamma_\omega$ on $\mathbb{R}$ and i.i.d. (independently, identically distributed) random variables $\alpha_\omega = (\alpha_{\omega,\gamma})_{\gamma \in \Gamma_\omega}$, we conclude that $H_{\Gamma_\omega,\alpha_\omega}$ is self-adjoint almost surely. Kostenko–Malamud [20] give the following remarkable result.

**Theorem 1** (Kostenko–Malamud [20]). Let $d = 1$. Let $\Gamma = \{\gamma_n\}_{n \in \mathbb{Z}}$ be a sequence of strictly increasing real numbers with $\lim_{n \to \pm \infty} \gamma_n = \pm \infty$. Assume

$$\sum_{n=-\infty}^{1} d_n^2 = \sum_{n=0}^{\infty} d_n^2 = \infty, \quad d_n = \gamma_{n+1} - \gamma_n.$$  

Then, $H_{\Gamma,\alpha}$ is self-adjoint for every $\alpha = (\alpha_\gamma)_{\gamma \in \Gamma}$.

Actually Kostenko–Malamud [20] state the result in the half-line case, but the result can be easily extended in the whole line case, as stated above. In the proof, Kostenko–Malamud construct an appropriate boundary triplet for $H_{\Gamma,\alpha}$. Moreover, Christ–Stolz [10] give a counter example of $(\Gamma,\alpha)$ so that $d = 1$, $d_* = 0$ and $H_{\Gamma,\alpha}$ is not self-adjoint. However, the proof of Minami [23] uses that the deficiency indices are not more than two for one-dimensional symmetric differential operator, and the proof of Kostenko–Malamud [20] uses the decomposition $L^2(\mathbb{R}) = \oplus_{n=-\infty}^{\infty} L^2((\gamma_n, \gamma_{n+1}))$. Both methods depend on the one-dimensionality of the space, and cannot directly be applied in two or three dimensional case.

In the present paper, we give a sufficient condition for the self-adjointness of $H_{\Gamma,\alpha}$, which is available even in the case $d_* = 0$ and $d = 2,3$. In the sequel, we denote $R$-neighborhood of a set $S$ by $(S)_R$, that is,

$$(S)_R := \{x \in \mathbb{R}^d; \ \text{dist}(x, S) < R\}.$$
where the distance $\text{dist}(S, T)$ between two sets $S$ and $T$ is defined by
\[
\text{dist}(S, T) := \inf_{x \in S, y \in T} |x - y|.
\]

**Assumption 2.** There exists $R > 0$ such that every connected component of $(\Gamma)_R$ is a bounded set.

The set $(\Gamma)_R$ is the union of $B_R(\gamma)$, an open disk of radius $R$ centered at $\gamma \in \Gamma$ (see Figure 1). Assumption 2 is a generalization of the uniform discreteness condition (4). Actually, if we call the set of points of $\Gamma$ in each connected component of $(\Gamma)_R$ a cluster, then the assumption says ‘the clusters of $\Gamma$ are uniformly discrete’.

**Figure 1:** The set $(\Gamma)_R$ in $(-5, 5)^2$ when $d = 2$ and $R = 0.4$. $\Gamma$ is a sample configuration of the Poisson configuration with intensity 1.

Our first main result is stated as follows.

**Theorem 3.** Let $d = 1, 2, 3$. Suppose Assumption 2 holds. Then, $H_{\Gamma, \alpha}$ is self-adjoint for any $\alpha = (\alpha_\gamma)_{\gamma \in \Gamma}$.

In the case $d = 1$, Theorem 3 is a special case of Theorem 1, since Assumption 2 implies there are infinitely many positive $n$ and negative $n$ such that $d_n \geq 2R$, so the assumption (5) holds. In the case $d = 2, 3$, Theorem 3 is new.

Theorem 3 is especially useful in the study of Schrödinger operators with random point interactions. There are a lot of studies about the Schrödinger operators with random point interactions (3, 11, 23, 8, 12, 17, 13), but in most of these results $\Gamma$ is assumed to be $\mathbb{Z}^d$ or its random subset, except Minami’s paper (23). Using Theorem 3, we can study more general random
point interactions so that \( d_\omega \) can be 0. In the present paper, we prove the self-adjointness of \( H_{\Gamma,\alpha} \) for the following two models. First one is the random displacement model, given as follows. Notice that \( d_\omega \) can be 0 for this model.

**Corollary 4.** Let \( d = 1, 2, 3 \). Let \( \{\delta_n(\omega)\}_{n \in \mathbb{Z}^d} \) be a sequence of i.i.d. \( \mathbb{R}^d \)-valued random variables defined on some probability space \( \Omega \) such that \( |\delta_n(\omega)| < \mathbf{C} \) for some positive constant \( \mathbf{C} \) independent of \( n \) and \( \omega \in \Omega \). Put

\[
\Gamma_{\omega} = \{n + \delta_n(\omega)\}_{n \in \mathbb{Z}^d}.
\]

Then, \( H_{\Gamma_{\omega},\alpha} \) is self-adjoint for any \( \alpha = (\alpha_\gamma)_{\gamma \in \Gamma_{\omega}} \).

The proof of Corollary 4 is an application of Theorem 3 via some auxiliary result (Corollary 13). Another one is the Poisson model, given as follows.

**Corollary 5.** Let \( d = 1, 2, 3 \). Let \( \Gamma_{\omega} \) be the Poisson configuration on \( \mathbb{R}^d \) with intensity measure \( \lambda dx \) for some positive constant \( \lambda \). Then, \( H_{\Gamma_{\omega},\alpha} \) is self-adjoint for any \( \alpha = (\alpha_\gamma)_{\gamma \in \Gamma_{\omega}}, \) almost surely.

Corollary 5 is proved by combining Theorem 3 with the theory of continuum percolation (Theorem 15). These results are new when \( d = 2, 3 \), and are not new when \( d = 1 \), as stated before.

The proof of Theorem 3 also enables us to determine the spectrum of \( H_{\Gamma,\alpha} \) for the point interactions of Poisson-Anderson type, defined as follows.

**Assumption 6.** (i) \( \Gamma_{\omega} \) is the Poisson configuration with intensity measure \( \lambda dx \) for some \( \lambda > 0 \).

(ii) The coupling constants \( \alpha_{\omega} = (\alpha_{\omega,\gamma})_{\gamma \in \Gamma_{\omega}} \) are real-valued i.i.d. random variables with common distribution measure \( \nu \) on \( \mathbb{R} \). Moreover, \( (\alpha_{\omega,\gamma})_{\gamma \in \Gamma_{\omega}} \) are independent of \( \Gamma_{\omega} \).

**Theorem 7.** Let \( d = 1, 2, 3 \). Let \( \Gamma_{\omega} \) and \( \alpha_{\omega} \) satisfy Assumption 6 and put \( H_{\omega} = H_{\Gamma_{\omega},\alpha_{\omega}} \). Then, the spectrum \( \sigma(H_{\omega}) \) of \( H_{\omega} \) is given as follows.

(i) When \( d = 1 \), we have

\[
\sigma(H_{\omega}) = \begin{cases} [0, \infty) & (\text{supp} \nu \subset [0, \infty)), \\ \mathbb{R} & (\text{supp} \nu \cap (-\infty, 0) \neq \emptyset), \end{cases}
\]

almost surely.

(ii) When \( d = 2, 3 \), we have \( \sigma(H_{\omega}) = \mathbb{R} \) almost surely.
Notice that there is no assumption on $\text{supp} \nu$ when $d = 2, 3$. Theorem 7 can be interpreted as a generalization of the corresponding result for the Schrödinger operator $-\Delta + V_\omega$ with random scalar potential of Poisson-Anderson type

$$V_\omega(x) = \sum_{\gamma \in \Gamma_\omega} \alpha_{\omega, \gamma} V_0(x - \gamma),$$

where $\Gamma_\omega$ and $\alpha_\omega$ satisfy Assumption 6, and $V_0$ is a real-valued scalar function having some regularity and decaying property. The spectrum $\sigma(-\Delta + V_\omega)$ is determined in [24, 5, 18], and the result says ‘the spectrum equals $[0, \infty)$ if $V_\omega$ is non-negative, and it equals $\mathbb{R}$ if $V_\omega$ has negative part’. When $d = 1$, the point interaction at $\gamma$ has the same sign as the sign of the coupling constant $\alpha_\gamma$ in the sense of quadratic form, that is,

$$(u, H_{\Gamma, \alpha} u) = \|\nabla u\|^2 + \sum_{\gamma \in \Gamma} \alpha_\gamma |u(\gamma)|^2$$

for $u \in D(H_{\Gamma, \alpha})$ with bounded support. When $d = 2, 3$, the sign of point interaction at $\gamma$ is in some sense negative for any $\alpha_\gamma \in \mathbb{R}$. Actually, in the approximation [11], the limiting operator $H$ is not the free operator $H_0$ only if the zero-energy resonance of $-\Delta + V_\omega$ exists, and the existence of the zero-energy resonance requires $V$ has negative part (see [2]). There is also qualitative difference between the proof of Theorem 7 in the case $d = 1$ and that in the case $d = 2, 3$. The spectrum $(-\infty, 0)$ is created by the accumulation of many points in one place when $d = 1$, while it is created by the meeting of two points when $d = 2, 3$ (see section 3.3). The latter fact reminds us Thomas collapse, which says the mass defect of the tritium $^3\text{H}$ becomes arbitrarily large as the distances between a proton and two neutrons become small enough (see [27]).

Let us give a brief comment on the magnetic case. The Schrödinger operator with a constant magnetic field plus infinitely many point interactions is studied in [14, 12], and the self-adjointness is proved under the uniform discreteness condition [10]. Theorem 3 can be generalized under the existence of a constant magnetic field, by using the magnetic translation operator. We will discuss this case elsewhere in the near future.

