Continuum limit of lattice Hamiltonians

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§1 Continuum limit

The problem we address here is the convergence of solutions for discrete Schrödinger equations to those for continuous Schrödinger equations. Let us begin with a simple case. Consider a discrete Schrödinger equation

$$(-\Delta_{disc,h} + V_h - E)u_h = f_h, \qquad (1)$$

where

$$-\Delta_{disc,h} = \frac{2}{h^2}\sum_{j=1}^{d}\Big(I - \frac{1}{2}(S_{h,j} + S^*_{h,j})\Big) \qquad (2)$$

is a discrete Laplacian on the square lattice with mesh size h, i.e.

$$\mathbf{Z}^d_h = \mathbf{R}^d/(h\mathbf{Z})^d = \{hn\,;\, n \in \mathbf{Z}^d\},$$

and V_h be a real-valued potential, i.e.

$$(V_h u)(n) = V_h(n)u_h(n).$$

Solving (1), we get a function $\{u_h(n)\}_{n\in\mathbf{Z}^d}$ on $\mathbf{Z}^d_h$. We interpolate it, i.e. construct a function $\{\widetilde{u}_h(x)\}_{n\in\mathbf{Z}^d}$ on $\mathbf{R}^d$ such that

$$\widetilde{u}_h(hn) = u_h(n), \quad \forall n \in \mathbf{Z}^d.$$

Letting $h \to 0$, we expect that

$$\widetilde{u}_h(x) \to \widetilde{u}(x),$$

where $\widetilde{u}(x)$ satisfies a continuous Schrödinger equation

$$(-\Delta_{cont} + V(x) - E)\widetilde{u} = \widetilde{f}, \qquad (3)$$

$$\Delta_{cont} = \sum_{j=1}^{d}\frac{\partial^2}{\partial x_j^2}.$$

The following problems are our concern.

- How to interpolate $u_h(n)$?
- Does $\widetilde{u}_h(x)$ converge?
- Can one deal with scattering solutions?

Here, by the scattering solution, we mean a solution to the Schrödinger equation (3) satisfying the radiation condition of Sommerfeld. Since it is the boundary condition at infinity, the last problem asks the behavior of solutions to the Schrödinger equation as $n \to \infty$ and $h \to 0$ at the same time.

In the above situation, we started from continuous model and considered its discretization. However, in solid state physics, one often starts from the discrete model (e.g. lattice), in which case the associated differential equation for the continuous model is not obvious. This sort of continuum limit problem has been basically open, especially for the case of scattering solutions, i.e. the ones describing the continuous spectrum. The aim of this work is to give a class of lattices for which this continuum limit can be computed. The applicability of our methods ranges over the following lattices:

- square lattice, triangular lattice $\Longrightarrow$ Schrödinger equation
- hexgonal lattice (graphen) $\Longrightarrow$ Schrödinger equation, Dirac equation
- ladder of lattices (e.g. graphite) $\Longrightarrow$ System of Schrödinger or Dirac equations

As regards to the Fourier analysis, our argument is based on the following fact. Let $\mathbf{T}_h^d$ be the torus associated with the lattice $\mathbf{Z}_h^d$:

$$\mathbf{T}_h^d = (S_h^1)^d = [-\frac{\pi}{h}, \frac{\pi}{h}]^d, \quad S_h^1 = \left\{e^{ih\theta}\,;\, -\frac{\pi}{h} \le \theta \le \frac{\pi}{h}\right\}. \tag{4}$$

We use the following notations for functions on $\mathbf{Z}_h^d$, $\mathbf{T}_h^d$ and $\mathbf{R}^d$:

$$u_h = (u_h(n)) \quad \text{on} \quad \mathbf{Z}_h^d, \tag{5}$$

$$\widehat{u}_h(\xi) = (\frac{h}{2\pi})^{d/2} \sum_{n \in \mathbf{Z}^d} e^{-ihn\cdot\xi} u_h(n) \quad \text{on} \quad \mathbf{T}_h^d, \tag{6}$$

$$\widetilde{u}_h(x) = (\frac{h}{2\pi})^{d/2} \int_{\mathbf{T}_h^d} e^{ix\cdot\xi} \widehat{u}_h(\xi) d\xi \quad \text{on} \quad \mathbf{R}^d. \tag{7}$$