The present paper is organized as follows. In section 2, we review some fundamental formulas about self-adjoint extensions of $H_{\Gamma, \min}$, and prove Theorem 3. The crucial fact is ‘bounded support functions are dense in $D(H_{\Gamma, \alpha})$ under Assumption 2’ (Proposition 12). In section 3, we prove the self-adjointness of Schrödinger operators with various random point interactions. We also determine the spectrum of $H_\omega = H_{\Gamma_\omega, \alpha_\omega}$ for Poisson-Anderson type.
point interactions, using the method of admissible potentials (Proposition 18; see also [19, 24, 5, 18]). In the proof, we again need Proposition 12, and also need to take care of the dependence of the operator domain $D(H_{\Gamma,\alpha})$ with respect to $\Gamma$ and $\alpha$. Once we establish the method of admissible potentials, the proof of Theorem 7 is reduced to the calculation of $\sigma(H_{\Gamma,\alpha})$ for admissible $(\Gamma, \alpha)$.

Let us explain the notation in the manuscript. The notation $A := B$ means $A$ is defined as $B$. The set $B_r(x)$ is the open ball of radius $r$ centered at $x \in \mathbb{R}^d$, that is, $B_r(x) := \{y \in \mathbb{R}^d; |y - x| < r\}$. The space $D(H)$ is the operator domain of a linear operator $H$ equipped with the graph norm $\|u\|_{D(H)}^2 = \|u\|^2 + \|Hu\|^2$. For an open set $U$, $C^\infty_0(U)$ is the set of compactly supported $C^\infty$ functions on $U$. The space $L^2(U)$ is the space of square integrable functions on $U$, and the inner product and the norm on $L^2(U)$ are defined as 

$$(u, v)_{L^2(U)} = \int_U \overline{u}v dx, \quad \|u\|_{L^2(U)} = (u, u)^{1/2}_{L^2(U)} = \left(\int_U |u|^2 dx\right)^{1/2}.$$ 

When $U = \mathbb{R}^d$, we often abbreviate the suffix $L^2(U)$. The space $H^2(U)$ is the Sobolev space of order 2 on $U$, and the norm is defined by 

$$\|u\|_{H^2(U)}^2 = \sum_{0 \leq |\alpha| \leq 2} \left\|\frac{\partial^{|\alpha|}u}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}\right\|_{L^2(U)}^2,$$

where $\alpha = (\alpha_1, \ldots, \alpha_d) \in (\mathbb{Z}_{\geq 0})^d$ is the multi-index and $|\alpha| = \alpha_1 + \cdots + \alpha_d$, and the derivatives are defined as elements of $\mathcal{D}'(U)$, the Schwartz distributions on $U$. The space $L^2_{\text{loc}}(U)$ is the set of the functions $u$ such that $\chi u \in L^2(U)$ for any $\chi \in C^\infty_0(U)$. The space $H^2_{\text{loc}}(U)$ is defined similarly.

2 Self-adjointness

2.1 Structure of $D(H_{\Gamma,\text{max}})$

First we review fundamental properties of the operator domain $D(H_{\Gamma,\text{max}})$ of the maximal operator $H_{\Gamma,\text{max}}$. Most of the results are already obtained under more general assumption (see e.g. [2, 9]), but we prove them here again for the completeness of the present manuscript.

Proposition 8. Let $d = 1, 2, 3$. 
(i) We have
\[ D(H_{\Gamma,\text{max}}) = \{ u \in L^2(\mathbb{R}^d) ; \Delta u \in L^2(\mathbb{R}^d) \} = \{ u \in L^2(\mathbb{R}^d) \cap H^2_{\text{loc}}(\mathbb{R}^d \setminus \Gamma) ; \Delta u \in L^2(\mathbb{R}^d) \}, \]
where \( \Delta u \) is defined as an element of \( D'(\mathbb{R}^d \setminus \Gamma) \).

(ii) Let \( \chi \in C_0^\infty(\mathbb{R}^d) \) such that \( \Gamma \cap \text{supp} \nabla \chi = \emptyset \). Then, for any \( u \in D(H_{\Gamma,\text{max}}) \), we have \( \chi u \in D(H_{\Gamma,\text{max}}) \).

Proof. (i) By definition, the statement \( u \in D(H_{\Gamma,\text{max}}) = D(H_{\Gamma,\text{min}}^*) \) is equivalent to \( u \in L^2(\mathbb{R}^d) \) and there exists \( v \in L^2(\mathbb{R}^d) \) such that \( (u, -\Delta \phi) = (v, \phi) \) for any \( \phi \in C_0^\infty(\mathbb{R}^d \setminus \Gamma) \). The latter statement is equivalent to \( v = -\Delta u \in L^2(\mathbb{R}^d) \), where \( \Delta u \) is defined as an element of \( D'(\mathbb{R}^d \setminus \Gamma) \). Moreover, by the elliptic inner regularity theorem (Corollary 24), we have \( u \in H^2_{\text{loc}}(\mathbb{R}^d \setminus \Gamma) \).

(ii) Let \( \chi \) satisfy the assumption, and \( u \in D(H_{\Gamma,\text{max}}) \). By the chain rule, we have
\[
\Delta (\chi u) = (\Delta \chi) u + 2 \nabla \chi \cdot \nabla u + \chi \Delta u.
\] (7)

Since \( u, \Delta u \in L^2(\mathbb{R}^d) \), the first term of (7) and the third belong to \( L^2(\mathbb{R}^d) \). Moreover, since \( \text{supp} \nabla \chi \) is a compact subset of \( \mathbb{R}^d \setminus \Gamma \) and \( u \in H^2_{\text{loc}}(\mathbb{R}^d \setminus \Gamma) \), the second term also belongs to \( L^2(\mathbb{R}^d) \). Thus \( \chi u, \Delta (\chi u) \in L^2(\mathbb{R}^d) \), and the statement follows from (i).

The assumption \( \Gamma \cap \text{supp} \nabla \chi = \emptyset \) above cannot be removed when \( d = 2, 3 \).

For example, consider the case \( d = 2 \), \( \Gamma = O := \{0\} \). Take functions \( u \in C^\infty(\mathbb{R}^2 \setminus O) \) and \( \chi \in C_0^\infty(\mathbb{R}^2) \) such that
\[
u(x) = \begin{cases} \log |x| & |x| < 1, \\ 0 & |x| > 2, \end{cases} \quad \chi(x) = \begin{cases} x_1 & |x| < 1, \\ 0 & |x| > 2. \end{cases}
\] (8)

Since \( \Delta \log |x| = 0 \) for \( x \neq 0 \), we see that \( u, \Delta u \in L^2(\mathbb{R}^2) \), so \( u \in D(H_{O,\text{max}}) \). However, the chain rule (7) implies
\[\Delta (\chi u) = \frac{2x_1}{|x|^2}\]
for \( |x| < 1 \), so \( \Delta (\chi u) \not\in L^2(\mathbb{R}^2) \). This fact is crucial in our proof of self-adjointness criterion (Theorem 3).

Next we define the (generalized) boundary values at \( \gamma \in \Gamma \) of \( u \in D(H_{\Gamma,\text{max}}) \). In the case \( d = 2, 3 \), similar argument is found in [2, 9].
Proposition 9.  
(i) Let \( d = 1 \), \( u \in D(H_{\Gamma, \text{max}}) \) and \( \gamma \in \Gamma \). Then, one-side limits \( u(\gamma \pm 0) \) and \( u'(\gamma \pm 0) \) exist.

(ii) Let \( d = 2, 3 \), \( u \in D(H_{\Gamma, \text{max}}) \) and \( \gamma \in \Gamma \). Let \( \epsilon \) be a small positive constant so that \( B_\epsilon(\gamma) \cap \Gamma = \{ \gamma \} \). Then, there exist unique constants \( u_{\gamma, 0} \) and \( u_{\gamma, 1} \), and \( \tilde{u} \in H^2(B_\epsilon(\gamma)) \) with \( \tilde{u}(\gamma) = 0 \), such that for \( x \in B_\epsilon(\gamma) \)

\[
\begin{align*}
  u(x) &= u_{\gamma, 0} \log |x - \gamma| + u_{\gamma, 1} + \tilde{u}(x) \quad (d = 2), \\
  u(x) &= u_{\gamma, 0} |x - \gamma|^{-1} + u_{\gamma, 1} + \tilde{u}(x) \quad (d = 3). 
\end{align*}
\]

Proof.  
(i) This is a consequence of the Sobolev embedding theorem, since the restriction of \( u \in D(H_{\Gamma, \text{max}}) \) on \( I \) belongs to \( H^2(I) \) for any connected component \( I \) of \( \mathbb{R} \setminus \Gamma \).

(ii) We consider the case \( d = 2 \). By a cut-off argument ((ii) of Proposition 8), we can reduce the proof to the case \( \Gamma \) equals one point set. With out loss of generality, we assume \( \Gamma = O \). Then, by von Neumann’s theory of self-adjoint extensions (see e.g. [25, Section X.1]), we have

\[
D(H_{O, \text{max}}) = D(H_{O, \text{min}}) \oplus K_{O,-} \oplus K_{O,+},
\]

where \( D(H_{O, \text{min}}) \) is the closure of \( D(H_{O, \text{min}}) \) with respect to the graph norm (or \( H^2 \)-norm), and \( K_{O, \pm} = \ker(H_{O, \text{max}} \mp i) \) are deficiency subspaces. It is known that \( K_{O, \pm} \) are one dimensional spaces spanned by

\[
\varphi_{\pm}(x) = H_0^{(1)}(\sqrt{\pm i} r),
\]

where \( H_0^{(1)} \) is the 0-th order Hankel function of the first kind, \( r = |x| \), and the branches of \( \sqrt{\pm i} \) are taken as \( \text{Im} \sqrt{\pm i} > 0 \) (see [2]). Thus we have inclusion

\[
D(H_{O, \text{max}}) \subset \{ u \in H^2(\mathbb{R}^2) ; u(0) = 0 \} \subset H^2(\mathbb{R}^2) \subset D(H_{O, \text{max}}).
\]

The first inclusion is due to the Sobolev embedding theorem. The second inclusion is clearly strict, and the third one is also strict since \( D(H_{O, \text{max}}) \) contains elements singular at 0, by (10) (see (12) below). The decomposition (10) also tells us \( \dim(D(H_{O, \text{max}}) / D(H_{O, \text{min}})) = 2 \), so the first inclusion in (11) must be equality, that is,

\[
D(H_{O, \text{min}}) = \{ u \in H^2(\mathbb{R}^2) ; u(0) = 0 \}.
\]

By the series expansion of the Hankel function, we have

\[
\varphi_\pm(x) = 1 + \frac{2i}{\pi} \left( \gamma E + \log \frac{\sqrt{\pm i} r}{2} \right) + O(r^2 \log r) \quad (r \to 0),
\]

(12)
where $\gamma_E$ is the Euler constant. It is easy to see the remainder term is in $H^2(B,0))$ and vanishes at 0. Thus by the decomposition (10), every $u \in D(H_{O,\text{max}})$ can be uniquely written as (9).

In the case $d = 3$, a basis of the deficiency subspace $K_{O,\pm}$ is

$$\varphi_{\pm}(x) = e^{i\sqrt{\pm r}} r = \frac{1}{r} + i\sqrt{\pm r} + O(r) \quad (r \to 0)$$

(see [2]). Using this expression, we can prove the statement for $d = 3$ similarly.

Next we introduce the generalized Green formula.

**Proposition 10.** Let $d = 1, 2, 3$. Let $u, v \in D(H_{\Gamma,\text{max}})$, and assume $\text{supp } u$ or $\text{supp } v$ is bounded. Then we have

$$\begin{align*}
(H_{\Gamma,\text{max}} u, v) - (u, H_{\Gamma,\text{max}} v) &= \sum_{\gamma \in \Gamma} (-\bar{u}'(\gamma - 0)v(\gamma - 0) + u(\gamma - 0)v'(\gamma - 0)) \\
&\quad + \bar{u}'(\gamma + 0)v(\gamma + 0) - u(\gamma + 0)v'(\gamma + 0)) \quad (d = 1), \\
&\quad \sum_{\gamma \in \Gamma} 2\pi(u_{\gamma,0}v_{\gamma,1} - \bar{u}_{\gamma,0}v_{\gamma,0}) \quad (d = 2), \\
&\quad \sum_{\gamma \in \Gamma} (-4\pi)(\bar{u}_{\gamma,0}v_{\gamma,1} - \bar{u}_{\gamma,1}v_{\gamma,0}) \quad (d = 3) .
\end{align*}$$

**Proof.** The proof in the case $d = 1$ is easy. Consider the case $d = 2$. By a cut-off argument, we can assume both $\text{supp } u$ and $\text{supp } v$ are bounded. We can also assume $\text{supp } u \cup \text{supp } v \subset B_R(0)$, and $\Gamma \cap \partial B_R(0) = \emptyset$. Then, we can decompose $u$ and $v$ as

$$u = \sum_{\gamma \in \Gamma \cap B_R(0)} (u_{\gamma,0}\phi_{\gamma} + u_{\gamma,1}\psi_{\gamma}) + \tilde{u}, \quad v = \sum_{\gamma \in \Gamma \cap B_R(0)} (v_{\gamma,0}\phi_{\gamma} + v_{\gamma,1}\psi_{\gamma}) + \tilde{v},$$

where $\tilde{u}, \tilde{v} \in \overline{D(H_{\Gamma,\text{min}})}$, and $\phi_{\gamma}, \psi_{\gamma} \in D(H_{\Gamma,\text{max}})$ are real-valued functions such that

$$\phi_{\gamma}(x) = \log |x - \gamma|, \quad \psi_{\gamma}(x) = 1 \quad \text{near } x = \gamma,$$

and $\text{supp } \phi_{\gamma} \cup \text{supp } \psi_{\gamma}$ is contained in some small neighborhood of $\gamma$ so that $\{\text{supp } \phi_{\gamma} \cup \text{supp } \psi_{\gamma}\}_{\gamma \in \Gamma \cap B_R(0)}$ are disjoint sets in $B_R(0)$.

We use the notation

$$[\phi, \psi] = (H_{\Gamma,\text{max}} \phi, \psi) - (\phi, H_{\Gamma,\text{max}} \psi).$$
Clearly \([\phi, \psi] = -[\psi, \phi]\), so \([\phi, \phi] = 0\) for real-valued \(\phi \in D(H_{\Gamma, \max})\). Moreover, \([\phi, \psi] = 0\) if \(\phi \in D(H_{\Gamma, \max})\) and \(\psi \in D(H_{\Gamma, \min})\). Thus we have

\[
[u, v] = \sum_{\gamma \in \Gamma \cap BR(0)} (\overline{u_{\gamma,0}}v_{\gamma,1} - \overline{u_{\gamma,1}}v_{\gamma,0}) [\phi_{\gamma}, \psi_{\gamma}],
\]

Let us calculate \([\phi_{\gamma}, \psi_{\gamma}]\). By translating the coordinate, we assume \(\gamma = 0\), and write \(\phi_{\gamma} = \phi, \psi_{\gamma} = \psi\). Then, since \(\phi = \log r\) and \(\psi = 1\) near \(x = 0\),

\[
[\phi, \psi] = \lim_{\epsilon \downarrow 0} \int_{B_\epsilon(0)} \left( (-\overline{\nabla \phi}) \psi + \overline{\phi} (\nabla \psi) \right) dx
\]

\[
= \lim_{\epsilon \downarrow 0} \int_{\partial B_\epsilon(0)} \left( (-\nabla \phi \cdot n) \psi + \phi (\nabla \psi \cdot n) \right) ds
\]

\[
= \lim_{r \downarrow 0} \int_{0}^{2\pi} \left( \frac{\partial \phi}{\partial r} \cdot \psi - \phi \cdot \frac{\partial \psi}{\partial r} \right) r d\theta
\]

\[
= 2\pi,
\]

where \(n\) is the unit inner normal vector on \(\partial B_\epsilon(0)\), \(ds\) is the line element, and \((r, \theta)\) is the polar coordinate. Thus the assertion for \(d = 2\) holds. The proof for the case \(d = 3\) is similar, but we take the function \(\phi_{\gamma}\) as

\[
\phi_{\gamma}(x) = |x - \gamma|^{-1} \quad \text{near } x = \gamma.
\]

If the uniform discreteness condition \(4\) holds, the results in this subsection can be formulated in terms of the boundary triplet for \(H_{\Gamma, \max}\), as is done in \([9]\). When \(d = 1\) and \(d_* = 0\), the boundary triplet for \(H_{\Gamma, \max}\) is constructed in \([20]\). The construction in the case \(d = 2, 3\) and \(d_* = 0\) seems to be unknown so far.

### 2.2 Proof of Theorem 3

Let \(\Gamma\) be a locally finite discrete set in \(\mathbb{R}^d\), and \(\alpha = (\alpha_\gamma)_{\gamma \in \Gamma}\) be a sequence of real numbers. In this subsection we write \(H = H_{\Gamma, \alpha}\), that is,

\[
Hu = -\Delta u, \quad D(H) = \{u \in D(H_{\Gamma, \max}) \mid u \text{ satisfies (BC)}_{\gamma} \text{ for every } \gamma \in \Gamma\},
\]

where \((BC)_{\gamma}\) is defined in \([3]\). We introduce an auxiliary operator \(H_b\) by

\[
H_bu = -\Delta u, \quad D(H_b) = \{u \in D(H) \mid \text{supp } u \text{ is bounded}\}.
\]

By the generalized Green formula (Proposition \([11]\)), we have the following.
Proposition 11. Let \( d = 1, 2, 3 \). For any \( \Gamma \) and \( \alpha \), the operator \( H_b \) is a densely defined symmetric operator, and \( H_b^* = H \).

Proof. We consider the case \( d = 2 \), since the case \( d = 1, 3 \) can be treated similarly. For \( u, v \in D(H_b) \), the generalized Green formula (13) and \((BC)_\gamma\) imply
\[
[u, v] := (Hu, v) - (u, Hv) = \sum_{\gamma \in \Gamma} 2\pi (u_{\gamma,0}v_{\gamma,1} - \overline{u_{\gamma,1}v_{\gamma,0}})
= \sum_{\gamma \in \Gamma} (2\pi)^2 \alpha_\gamma (-\overline{u_{\gamma,0}}v_{\gamma,0} + \overline{u_{\gamma,0}}v_{\gamma,0}) = 0.
\]
Thus \( H_b \) is a symmetric operator.

The equality (14) also holds for any \( u \in D(H_b) \) and \( v \in D(H_b) \), so \( D(H_b^*) \subset D(H_b) \). Conversely, let \( v \in D(H_b^*) \). By definition, \([u, v] = 0\) holds for any \( u \in D(H_b) \). For \( \gamma \in \Gamma \), take \( u \in D(H_b) \) such that \( u_{\gamma,0} = 1/(2\pi) \), \( u_{\gamma,1} = -\alpha_\gamma \), and \( u_{\gamma',0} = u_{\gamma',1} = 0 \) for \( \gamma' \neq \gamma \). Since \( D(H_b^*) \subset D(H_{\Gamma,\min}^*) = D(H_{\Gamma,\max}) \), we have by the generalized Green formula (13)
\[
[u, v] = v_{\gamma,1} + 2\pi \alpha_\gamma v_{\gamma,0} = 0.
\]
Thus \( v \) satisfies \((BC)_\gamma\) for every \( \gamma \in \Gamma \), and we conclude \( v \in D(H) \). This means \( H = H_b^* \).