The formula (7), expanded into a Fourier series by using (6), is called a Cardinal series. Let us consider a series of transformations for $\varphi \in \mathcal{S}(\mathbf{R}^d)$:

$$\varphi \Longrightarrow \varphi_h \Longrightarrow \widehat{\varphi}_h \Longrightarrow \widetilde{\varphi}_h,$$

where $\varphi_h(n) = \varphi(hn)$.

Lemma 1.1 *$\widetilde{\varphi}_h$ is an interpolation of φ_h, and $\widetilde{\varphi}_h \to \varphi$ as $h \to 0$.*

In fact, recall that $\left\{\left(\frac{h}{2\pi}\right)^{d/2} e^{-ihn\cdot\xi}\right\}_{n\in\mathbf{Z}^d}$ is a C.O.N.S. of $L^2(\mathbf{T}_h^d)$. Take $\varphi(x) \in \mathcal{S}(\mathbf{R}^d)$, and put $\varphi_h(n) = \varphi(hn)$. Then

$$\widehat{\varphi}_h(\xi) = \left(\frac{h}{2\pi}\right)^{d/2} \sum_n e^{-ihn\cdot\xi}\varphi_h(n),$$

$$\varphi(hn) = \varphi_h(n) = \left(\frac{h}{2\pi}\right)^{d/2} \int_{\mathbf{T}_h^d} e^{ihn\cdot\xi}\widehat{\varphi}_h(\xi)d\xi,$$

by the inversion formula of Fourier series. So, $\widetilde{\varphi}_h(hn) = \varphi(hn)$. Let $h \to 0$ and $n \to \infty$ so that $hn \to x$. Then

$$h^{d/2}\widehat{\varphi}_h(\xi) = (2\pi)^{-d/2} \sum_n e^{-ihn\cdot\xi}\varphi(hn)h^d \to (2\pi)^{-d/2} \int_{\mathbf{R}^d} e^{-ix\cdot\xi}\varphi(x)dx.$$

The inversion formula of Fourier transform implies that $\varphi(hn) \to \varphi(x)$ (at least in $\mathcal{S}'$).

Now we return to the equations (1) and (3).

Assume : $V(x) \in C_0^\infty(\mathbf{R}^d)$, real-valued.

We also assume that the potential $V_h(n)$ satisfies

$$(V_{disc,h}u)(n) = V(hn)u(n), \quad \forall n \in \mathbf{Z}^d. \tag{8}$$

Then, the equations (1) and (3) have a unique solution satisfying the radiation condition, respectively. Here, one must pay attention to the radiation condition for the discrete equation, which we explain later.

Given $f \in \mathcal{S}(\mathbf{R}^d)$, we put

$$f_h(n) = f(hn),$$

and let $u_h(n)$ be a solution to the equation (1), and $\widehat{u}_h(n)$ and $\widetilde{u}_h(x)$ be defined by (6) and (7). As is proved above,

$$\widetilde{u}_h(hn) = u_h(n), \tag{9}$$

hence $\widetilde{u}_h(x)$ is an interpolation of $(u_h(n))_{n\in\mathbf{Z}^d}$. For $s \in \mathbf{R}$, we define the weighted L^2 space by

$$u \in L^{2,s}(\mathbf{R}^d) \Longleftrightarrow \|(1+|x|)^s u(x)\|_{L^2(\mathbf{R}^d)} < \infty.$$

Then, the following theorem holds.

Theorem 1.2 *As $h \to 0$, $\widetilde{u}_h(x) \to \widetilde{u}(x)$, in $L^{2,-s}(\mathbf{R}^d)$ for $s > 1/2$, where $\widetilde{u}(x)$ is a solution to (3) satisfying the radiation condition.*

§2 Limiting absorption principle

The proof of Theorem 1.2 traces the classical idea of limiting absorption principle, which we briefly review. Let H be a self-adjoint operator in a Hilbert space $\mathcal{H}$. If $\lambda \in \sigma_c(H)$, the limit $\lim_{\epsilon\to 0}(H-\lambda\mp i\epsilon)^{-1} : \mathcal{H} \to \mathcal{H}$ does not exist. However, by preparing Banach spaces $\mathcal{Y}$, $\mathcal{X}$ satisfying $\mathcal{Y} \subset \mathcal{H} \subset \mathcal{X}$ with dense and continuous inclusions, one can sometimes prove the existence of the limit

$$\lim_{\epsilon\to 0}(H-\lambda\mp i\epsilon)^{-1} : \mathcal{Y} \to \mathcal{X}.$$

This is called the limiting absorption principle (LAP). The proof consists in the following lemma from elementary topology.

Lemma 2.1 *Let X be a complete metric space, and $\{x_i\}_{i=1}^{\infty}$ a precompact sequence in X with unique accumulation point $x \in X$. Then, $x_i \to x$.*

To prove LAP for the continuous operator $H = -\Delta + V(x)$, put

$$u_\epsilon = (H - E - i\epsilon)^{-1} f, \quad f \in L^{2,s}(\mathbf{R}^d), \quad s > 1/2.$$

Then, one can show

- $\{u_\epsilon\}_{0<\epsilon<\epsilon_0}$ is precompact in $L^{2,-s}$, $\forall s > 1/2$,
- u_ϵ $(0 < \epsilon < \epsilon_0)$ satisfies the radiation condition

$$\Big(\frac{1}{i}\frac{\partial}{\partial r} - \sqrt{E+i\epsilon}\Big)u_\epsilon \in L^{2,-\delta}, \quad \delta > 1/2 \tag{10}$$

  uniformly in $\epsilon > 0$.

The key fact is the following.

Lemma 2.2 *The solution of the equation $(-\Delta + V - E)u = f$ satisfying the radiation condition is unique.*

Then, we are done by virtue of Lemma 2.1. This is the method due to Eidus [3], and has been frequently used in the spectral and scattering theory.

To prove Lemmas 2.1 and 2.2, the main issues are

- Precompactness $\to$ a-priori estimates in suitable weighted spaces,
- Uniqueness of accumulation points $\to$ Rellich type theorem for scattering solutions.

Both of them boil down to elliptic boundary value problems in an infinite domain.

One can use the same idea for discrete cases. In our previous paper [2], we have already discussed

- Uniform estimates and precompactness of solutions to the discrete equation
$$(-\Delta_{disc,h} + V_h - E)u_h = f_h,$$
- Radiation condition,

which enabled us to prove LAP for a class of lattice Schrödinger equations.

A new problem in the continuum limit is that the radiation conditions for continuous operator and discrete operator must be compatible. Our radiation condition in [2] fulfils this requirement.

§3 Proof of Theorem 1.2

First we consider the continuous case. Let $R(z) = (H - z)^{-1}$. Then, we know that for $E > 0$,

$$R(E + i0) \in \mathbf{B}(L^{2,s}; L^{2,-s}), \quad s > 1/2.$$

Consider a pseudo-differential operator (ΨDO) $p_-(x, D_x)$ with symbol $p_-(x, \xi)$ satisfying

$$|\partial_x^\alpha \partial_\xi^\beta p_-(x, \xi)| \leq C_{\alpha\beta} \langle x \rangle^{-|\alpha|} \langle \xi \rangle^{-|\beta|},$$

$$p_-(x, \xi) = 0, \quad if \quad \frac{x}{|x|} \cdot \frac{\xi}{|\xi|} > 1 - \epsilon.$$