Now Theorem 3 is a corollary of the following proposition.

Proposition 12. Suppose Assumption 2 holds. Then, \( \overline{H_b} = H \). In other words, \( D(H_b) \) is an operator core for the operator \( H \).

Proof. Let \( R \) be the constant in Assumption 2. For a positive integer \( n \), let \( S_n \) be the connected component of \( B_n(0) \cup (\Gamma)_R \) containing \( B_n(0) \) (see Figure 2).

By assumption, \( S_n \) is a bounded open set in \( \mathbb{R}^d \). Let \( \eta \in C_0^\infty(\mathbb{R}^d) \) be a rotationally symmetric function such that \( \eta \geq 0 \), \( \text{supp} \eta \subset B_{R/3}(0) \), and \( \int_{\mathbb{R}^d} \eta dx = 1 \). Put
\[
\chi_n(x) = \int_{S_n} \eta(x - y) dy.
\]
The function \( \chi_n \) has the following properties.

(i) \( \chi_n \in C_0^\infty(\mathbb{R}^d) \), \( 0 \leq \chi_n(x) \leq 1 \), and
\[
\chi_n(x) = \begin{cases} 
1 & (x \in S_n, \ \text{dist}(x, \partial S_n) > R/3), \\
0 & (x \notin S_n, \ \text{dist}(x, \partial S_n) > R/3).
\end{cases}
\]
In particular, \( \chi_n(x) \to 1 \) as \( n \to \infty \) for every \( x \in \mathbb{R}^d \).
(ii) supp $\nabla \chi_n \subset (\partial S_n)_{R/3}$, and supp $\nabla \chi_n \cap \Gamma = \emptyset$.

(iii) $\|\nabla \chi_n\|_\infty$, $\|\Delta \chi_n\|_\infty$ are bounded uniformly with respect to $n$, where $\|\cdot\|_\infty$ denotes the sup norm.

Let $u \in D(H)$. By (i), (ii) and Proposition 8, $\chi_n u \in D(H_b)$. By the dominated convergence theorem and (i), $\chi_n u \to u$ in $L^2(\mathbb{R}^d)$. Moreover,

$$\Delta (\chi_n u) - \Delta u = (\chi_n - 1)\Delta u + 2\nabla \chi_n \cdot \nabla u + (\Delta \chi_n) u. \quad (15)$$

Since $u, \Delta u \in L^2$, the first term of (15) and the third tend to 0 in $L^2(\mathbb{R}^d)$ by the dominated convergence theorem. As for the second term, we apply the elliptic inner regularity estimate (Corollary 24) for $U = (\partial S_n)_{R/2}$ and $V = (\partial S_n)_{R/3}$, and obtain

$$\|\nabla \chi_n \cdot \nabla u\|_{L^2(\mathbb{R}^d)} \leq \|\nabla \chi_n\|_\infty \|\nabla u\|_{L^2(V)} \leq C \|\nabla \chi_n\|_\infty \left(\|\Delta u\|_{L^2(U)} + \|u\|_{L^2(U)}\right) \leq C \|\nabla \chi_n\|_\infty \left(\|\Delta u\|_{L^2(B_n-R/2(0)^c)} + \|u\|_{L^2(B_n-R/2(0)^c)}\right).$$

Here the constant $C$ is independent of $n$, since dist($V, \partial U$) $\geq R/6$ and the lower bound is independent of $n$. The last expression tends to 0 as $n \to \infty$, so $\Delta (\chi_n u) - \Delta u \to 0$ in $L^2(\mathbb{R}^d)$. Thus $\chi_n u \in D(H_b)$ converges to $u$ in $D(H)$, and we conclude $D(H_b)$ is dense in $D(H)$. $\square$
Proof of Theorem 3. Proposition 11 implies $H = H_b^*$, and $H_b^* = (\overline{H_b})^*$ always holds. On the other hand, Proposition 12 says $\overline{H_b} = H_b$, so $H = H_b^* = (\overline{H_b})^* = H^*$. Thus $H$ is self-adjoint.

3 Random point interactions

Using Theorem 3 we study the Schrödinger operators with random point interactions so that $d_\gamma$ can be 0.

3.1 Self-adjointness

First we give a simple corollary of Theorem 3.

**Corollary 13.** Assume that there exists $R_0 > 0$ and $M > 0$ such that $\#(\Gamma \cap B_{R_0}(x)) \leq M$ for every $x \in \mathbb{R}^d$. Then, $H_{\Gamma, \alpha}$ is self-adjoint for any $\alpha = (\alpha_\gamma)_{\gamma \in \Gamma}$.

**Proof.** The assumption implies Assumption 2 holds with $R = R_0/(2M)$, since the connected component of $(\Gamma)_R$ containing $x \in \mathbb{R}^d$ is contained in the bounded set $B_{R_0}(x)$. □

The assumption of Corollary 13 is satisfied for random displacement model (Corollary 4).

**Proof of Corollary 4.** Under the assumption of Corollary 4 we have

$$\#(\Gamma \cap B_1(x)) \leq \#(\mathbb{Z}^d \cap B_{C+1}(x)) \leq \left| B_{C+1+\sqrt{d}/2}(0) \right|,$$

where $|S|$ denotes the Lebesgue measure of a measurable set $S$. Thus the assumption of Corollary 13 is satisfied. □

Next, we consider the case $\Gamma = \Gamma_\omega$ is the Poisson configuration (Corollary 5). We review the definition of the Poisson configuration (see e.g. [24], [5], [18], [26]).

**Definition 14.** Let $\mu_\omega$ be a random measure on $\mathbb{R}^d$ ($d \geq 1$) dependent on $\omega \in \Omega$ for some probability space $\Omega$. For a positive constant $\lambda$, we say $\mu_\omega$ is the Poisson point process with intensity measure $\lambda dx$ if the following conditions hold.
(i) For every Borel measurable set $E \in \mathbb{R}^d$ with the Lebesgue measure $|E| < \infty$, $\mu_\omega(E)$ is an integer-valued random variable on $\Omega$ and

$$
\mathbb{P}(\mu_\omega(E) = k) = \frac{(\lambda |E|)^k}{k!} e^{-\lambda |E|}
$$

for every non-negative integer $k$.

(ii) For any disjoint Borel measurable sets $E_1, \ldots, E_n$ in $\mathbb{R}^d$ with finite Lebesgue measure, the random variables $\{\mu_\omega(E_j)\}_{j=1}^n$ are independent.

We call the support $\Gamma_\omega$ of the Poisson point process measure $\mu_\omega$ the Poisson configuration.

We introduce a basic result in the theory of continuum percolation (see e.g. [22]).

**Theorem 15** (Continuum percolation). Let $\Gamma = \Gamma_\omega$ be the Poisson configuration on $\mathbb{R}^d$ ($d \geq 2$) with intensity measure $\lambda dx$, where $\lambda$ is a positive constant. For $R > 0$, let $\theta_R(\lambda)$ be the probability of the event ‘the connected component of $(\Gamma)_R$ containing the origin is unbounded’. Then, for any $R > 0$, there exists a positive constant $\lambda_c(R)$, called the critical density, such that

$$\begin{cases}
\theta_R(\lambda) = 0 & (\lambda < \lambda_c(R)), \\
\theta_R(\lambda) > 0 & (\lambda > \lambda_c(R)).
\end{cases}$$

Moreover, the scaling property

$$\lambda_c(R) = R^{-d} \lambda_c(1) \tag{16}$$

holds for any $R > 0$.

When $d = 1$, it is easy to see $\theta_R(\lambda) = 0$ for every $R > 0$ and $\lambda > 0$, so we put $\lambda_c(R) = \infty$.

**Proof of Corollary 5.** By the scaling property (16), the condition $\lambda < \lambda_c(R)$ is satisfied if we take $R$ sufficiently small. Then, since the Poisson point process is statistically translationally invariant and $\mathbb{R}^d$ has a countable dense subset, we see that every connected component of $(\Gamma_\omega)_R$ is bounded, almost surely. Thus Theorem 15 implies the conclusion. \(\square\)
3.2 Admissible potentials for Poisson-Anderson type point interactions

By Corollary 5, we can define the Schrödinger operator with random point interactions of Poisson-Anderson type, that is, \((\Gamma_\omega, \alpha_\omega)\) satisfies Assumption \(6\). We write \(H_\omega = H_{\Gamma_\omega, \alpha_\omega}\) for simplicity, and study the spectrum of \(H_\omega\). For this purpose, we use the method of admissible potentials, which is a useful method when we determine the spectrum of the random Schrödinger operators (see e.g. [19, 24, 5, 18]).

Definition 16. Let \(\nu\) be the single-site measure in (ii) of Assumption \(\alpha\).

(i) We say a pair \((\Gamma, \alpha)\) belongs to \(A_F\) if \(\Gamma\) is a finite set in \(\mathbb{R}^d\) and \(\alpha = (\alpha_\gamma)_{\gamma \in \Gamma}\) with \(\alpha_\gamma \in \text{supp}\ \nu\) for every \(\gamma \in \Gamma\).

(ii) We say a pair \((\Gamma, \alpha)\) belongs to \(A_P\) if \(\Gamma\) is expressed as

\[
\Gamma = \bigcup_{k=1}^{n} \left( \gamma_k + \bigoplus_{j=1}^{d} \mathbb{Z}e_j \right)
\]

for some \(n = 0, 1, 2, \ldots\), some vectors \(\gamma_1, \ldots, \gamma_n \in \mathbb{R}^d\) and independent vectors \(e_1, \ldots, e_d \in \mathbb{R}^d\), and \(\alpha = (\alpha_\gamma)_{\gamma \in \Gamma}\) is a \(\text{supp}\ \nu\)-valued periodic sequence on \(\Gamma\), i.e., \(\alpha_\gamma \in \text{supp}\ \nu\) for every \(\gamma \in \Gamma\) and \(\alpha_{\gamma + e_j} = \alpha_\gamma\) for every \(\gamma \in \Gamma\) and \(j = 1, \ldots, d\).

Notice that \((\Gamma, \alpha)\) belongs to both \(A_F\) and \(A_P\) if \(\Gamma = \emptyset\).

We need a lemma about the continuous dependence of the operator domain \(D(H_{\Gamma, \alpha})\) with respect to \((\Gamma, \alpha)\).

Lemma 17. Let \(\Gamma = \{\gamma_j\}_{j=1}^{n}\) be an \(n\)-point set and \(\alpha = (\alpha_j)_{j=1}^{n}\) a real-valued sequence on \(\Gamma\), where we denote \(\alpha_{\gamma_j}\) by \(\alpha_j\). Let \(\delta = \min_{j \neq k} |\gamma_j - \gamma_k|\). Let \(\epsilon > 0\), \(E \in \mathbb{R}\), and \(U\) be a bounded open set. Suppose that there exists \(u_\epsilon \in D(H_{\Gamma, \alpha})\) such that \(\|u_\epsilon\| = 1\), \(\text{supp}\ u_\epsilon \subset U\), and \(\|(H_{\Gamma, \alpha} - E)u_\epsilon\| \leq \epsilon\). Then the following holds.

(i) There exists \(\epsilon' > 0\) satisfying the following property; for any \(\tilde{\Gamma} = \{\tilde{\gamma}_j\}_{j=1}^{n}\) with \(|\gamma_j - \tilde{\gamma}_j| \leq \epsilon'\), there exists \(v_\epsilon \in H_{\Gamma, \alpha}\) such that \(\|v_\epsilon\| = 1\), \(\text{supp}\ v_\epsilon \subset U\), and \(\|(H_{\Gamma, \alpha} - E)v_\epsilon\| \leq 2\epsilon\).

(ii) There exists \(\epsilon'' > 0\) satisfying the following property; for any \(\tilde{\alpha} = (\tilde{\alpha}_j)_{j=1}^{n}\) with \(|\alpha_j - \tilde{\alpha}_j| \leq \epsilon''\), there exists \(v_\epsilon \in H_{\Gamma, \tilde{\alpha}}\) such that \(\|v_\epsilon\| = 1\), \(\text{supp}\ v_\epsilon \subset U\), and \(\|(H_{\Gamma, \tilde{\alpha}} - E)v_\epsilon\| \leq 2\epsilon\). Moreover, \(\epsilon''\) can be taken uniformly with respect to \(\Gamma\) so that \(\delta = \delta(\Gamma)\) is bounded uniformly from below.
Proof. (i) Let \( \eta \in C_0^\infty(\mathbb{R}^d) \) such that \( 0 \leq \eta \leq 1 \), \( \eta(x) = 1 \) for \( x \leq \delta/4 \), and \( \eta(x) = 0 \) for \( x \geq \delta/3 \). Let \( \tilde{\Gamma} = \{ \tilde{\gamma}_j \}^n_{j=1} \) with \( |\gamma_j - \tilde{\gamma}_j| \leq \epsilon' \) for sufficiently small \( \epsilon' \) (specified later). Consider the map

\[
\Phi(x) = x + \sum_{j=1}^n \eta(x - \gamma_j) \cdot (\tilde{\gamma}_j - \gamma_j). \tag{17}
\]

By definition, \( \Phi \) is a \( C^\infty \) map from \( \mathbb{R}^d \) to itself, \( \Phi(\gamma_j) = \tilde{\gamma}_j \), and

\[
|\Phi(x) - x| + |\nabla(\Phi(x) - x)| + |\Delta(\Phi(x) - x)| \leq C \epsilon'
\]

for some positive constant \( C \). Thus, by Hadamard’s global inverse function theorem, \( \Phi \) is a diffeomorphism from \( \mathbb{R}^d \) to itself, for sufficiently small \( \epsilon' \).

Put \( w_\epsilon := u_\epsilon \circ \Phi^{-1} \). We can easily check \( w_\epsilon \in D(\tilde{\Gamma}_\epsilon) \), since the map \( \Phi \) is just a translation in \( B_{\delta/4}(\gamma_j) \). We use the the coordinate change \( x = \Phi(y) \) or \( y = \Phi^{-1}(x) \). By (17) and the inverse function theorem, we have estimates

\[
\frac{\partial x_j}{\partial y_k}(y) = \delta_{jk} + O(\epsilon'), \quad \frac{\partial y_j}{\partial x_k}(x) = \delta_{jk} + O(\epsilon'), \quad \frac{\partial^2 y_j}{\partial x_k \partial x_\ell}(x) = O(\epsilon'),
\]

\[
det \left( \frac{\partial x}{\partial y} \right) = 1 + O(\epsilon') \tag{18}
\]

as \( \epsilon' \to 0 \), where \( \delta_{jk} \) is Kronecker’s delta, and \( \partial x/\partial y = (\partial x_j/\partial y_k)_{jk} \) is the Jacobian matrix. The remainder terms are uniform with respect to \( x \) (or \( y \)), and are equal to 0 for \( x \not\in \bigcup_j (B_{\delta/3}(\gamma_j) \setminus B_{\delta/4}(\gamma_j)) \). Thus we have by (18)

\[
\|w_\epsilon\|^2 = \int_{\mathbb{R}^d} |u_\epsilon(y)|^2 \, dx = \int_{\mathbb{R}^d} |u_\epsilon(y)|^2 \left| \det \left( \frac{\partial x}{\partial y} \right) \right| \, dy = 1 + O(\epsilon').
\]

Next, by the chain rule

\[
\Delta u_\epsilon(x) = \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} u_\epsilon(y)
\]

\[
= \sum_{j=1}^d \frac{\partial}{\partial x_j} \left( \sum_{k=1}^d \frac{\partial u_\epsilon(y)}{\partial y_k} \cdot \frac{\partial y_k}{\partial x_j}(x) \right)
\]

\[
= \sum_{j=1}^d \sum_{k=1}^d \left( \sum_{\ell=1}^d \frac{\partial^2 u_\epsilon}{\partial y_k \partial y_\ell}(y) \cdot \frac{\partial y_k}{\partial x_j}(x) \cdot \frac{\partial y_\ell}{\partial x_j}(x) + \frac{\partial u_\epsilon(y)}{\partial y_k} \cdot \frac{\partial^2 y_k}{\partial x_j^2}(x) \right).
\]
Thus we have by \((18)\)
\[
\|(H_{\Gamma,\alpha} - E)w_\epsilon\|^2 \\
\int_{\mathbb{R}^d}|(-\Delta x - E)w_\epsilon(x)|^2 dx \\
= \int_{\mathbb{R}^d}|(-\Delta y - E)u_\epsilon(y)|^2 dy \cdot (1 + O(\epsilon')) + \frac{1}{n} \sum_{j=1}^{n} \|u_\epsilon\|_{H^2(B_{\delta/3}(\gamma_j)) \setminus B_{\delta/4}(\gamma_j)}^2 \cdot O(\epsilon').
\]
\[
\leq \epsilon^2 (1 + O(\epsilon')) + \frac{1}{n} \sum_{j=1}^{n} \|u_\epsilon\|_{H^2(B_{\delta/3}(\gamma_j)) \setminus B_{\delta/4}(\gamma_j)}^2 \cdot O(\epsilon').
\]
By the elliptic inner regularity estimate (Corollary 24)
\[
\sum_{j=1}^{n} \|u_\epsilon\|_{H^2(B_{\delta/3}(\gamma_j)) \setminus B_{\delta/4}(\gamma_j)}^2 \leq C \sum_{j=1}^{n} \left(\|(-\Delta u_\epsilon - E)u_\epsilon\|_{L^2(B_{\delta/2}(\gamma_j))}^2 + \|u_\epsilon\|_{L^2(B_{\delta/2}(\gamma_j))}^2\right) \leq C(\epsilon^2 + 1),
\]
where \(C\) is a positive constant independent of \(u_\epsilon\). Taking \(\epsilon'\) sufficiently small and putting \(v_\epsilon = w_\epsilon/\|w_\epsilon\|\), we conclude \(v_\epsilon\) has the desired property.

(ii) We give the proof only in the case \(d = 2\) (the case \(d = 1, 3\) can be treated similarly). Let \(\phi_j = \phi_{\gamma_j}\) and \(\psi_j = \psi_{\gamma_j}\) be the functions introduced in the proof of Proposition 10. Then, the function \(u_\epsilon\) can be uniquely expressed as
\[
u_\epsilon = \sum_{j=1}^{d} C_j(\phi_j - 2\pi \alpha_j \psi_j) + \tilde{u}_\epsilon,
\]
where \(C_j\) is a constant and \(\tilde{u}_\epsilon \in H^2(\mathbb{R}^2)\) such that \(\tilde{u}_\epsilon(\gamma_j) = 0\) for every \(j\).