We say that a solution u to $(-\Delta + V - E)u = f$ satisfies the outgoing radiation condition if there exist $\delta < 1/2 < s$ such that

$$u \in L^{2,-s}, \quad p_-(x, D_x)u \in L^{2,-\delta}$$

for all such $p_-(x, D_x)$. Then, the resolvent $R(E + i0)$ satisfies this radiation condition. Moreover, the solution to $(-\Delta + V - E)u = f$ satisfying this radiation condition is unique. This formulation of radiation condition is equivalent to the classical one:

$$\Big(\frac{\partial}{\partial r} - i\sqrt{E}\Big)u \in L^{2,-\delta}.$$

Next we consider the discrete case. The free equation is

$$(-\Delta_{disc,h} - z)u_h = f_h, \quad z = E + i\epsilon.$$

Passing to the Fourier series, we have

$$(P_h(\xi) - z)\widehat{u}_h = \frac{4}{h^2}\widehat{f}_h,$$

where $P_h(\xi)$ is given as follows and behaves like

$$P_h(\xi) = \frac{4}{h^2}\sum_{j=1}^{d}\sin^2\Big(\frac{h\xi_j}{2}\Big) \sim |\xi|^2$$

as $h \to 0$. We define the characteristic surface $M_{E,h}$ by

$$M_{E,h} = \{\xi\,;\, P_h(\xi) = E\}.$$

We are interested in the regularity of $\widehat{u}_h(\xi)$, since we are concerned with the behavior of $u_h(n)$ as $|n| \to \infty$. Then, one can easily see:

- Outside $M_{E,h}$, $\widehat{u}_h(\xi)$ has the same regularity as $\widehat{f}_h(\xi)$.
- Near $M_{E,h}$, $\widehat{u}_h(\xi)$ can be dealt with in the same way as in the continuous case.

Now, let us recall the Agmon-Hörmander approach to LAP [1]. Consider a differential equation of constant coefficients:

$$(P(D) - \lambda)u = f.$$

Assume that $P(\xi)-\lambda$ is simple characteristic. Then, one can factrize $P(\xi)-\lambda$ as

$$P(\xi) - \lambda = (\xi_1 - p(\xi'))q(\xi,\lambda), \quad q(\xi,\lambda) \neq 0,$$

and transform the above equation into the following one:

$$(\xi_1 - p(\xi'))v = g.$$

By the partial Fourier transform, we then have

$$\Big(\frac{1}{i}\frac{d}{dx_1} - p(\xi')\Big)\widetilde{v} = \widetilde{g}, \quad \widetilde{v} = \int_{-\infty}^{x_1} e^{ip(\xi')y_1}\widetilde{g}(y_1,\xi')dy_1.$$

The Sobolev space on $\mathbf{T}^d_h$ is then defined by

$$f \in L^{2,s}(\mathbf{Z}^d_h) \Longleftrightarrow \widehat{f}_h(\xi) \in H^s(\mathbf{T}^d_h).$$

If supp $\widehat{f}_h(\xi)$ is localized near $M_{E,h}$, this is equivalent to $\widehat{f}_h \in H^s(\mathbf{R}^d)$.

Arguing in this way, one can show that the resolvent of $-\Delta_{disc,h}$ satisfies the same estimates as the continuous case. The radiation condition formulated by ΨDO is also satisfied. By the perturbation theory, it is not difficult to include the potential $V_h(n)$. Moreover, the resolvent estimates thus obtained are uniform with respect to $0 < h < h_0$. In summary, the following lemma holds.

Lemma 3.1

$$(-\Delta_{disc,h} + V_h - z)^{-1} : L^{2,s} \to L^{2,-s},$$

$$P_-(-\Delta_{disc,h} + V_h - z)^{-1} : L^{2,s} \to L^{2,-\delta}$$

for $\delta < 1/2 < s$, *uniformly with respect to* $0 < \mathrm{Im}\, z < 1$, $0 < h < h_0$.

Letting $\mathrm{Im}\, z \to 0$, we have

$$(-\Delta_{disc,h} + V_h - E - i0)^{-1} : L^{2,s} \to L^{2,-s},$$
$$P_-(-\Delta_{disc,h} + V_h - E - i0)^{-1} : L^{2,s} \to L^{2,-\delta}$$

for $\delta < 1/2 < s$, uniformly with respect to $0 < h < h_0$.