Suppose \(|\tilde{\alpha}_j - \alpha_j| \leq \epsilon''\) for sufficiently small \(\epsilon''\), and put
\[
u_\epsilon = \sum_{j=1}^{d} C_j(\phi_j - 2\pi \tilde{\alpha}_j \psi_j) + \tilde{u}_\epsilon,
\]
and \(v_\epsilon = w_\epsilon/\|w_\epsilon\|.\) Then we can prove that \(v_\epsilon\) has the desired property. \(\square\)

Proposition 18. Let \(d = 1, 2, 3,\) and \(\Gamma_\omega\) and \(\alpha_\omega\) satisfy Assumption 6. Then, for \(H_\omega = H_{\Gamma_\omega,\alpha_\omega}\),
\[
\sigma(H_\omega) = \bigcup_{(\Gamma,\alpha) \in A_F} \sigma(H_{\Gamma,\alpha}) = \bigcup_{(\Gamma,\alpha) \in A_F} \sigma(H_{\Gamma,\alpha}) (19)
\]
holds almost surely.
Proof. First, let
\[ \Sigma = \bigcup_{(\Gamma, \alpha) \in \mathcal{A}_F} \sigma(H_{\Gamma, \alpha}), \]
and prove \( \sigma(H_\omega) = \Sigma \) holds almost surely.

Recall that \( \Gamma_\omega \) is a locally finite discrete subset satisfying Assumption \( \text{II-2.1.3} \) (so \( H_\omega \) is self-adjoint), almost surely. For such \( \omega \), let \( E \in \sigma(H_\omega) \). Then, by Proposition \( \text{II-2.1.3} \) for any \( \epsilon > 0 \) there exists \( u_\epsilon \in D(H_\omega) \) such that \( \text{supp } u_\epsilon \) is bounded, \( \|u_\epsilon\| = 1 \), and \( \|H_\omega - E\)\( u_\epsilon \| \leq \epsilon \). Let \( \tilde{\Gamma} = \Gamma_\omega \cap \text{supp } u_\epsilon \) and \( \tilde{\alpha} = (\alpha_{\omega, \gamma})_{\gamma \in \tilde{\Gamma}} \). Then, \((\tilde{\Gamma}, \tilde{\alpha}) \in \mathcal{A}_F \), \( u_\epsilon \in D(H_{\tilde{\Gamma}, \tilde{\alpha}}) \) and \( \|H_{\tilde{\Gamma}, \tilde{\alpha}} - E\)\( u_\epsilon \| \leq \epsilon \). This implies \( \text{dist}(E, \Sigma) \leq \epsilon \) for any \( \epsilon > 0 \), so \( E \in \Sigma \). Thus we conclude \( \sigma(H_\omega) \subset \Sigma \) almost surely.

Conversely, let \( E \in \sigma(H_{\Gamma, \alpha}) \) for some \((\Gamma, \alpha) \in \mathcal{A}_F \). Then, for any \( \epsilon > 0 \), there exists \( u_\epsilon \in D(H_{\Gamma, \alpha}) \) such that \( \text{supp } u_\epsilon \) is contained in some bounded open set \( U \), \( \|u_\epsilon\| = 1 \), and \( \|H_{\Gamma, \alpha} - E\)\( u_\epsilon \| \leq \epsilon \). We write \( \Gamma := \Gamma \cap U = \{\gamma_j\}_{j=1} \) and \( \alpha_j = \alpha_\gamma \). By the ergodicity of \((\Gamma_\omega, \alpha_\omega)\), for any \( \epsilon', \epsilon'' > 0 \) we can almost surely find \( y \in \mathbb{R}^d \) such that \( \Gamma_{\epsilon'} := \Gamma_\omega \cap (y + U) = \{\gamma'_j\}_{j=1} \), \( \gamma'_j = \gamma_j + y + \epsilon'_j \) with \( |\epsilon'_j| \leq \epsilon' \), and \( \alpha_{\omega, \gamma'_j} = \alpha_j + \epsilon''_j \) with \( |\epsilon''_j| \leq \epsilon'' \). Taking \( \epsilon' \) and \( \epsilon'' \) sufficiently small and applying Lemma \( \text{I-2.1.3} \) we can almost surely find \( v_\epsilon \in D(H_\omega) \) such that \( \text{supp } v_\epsilon \) is bounded, \( \|v_\epsilon\| = 1 \), and \( \|H_\omega - E\)\( v_\epsilon \| \leq 4\epsilon \). Then we have \( \text{dist}(\sigma(H_\omega), E) \leq 4\epsilon \) for any \( \epsilon > 0 \), so \( E \in \sigma(H_\omega) \) almost surely. Thus \( \Sigma \subset \sigma(H_\omega) \), and the first equality in \( \text{II-2.1.3} \) holds.

The proof of the second equality in \( \text{II-2.1.3} \) is similar; we have only to replace \( \mathcal{A}_F \) by \( \mathcal{A}_P \), and \((\Gamma, \tilde{\alpha}) \) in the first part of the proof by its periodic extension.

\( \square \)

### 3.3 Calculation of the spectrum

By Proposition \( \text{II-2.1.3} \), the proof of Theorem \( \text{II-2.1.3} \) is reduced to the calculation of the spectrum of \( H_{\Gamma, \alpha} \) for \((\Gamma, \alpha) \in \mathcal{A}_F \) or \( \mathcal{A}_P \).

First we consider the case \( d = 1 \) and the interactions are non-negative.

**Lemma 19.** Let \( d = 1 \). Let \( \Gamma \) be a finite set and \( \alpha = (\alpha_\gamma)_{\gamma \in \Gamma} \) with \( \alpha_\gamma \geq 0 \) for every \( \gamma \in \Gamma \). Then, \( \sigma(H_{\Gamma, \alpha}) = [0, \infty) \).

**Proof.** Under the assumption of the lemma, we have
\[
(u, H_{\Gamma, \alpha}u) = \|\nabla u\|^2 + \sum_{\gamma \in \Gamma} \alpha_\gamma |u(\gamma)|^2 \geq 0
\]
for any \( u \in D(H_{\Gamma, \alpha}) \). Thus \( \sigma(H_{\Gamma, \alpha}) \subset [0, \infty) \). The inverse inclusion \( \sigma(H_{\Gamma, \alpha}) \supset [0, \infty) \) follows from \( \text{II-2.1.3} \).

\( \square \)
Lemma 19 seems obvious, but the same statement does not hold when $d = 2, 3$, since the point interaction is always negative in that case, as stated in the introduction.

Next we consider the other cases. In the following lemmas, the sequence $\alpha = (\alpha_\gamma)_{\gamma \in \Gamma}$ is assumed to be a constant sequence, that is, all the coupling constants $\alpha_\gamma$ are the same. We denote the common coupling constant $\alpha_\gamma$ also by $\alpha$, by abuse of notation.

**Lemma 20.** Let $d = 1$, and $x_1, \ldots, x_N$ be $N$ distinct points in $\mathbb{R}$ with $2 \leq N < \infty$. For $L > 0$, put $\Gamma_{N,L} = \{Lx_j\}_{j=1}^N$. Let $\alpha$ be a constant sequence on $\Gamma_{N,L}$ with common coupling constant $\alpha < 0$. Then, the following holds.

(i) Let $N = 2$ and $|x_1 - x_2| = 1$. Then, $H_{\Gamma_{2,L},\alpha}$ has only one negative eigenvalue $E_1(L)$ for $L \leq -2/\alpha$, and two negative eigenvalues $E_1(L)$ and $E_2(L)$ ($E_1(L) < E_2(L)$) for $L > -2/\alpha$. The function $E_1(L)$ (resp. $E_2(L)$) is continuous and monotone increasing (resp. decreasing) with respect to $L \in (0, \infty)$ (resp. $L \in (-2/\alpha, \infty)$), and

$$\lim_{L \to -2/\alpha} E_1(L) = 0, \quad \lim_{L \to \infty} E_1(L) = -\alpha^2/4,$$

$$\lim_{L \to +0} E_2(L) = -\alpha^2/4.$$

(ii) Let $N \geq 3$. Then the operator $H_{\Gamma_{N,L},\alpha}$ has at least one negative eigenvalue for any $L > 0$. The smallest eigenvalue $E_1(L)$ is simple, continuous and monotone increasing with respect to $L \in (0, \infty)$, and

$$\lim_{L \to +0} E_1(L) = -\frac{(N\alpha)^2}{4}, \quad \lim_{L \to \infty} E_1(L) = -\alpha^2/4.$$

**Proof.** According to [2, Theorem II-2.1.3], $H_{\Gamma_{N,L},\alpha}$ has a negative eigenvalue $E = -s^2$ ($s > 0$) if and only if $\det M = 0$, where $M = (M_{jk})$ is the $N \times N$ matrix given by

$$M_{jk} = \begin{cases} -\alpha^{-1} - (2s)^{-1} & (j = k), \\ -(2s)^{-1}e^{-sL|x_j-x_k|} & (j \neq k). \end{cases}$$

Let $\widetilde{M} = (\widetilde{M}_{jk})$ be the $N \times N$-matrix given by $\widetilde{M}_{jk} = e^{-sL|x_j-x_k|}$. Then, since $M = -(2s)^{-1}(2s/\alpha \cdot I + \widetilde{M})$ ($I$ is the identity matrix),

$$\det M = 0 \iff M \text{ has eigenvalue } 0 \iff -2s/\alpha \text{ coincides with one of eigenvalues of } \widetilde{M}.$$
(i) Let $N = 2$ and $|x_1 - x_2| = 1$. Then the eigenvalues of $\tilde{M}$ are $1 \pm e^{-sL}$. So we have $E_1(L) = -s_1(L)^2$ and $E_2(L) = -s_2(L)^2$, where $s = s_1(L)$ and $s = s_2(L)$ are solutions of
\[
\frac{-2s}{\alpha} = 1 + e^{-sL}, \quad \frac{2s}{\alpha} = 1 - e^{-sL},
\]
respectively, if the solutions exist. Then the statement can be proved by inspecting the graphs of both sides of (20) (see Figure 3, 4).