By a little more computation, one can prove the precompactness of $(-\Delta_{disc,h} + V_h - E - i0)^{-1}$.

From this, we can conclude the theorem.

§4 S-matrix

As an application of Theorem 1.2, we show that the S-matrix of continuous Schrödinger operator is approximated by that of the discrete Schrödinger operator. Put for $\omega \in S^{d-1}$

$$\varphi(x, \sqrt{E}, \omega) = e^{i\sqrt{E}\omega\cdot x} - (- \Delta + V(x) - E - i0)^{-1}(V(x)e^{i\sqrt{E}\omega\cdot x}).$$

It satisfies

$$(- \Delta + V(x) - E)\varphi(x, E, \omega) = 0.$$

$$\varphi(x, E, \omega) \sim e^{-\sqrt{E}\omega\cdot x} - C(E)\frac{e^{i\sqrt{E}r}}{r^{(d-1)/2}}A(E, \theta, \omega), \quad \theta = x/r$$

Heisenberg's S-matrix is then defined by

$$S(E, \theta, \omega) = \delta(\theta - \omega) - c(E)A(E, \theta, \omega),$$

where the scattering amplitude $A(E, \theta, \omega)$ is defined by

$$\begin{aligned} A(E, \theta, \omega) &= \int_{\mathbf{R}^d} e^{-i\sqrt{E}(\theta-\omega)\cdot x}V(x)dx \\ &- \int_{\mathbf{R}^d} e^{-i\sqrt{E}\theta\cdot x}V(x)\Big(- \Delta + V(x) - E - i0\Big)^{-1}\Big(V(x)e^{i\sqrt{E}\omega\cdot x}\Big)dx. \end{aligned}$$

The scattering amplitude $A_h(E, \theta, \omega)$ for the square lattice is almost the same. Replace

$$\textit{Fourier transform} \ \to \ \textit{Fourier series},$$

$$S^{d-1} \to M_{E,h}.$$

Note

$$M_{E,h} \sim S^{d-1} \quad (\textit{diffeomorphic})$$

By Theorem 1.2, we have

Theorem 4.1 *For any* $E > 0$, *and* $\theta, \omega \in S^{d-1}$, *we have* $A_h(E, \theta, \omega) \to A(E, \theta, \omega)$ *as* $h \to 0$.

§5 General scheme for convergence of discrete operators to continuous operators

We start from the discrete operator and consider the passage to continuous operators. We denote the Fourier transformation on $\mathbf{R}^d$ by

$$(\mathcal{F}_{cont} f)(\xi) = (2\pi)^{-d/2} \int_{\mathbf{R}^d} e^{-ix\cdot\xi} f(x)dx,$$

the shift operator $S_{h,j}$ by

$$(S_{h,j} f)(x) = f(x - h\mathbf{e}_j),$$

$$\mathbf{e}_1 = (1, 0, \cdots, 0), \cdots, \mathbf{e}_d = (0, \cdots, 0, 1),$$

and put

$$S_h = (S_{h,1}, \cdots, S_{h,d}).$$

Then, we have

$$\mathcal{F}_{cont} S_{h,j} = e^{-ih\xi_j} \mathcal{F}_{cont}.$$

Similarly, we have for the discrete Fourier transform, i.e. Fourier series, cf. (7),

$$\mathcal{F}_{disc,h} S_{h,j} = e^{-ih\xi_j} \mathcal{F}_{disc,h}.$$

The discrete Laplacian is a matrix whose entries are shift operators. Therefore, it is transformed to a matrix of trigonometric polynomials.