![Figure 3: Graphs of both sides of (20) for $\alpha = -1$ and $L = 2^n$ ($n = -4, \ldots, 1$).](image)

![Figure 4: Graphs of both sides of (20) for $\alpha = -1$ and $L = 2^n$ ($n = 2, \ldots, 4$).](image)

(ii) Let $N \geq 3$. Let $\mu_1(s, L)$ be the largest eigenvalue of $\tilde{M}$. Since $\tilde{M}$ is a symmetric matrix with positive components, we can prove the following properties by the Perron–Frobenius theorem and the min-max principle.

- The eigenvalue $\mu_1(s, L)$ is simple and positive, and there is an eigenvector with only positive components.
- $\mu_1(s, L)$ is continuous and strictly monotone decreasing with respect to $sL \in (0, \infty)$.
- For fixed $L > 0$, $\lim_{s \to 0} \mu_1(s, L) = N$, $\lim_{s \to \infty} \mu_1(s, L) = 1$. The same properties also hold if we replace $s$ and $L$.

In Figure 5, 6 we give the graphs of $-\alpha s/2$ and eigenvalues of $\tilde{M}$ for $N = 4$, $x_j = j$ ($j = 1, \ldots, 4$), $\alpha = -1$ and $L = 1/16, 4$.

By the above properties and $\alpha < 0$, there exists a unique positive solution $s = s_1(L)$ of the equation $-2s/\alpha = \mu_1(s, L)$. The function $s_1(L)$ is continuous and strictly monotone decreasing on $(0, \infty)$. Moreover, by inspecting the
Figure 5: Graphs of $-2s/\alpha$ and eigenvalues of $\tilde{M}$ for $N = 4, \alpha = -1$ and $L = 1/16$.

Figure 6: Graphs of $-2s/\alpha$ and eigenvalues of $\tilde{M}$ for $N = 4, \alpha = -1$ and $L = 4$.

The limiting equation $-2s/\alpha = \mu_1(s, 0) = N$ and $-2s/\alpha = \mu_1(s, \infty) = 1$, we see that

$$\lim_{L \to 0} s_1(L) = -\frac{N\alpha}{2}, \quad \lim_{L \to \infty} s_1(L) = -\frac{\alpha}{2}.$$ 

Since $E_1(L) = -s_1(L)^2$, the statement holds.

Lemma 21. Let $d = 2$. For $L > 0$, let $\Gamma_L = \{\gamma_1, \gamma_2\}$ with $|\gamma_1 - \gamma_2| = L$. Let $\alpha$ be a constant sequence on $\Gamma_L$ with common coupling constant $\alpha \in \mathbb{R}$. Then, $H_{\Gamma_L, \alpha}$ has only one negative eigenvalue $E_1(L)$ for $L \leq e^{2\pi\alpha}$, and two negative eigenvalues $E_1(L)$ and $E_2(L)$ ($E_1(L) < E_2(L)$) for $L > e^{2\pi\alpha}$. The function $E_1(L)$ (resp. $E_2(L)$) is continuous, monotone increasing (resp. decreasing) with respect to $L \in (0, \infty)$ (resp. $L \in (e^{2\pi\alpha}, \infty)$), and

$$\lim_{L \to +0} E_1(L) = -\infty, \quad \lim_{L \to \infty} E_1(L) = -4e^{-4\pi\alpha-2\gamma_E},$$

$$\lim_{L \to -e^{2\pi\alpha}+0} E_2(L) = 0, \quad \lim_{L \to \infty} E_2(L) = -4e^{-4\pi\alpha-2\gamma_E},$$

where $\gamma_E$ is the Euler constant.

Proof. By [2, Theorem II-4.2], $H_{\Gamma_L, \alpha}$ has a negative eigenvalue $E = -s^2$ ($s > 0$) if and only if $\det M = 0$, where $M = (M_{jk})$ is a $2 \times 2$-matrix given by

$$M_{jk} = \begin{cases} (2\pi)^{-1}(2\pi\alpha + \gamma_E + \log(s/2)) & (j = k), \\ -\frac{1}{4}H_0^{(1)}(isL) & (j \neq k). \end{cases}$$
Here $H_0^{(1)}$ is the 0-th order Hankel function of the first kind. By [1 9.6.4], we have

\[-\frac{i}{4}H_0^{(1)}(isL) = -\frac{1}{2\pi}K_0(sL),\]

where $K_\nu(z)$ is the $\nu$-th order modified Bessel function of the second kind. Thus $\det M = 0$ if and only if one of the following two equations hold.

\[f(s, L) := 2\pi\alpha + \gamma_E + \log \frac{s}{2} - K_0(sL) = 0, \tag{21}\]

\[g(s, L) := 2\pi\alpha + \gamma_E + \log \frac{s}{2} + K_0(sL) = 0. \tag{22}\]

Let us review formulas for the modified Bessel functions [1 9.6.23,9.6.27,9.6.13,9.7.2].

\[K_\nu(z) = \frac{\pi^{1/2}}{\Gamma(\nu + 1/2)} \left(\frac{z}{2}\right)^\nu \int_1^\infty e^{-zt}(t^2 - 1)^{-1/2}dt \quad (|\arg z| < \frac{\pi}{2}), \tag{23}\]

\[K'_0(z) = -K_1(z), \tag{24}\]

\[K_0(z) = -\log \frac{z}{2} - \gamma_E + O(z^2 \log z) \quad \text{as} \quad z \to 0, \tag{25}\]

\[K_0(z) = \sqrt{\frac{\pi}{2z}}e^{-z}(1 + O(z^{-1})) \quad \text{as} \quad z \to +\infty. \tag{26}\]

By (23)-(26), we see that $K_\nu(z) > 0$ for $z > 0$ and $\nu > -1/2$, and

\[
\frac{\partial f}{\partial s} = \frac{1}{s} + LK_1(sL) > 0, \quad \frac{\partial f}{\partial L} = sK_1(sL) > 0,
\]

\[
\lim_{s \to +0} f(s, L) = -\infty, \quad \lim_{s \to \infty} f(s, L) = \infty,
\]

\[
\lim_{L \to +0} f(s, L) = -\infty, \quad \lim_{L \to \infty} f(s, L) = 2\pi\alpha + \gamma_E + \log \frac{s}{2}.
\]

The graphs of $y = f(s, L)$ are given as curves below the dashed curve in Figure 7-8. Here the dashed curve is the limiting curve $y = 2\pi\alpha + \gamma_E + \log s/2$.

By these properties, we conclude that the equation (21) has unique positive solution $s = s_1(L)$ for any $L > 0$, and

\[
\lim_{L \to +0} s_1(L) = \infty, \quad \lim_{L \to \infty} s_1(L) = 2e^{-2\pi\alpha - \gamma_E}.
\]
Next, again by (23)-(26),
\[
\frac{\partial g}{\partial s} = \frac{1}{s} - LK_1(sL) = \frac{1}{s} - sL^2 \int_1^{\infty} e^{-sLt} (t^2 - 1)^{1/2} dt > \frac{1}{s} - sL^2 \int_0^{\infty} e^{-sLt} dt = 0,
\]
\[
\frac{\partial g}{\partial L} = -sK_1(sL) < 0,
\]
\[
\lim_{s \to \pm 0} g(s, L) = 2\pi\alpha - \log L, \quad \lim_{s \to \infty} g(s, L) = \infty, \\
\lim_{L \to \pm 0} g(s, L) = \infty, \quad \lim_{L \to \infty} g(s, L) = 2\pi\alpha + \gamma \log s/2.
\]

The graphs of \( y = g(s, L) \) are given as curves above the dashed curve in Figure 7, 8. By these properties, we conclude the equation (22) has no positive solution for \( L \leq e^{2\pi\alpha} \), has unique positive solution \( s = s_2(L) \) for \( L > e^{2\pi\alpha} \), and
\[
\lim_{L \to e^{2\pi\alpha} + 0} s_2(L) = 0, \quad \lim_{L \to \infty} s_2(L) = 2e^{-2\pi\alpha - \gamma \log s/2}.
\]

Since \( E_1(L) = -s_1(L)^2 \) and \( E_2(L) = -s_2(L)^2 \), the statements hold.\( \square \)

**Lemma 22.** Let \( d = 3 \). For \( L > 0 \), let \( \Gamma_L = \{\gamma_1, \gamma_2\} \) with \( |\gamma_1 - \gamma_2| = L \). Let \( \alpha \) be a constant sequence on \( \Gamma_L \) with common coupling constant \( \alpha \in \mathbb{R} \). Then, the following holds.

(i) Assume \( \alpha \geq 0 \). Then, \( H_{\Gamma_L, \alpha} \) has no negative eigenvalue for \( L \geq 1/(4\pi\alpha) \), and has one negative eigenvalue \( E_1(L) \) for \( 0 < L < 1/(4\pi\alpha) \).
(when \( \alpha = 0 \), we interpret \( 1/(4\pi\alpha) = \infty \) and the first case does not occur). The function \( E_1(L) \) is continuous, monotone increasing with respect to \( L \in (0, 1/(4\pi\alpha)) \), and

\[
\lim_{L \to +0} E_1(L) = -\infty, \quad \lim_{L \to 1/(4\pi\alpha) - 0} E_1(L) = 0.
\]

(ii) Assume \( \alpha < 0 \). Then, \( H_{\Gamma_{L,\alpha}} \) has one negative eigenvalue \( E_1(L) \) for \( L \leq 1/(\alpha - 4\pi\alpha) \), and two negative eigenvalues \( E_1(L) \) and \( E_2(L) \) (\( E_1(L) < E_2(L) \)) for \( L > 1/(\alpha - 4\pi\alpha) \). The function \( E_1(L) \) (resp. \( E_2(L) \)) is continuous, monotone increasing (resp. decreasing) with respect to \( L \in (0, \infty) \) (resp. \( L \in (1/(\alpha - 4\pi\alpha), \infty) \)), and

\[
\lim_{L \to +0} E_1(L) = -\infty, \quad \lim_{L \to \infty} E_1(L) = -(4\pi\alpha)^2, \\
\lim_{L \to 1/(\alpha - 4\pi\alpha) + 0} E_2(L) = 0, \quad \lim_{L \to \infty} E_2(L) = -(4\pi\alpha)^2.
\]

Proof. By [2, Theorem II-1.1.4], \( H_{\Gamma_{L,\alpha}} \) has a negative eigenvalue \( E = -s^2 \) (\( s > 0 \)) if and only if \( \det M = 0 \), where \( M = (M_{jk}) \) is a \( 2 \times 2 \)-matrix given by

\[
M_{jk} = \begin{cases} 
\alpha + \frac{s}{4\pi} & (j = k), \\
-\frac{e^{-sL}}{4\pi L} & (j \neq k).
\end{cases}
\]

So \( \det M = 0 \) if and only if one of the following equations holds.

\[
4\pi\alpha + s = \frac{e^{-sL}}{L}, \quad (27)
\]

\[
4\pi\alpha + s = -\frac{e^{-sL}}{L}. \quad (28)
\]

The graphs of both sides of (27) and (28) are given in Figure 9 [10].

By inspecting the graphs, we conclude the following.

(i) For \( \alpha \geq 0 \), the equation (27) has no positive solution for \( L \geq 1/(4\pi\alpha) \), and has one positive solution \( s = s_1(L) \) for \( 0 < L < 1/(4\pi\alpha) \). Moreover, \( \lim_{L \to +0} s_1(L) = \infty, \lim_{L \to 1/(4\pi\alpha) - 0} s_1(L) = 0 \). The equation (28) has no positive solution.

(ii) For \( \alpha < 0 \), the equation (27) has one positive solution \( s = s_1(L) \) for any \( L > 0 \), and \( \lim_{L \to +0} s_1(L) = \infty, \lim_{L \to \infty} s_1(L) = -4\pi\alpha \). The equation (28)
has no positive solution for $L \leq 1/(-4\pi \alpha)$, has one positive solution $s = s_2(L)$ for $L > 1/(-4\pi \alpha)$, and

$$\lim_{L \to 1/(-4\pi \alpha)} s_2(L) = 0, \quad \lim_{L \to \infty} s_2(L) = -4\pi \alpha.$$ 

These facts and $E_1(L) = -s_1(L)^2$, $E_2(L) = -s_2(L)^2$ imply the statements.

**Proof of Theorem 7.** Put

$$\Sigma = \bigcup_{(\Gamma, \alpha) \in \mathcal{A}_F} \sigma(H_{\Gamma, \alpha}).$$

By Proposition 18, we have $\sigma(H_\omega) = \Sigma$ almost surely.

First consider the case $d = 1$ and supp $\nu \subset [0, \infty)$. Then, for any $(\Gamma, \alpha) \in \mathcal{A}_F$, we have $\sigma(H_{\Gamma, \alpha}) = [0, \infty)$ by Lemma 19. So $\Sigma = [0, \infty)$.

In all other cases, we have to prove $\Sigma = \mathbb{R}$. Since $\sigma(H_{\Gamma, \alpha}) = [0, \infty)$ for $\Gamma = \emptyset$, we have only to prove $(-\infty, 0) \subset \Sigma$.

Consider the case $d = 1$ and supp $\nu \cap (-\infty, 0) \neq \emptyset$. Let $\Gamma_{N,L}$ given in Lemma 20 and $\alpha$ be a constant sequence on $\Gamma_{N,L}$ with common coupling constant $\alpha \in \text{supp} \nu \cap (-\infty, 0)$. Then $(\Gamma_{N,L}, \alpha) \in \mathcal{A}_F$ for any $N \geq 2$ and $L > 0$, so

$$\Sigma \supset \bigcup_{N \geq 2, L > 0} \sigma(H_{\Gamma_{N,L}, \alpha}).$$

By Lemma 20 the right hand side contains $(-\infty, 0)$. When $d = 2, 3$, the statement can be proved similarly by using Lemma 21 22.

In the case $d = 1$ and sup$\nu$ has negative part, there is a simple another proof using the spectrum of the Kronig–Penney model (see 21 22).
Another proof of Theorem 7 (i). Put

$$\Sigma = \bigcup_{(\Gamma, \alpha) \in A_P} \sigma(H_{\Gamma, \alpha}).$$

By Proposition 18, we have $\sigma(H_\omega) = \Sigma$ almost surely.

Assume $d = 1$ and $(-\infty, 0) \cap \text{supp} \nu \neq \emptyset$. It is sufficient to show $\Sigma \supset (-\infty, 0)$. For $L > 0$, let $\Gamma_L = LZ$, and $\alpha$ be a constant sequence on $\Gamma_L$ with common coupling constant $\alpha \in \text{supp} \nu \cap (-\infty, 0)$. Then $(\Gamma_L, \alpha) \in A_P$. By [2, Theorem III.2.3.1], the spectrum of $H_{\Gamma_L, \alpha}$ is given by

$$\sigma(H_{\Gamma_L, \alpha}) = \{k^2 \in \mathbb{R} \mid |\cos(kL) + \alpha/(2k)\sin(kL)| \leq 1\}.$$ 

Put $k = is$ for $s > 0$. Then, $E = -s^2 \in \sigma(H_{\Gamma_L, \alpha})$ if and only if

$$|\cosh(sL) + \alpha/(2s)\sinh(sL)| \leq 1. \quad (29)$$

Take arbitrary $s_0 > 0$, and let $s \in (0, s_0)$. Consider the Taylor expansion with respect to $L$

$$f(s, L) := \cosh(sL) + \frac{\alpha}{2s} \sinh(sL) = 1 + \frac{\alpha}{2}L + O(L^2) \quad \text{as } L \to 0. \quad (30)$$

The remainder term is uniform with respect to $s \in (0, s_0]$. Since $\alpha < 0$, (30) implies (29) holds for sufficiently small $L$ uniformly with respect to $s \in (0, s_0]$ (see also Figure 11). Thus $[-s_0^2, 0) \subset \sigma(H_{\Gamma_L, \alpha})$ for sufficiently small $L$, so $(-\infty, 0) \subset \Sigma$.

Figure 11: Graphs of $y = f(s, L)$ for $L = 2^{-n}$ ($n = 3, \ldots, 6$). As $L \to +0$, the negative band becomes longer and longer.
4 Appendix

4.1 Elliptic inner regularity estimate

The following is a special case of the elliptic inner regularity theorem ([4, Theorem 6.3]).

Theorem 23. Let $U$ be an open set in $\mathbb{R}^d$ and $u \in L^2(U)$. Assume that there exists a positive constant $M$ such that

\begin{equation}
| (u, \Delta \phi)_{L^2(U)} | \leq M \| \phi \|_{L^2(U)}
\end{equation}

holds for every $\phi \in C_0^{\infty}(U)$. Then, $u \in H^2_{\text{loc}}(U)$. Moreover, for any open set $V$ such that $\overline{V}$ is a compact subset of $U$, there exists a positive constant $C$ dependent only on $U$ and $V$ such that

\begin{equation}
\| u \|_{H^2(V)} \leq C (M + \| u \|_{L^2(U)}),
\end{equation}

where $M$ is the constant in (31).

From Theorem 23 we have the following corollary useful for our purpose.

Corollary 24. Let $U, V$ be open sets in $\mathbb{R}^d$ such that $\overline{V} \subset U$ and

\begin{equation}
\text{dist}(\partial U, V) \geq \delta
\end{equation}

for some positive constant $\delta$. Let $u \in L^2(U)$ such that $\Delta u \in L^2(U)$ in the distributional sense. Then, $u \in H^2_{\text{loc}}(U)$, and there exists a constant $C$ dependent only on $\delta$ and the dimension $d$ such that

\begin{equation}
\| u \|^2_{H^2(V)} \leq C \left( \| \Delta u \|^2_{L^2(U)} + \| u \|^2_{L^2(U)} \right).
\end{equation}

Proof. Put $\epsilon = \delta/(2d)$. For $x_0 \in \mathbb{R}^d$, consider open cubes $Q = x_0 + (-\epsilon, \epsilon)^d$ and $Q' = x_0 + (-\epsilon/2, \epsilon/2)^d$. When $Q \subset U$, we have

\begin{align*}
| (u, \Delta \phi)_{L^2(Q)} | &= | (\Delta u, \phi)_{L^2(Q)} | \leq \| \Delta u \|_{L^2(Q)} \| \phi \|_{L^2(Q)}
\end{align*}

for every $\phi \in C_0^{\infty}(Q)$. Then the assumption of Theorem 23 is satisfied with $U = Q$, $V = Q'$, and $M = \| \Delta u \|_{L^2(Q)}$, and we have

\begin{equation}
\| u \|^2_{H^2(Q')} \leq C (\| \Delta u \|^2_{L^2(Q)} + \| u \|^2_{L^2(Q)})
\end{equation}
for some positive constant $C$ dependent only on $\delta$ and dimension $d$. We collect all the cubes $Q'$ such that the center $x_0 \in \epsilon \mathbb{Z}^d$ and $Q' \cap V \neq \emptyset$. Notice that $Q \subset U$ for such $Q'$. Thus we have by (33)

$$\|u\|^2_{H^2(V)} \leq \sum_{Q'} \|u\|^2_{H^2(Q')} \leq C \sum_{Q'} \left( \|\Delta u\|^2_{L^2(Q)} + \|u\|^2_{L^2(Q)} \right) \leq 2^d C \left( \|\Delta u\|^2_{L^2(U)} + \|u\|^2_{L^2(U)} \right),$$

where we use the fact $Q$ can overlap at most $2^d$ times.

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