§5.1 Expansion of the characteristic roots

Conider the case $h = 1$. A lattice Hamiltonian is an $s \times s$ matrix

$$\mathcal{L}(S) = \Big(\mathcal{L}_{ij}(S)\Big),$$

where $\mathcal{L}_{ij}(z)$ is a polynomial of $z \in \mathbf{C}^d$ and $\overline{z}$. Let $\lambda(\eta)$ be one of its characteristic roots:

$$\det\left(\mathcal{L}(e^{-i\eta}) - \lambda\right) = 0,$$

where we use the notation

$$\eta \in \mathbf{R}^d, \quad e^{-i\eta} = (e^{-i\eta_1}, \cdots, e^{-i\eta_d}).$$

Assume that at a point $\eta = d_1 \in \mathbf{T}^d$, $\lambda(\eta)$ takes a local minimum:

$$\lambda(\eta) \geq E_0, \quad \lambda(d_1) = E_0.$$

We call E_0 the *reference energy*.

Consider a scaled Hamiltonian on $\mathbf{T}^d_h$:

$$\mathcal{L}_h(e^{-ih\eta}) = \frac{1}{h^\nu}\Big(\mathcal{L}(e^{-ih\eta}) - E_0\Big).$$

Here, ν in $\frac{1}{h^\nu}$ depends on E_0, and is chosen so that the following arguments work well. Letting $d_h = d_1/h$ and making a change of variable $\eta = \xi + d_h$, consider

$$P_h(\xi) = \lambda(h\eta) = \lambda(h(\xi + d_h)) = \lambda(h\xi + d_1).$$

Assume that

$$P_h(\xi) \to P(\xi) \quad as \quad h \to 0.$$

Near d_h, we pass to a gauge transformation

$$\mathcal{L}_h(S_h) \to \mathcal{G}_h^* \mathcal{L}_h(S_h)\mathcal{G}_h,$$

$$(\mathcal{G}_h a)(n) = e^{ihn\cdot d_h} a(n), \quad d_h = d_1/h.$$

We expect that the term $\mathcal{G}_h^* \mathcal{L}_h(S_h)\mathcal{G}_h$ converges to a differential operator (more generally ΨDO):

$$\mathcal{G}_h^* \mathcal{L}_h(S_h)\mathcal{G}_h \to P(D_x), \quad \text{as} \quad h \to 0.$$

Let us examine it for basic examples.

§5.2 Triangular lattice

The Laplacian for the triangular lattice is defined by

$$\begin{aligned}(\Delta_{disc,h} f)(n) \;=\; & \frac{1}{h^2}\Big[f(n) - \frac{1}{6}\Big(\widehat{f}(n_1+1, n_2) + \widehat{f}(n_1-1, n_2) + \widehat{f}(n_1, n_2+1) \\ & + \widehat{f}(n_1, n_2-1) + \widehat{f}(n_1+1, n_2-1) + \widehat{f}(n_1-1, n_2+1)\Big)\Big].\end{aligned}$$

Passing to the Fourier series, $-\Delta_{disc,h}$ is rewritten as

$$\begin{aligned}\mathcal{L}_h(e^{-ih\xi}) &= \frac{1}{3h^2}(3 - \cos h\xi_1 - \cos h\xi_2 - \cos(h\xi_1 - h\xi_2)) \\ &= \frac{2}{3h^2}\Big(\sin^2\frac{h\xi_1}{2} + \sin^2\frac{h\xi_2}{2} + \sin^2\frac{h(\xi_1-\xi_2)}{2}\Big).\end{aligned}$$

Arguing as in the case of the square lattice, one can show :

Theorem 5.1 *The scattering solution of the triangular lattice converges to that of the equation*[1]

$$\Big(-\frac{1}{6}\big(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + (\frac{\partial}{\partial x_1} - \frac{\partial}{\partial x_2})^2\big) + V(x) - E\Big)u = f$$

The S-matrix also converges.

[1] For the topology of convergence, see Theorem 7.1.

§5.3 Hexagonal lattice

The hexagonal lattice is a 2×2 system, hence has 2 characteristic roots. When they cross, the solution of the lattice Schrödinger equation behaves differently.

5.3.1 Dirac points The Laplacian for the Hexagonal lattice is given by

$$-\Delta_{disc,h} = -\frac{1}{3h}\begin{pmatrix} 0 & 1+S_{h,1}^*+S_{h,2}^* \\ 1+S_{h,1}+S_{h,2} & 0 \end{pmatrix} = \mathcal{L}_h(S_h).$$

Its symbol is

$$\mathcal{L}_h(e^{-ih\eta}) = -\frac{1}{3h}\begin{pmatrix} 0 & 1+e^{ih\eta_1}+e^{ih\eta_2} \\ 1+e^{-ih\eta_1}+e^{-ih\eta_2} & 0 \end{pmatrix}.$$

We put

$$b_2(z) = \cos z_1 + \cos z_2 + \cos(z_1 - z_2), \quad z = (z_1, z_2) \in \mathbf{C}^2.$$

Then, we have

$$|1 + e^{i\eta_1} + e^{i\eta_2}|^2 = 3 + 2b_2(\eta), \quad \eta = (\eta_1, \eta_2) \in \mathbf{R}^2.$$

The characteristic roots of $\mathcal{L}_h(S_h)$ are

$$\lambda_h^{(\pm)}(\eta) = \pm\frac{\sqrt{3+2b_2(h\eta)}}{3h}.$$

By elementary geometry, we have

$$\begin{aligned} 3 + 2b_2(\eta) = 0 &\iff \eta = (\frac{2\pi}{3}, -\frac{2\pi}{3}),\ (-\frac{2\pi}{3}, \frac{2\pi}{3}), \\ 3 + 2b_2(\eta) = 9 &\iff \eta = (0, 0). \end{aligned}$$

The spectrum of $-\Delta_{\Gamma_h}$ is

$$\sigma(-\Delta_{\Gamma_h}) = [-1/h, 1/h].$$

We say that η_0 is a *Dirac point* if $\det(\mathcal{L}_h(ih\eta) - \lambda) = 0$ has a multiple root at $\eta = \eta_0$.

5.3.2 Derivation of Dirac equations. We expand the discerete equation near the center of the energy, i.e. 0 of $\sigma(-\Delta_{\Gamma_h})$. Let $d_h^{(\pm)}$ be the Dirac points for the hexagonal lattice, i.e.

$$d_h^{(\pm)} = \pm\frac{1}{h}(\frac{2\pi}{3}, -\frac{2\pi}{3}),$$

and take open sets $\mathcal{K}_0^{(\pm)} \subset \mathbf{T}^d$ such that

$$d_1^{(\pm)} \in \mathcal{K}_0^{(\pm)} \setminus \mathcal{K}_0^{(\mp)}, \quad \mathbf{T}^d = \mathcal{K}_0^{(+)} \cup \mathcal{K}_0^{(-)}.$$

We take $\chi^{(\pm)}(\eta) \in C^\infty(\mathbf{T}^d)$ such that

$$\operatorname{supp} \chi^{(\pm)} \subset \mathcal{K}_0^{(\pm)}, \quad \chi^{(+)} + \chi^{(-)} = 1 \quad \text{on} \quad \mathbf{T}^d.$$

In particular, $\chi^{(\pm)} = 1$ in a neighborhood of $d_h^{(\pm)}$, and $\chi^{(\pm)} = 0$ in a neighborhood of $d_h^{(\mp)}$.

We put

$$P_h^{(\pm)}(\xi) = \frac{\sqrt{3 + 2b_2(h(\xi + d_h^{(+)}))}}{3h},$$

$$\mathcal{K}^{(\pm)} = \mathcal{K}_0^{(\pm)} - d_1^{(\pm)}.$$

On $\mathcal{K}^{(\pm)}/h$, $P_h^{(\pm)}(\xi)$ vanishes only at $\xi = 0$. Moreover, there exists a constant $C > 0$ such that

$$P_h^{(\pm)}(\xi) \geq C|\xi|, \quad \xi \in \mathcal{K}^{(\pm)}/h.$$

The next step is the *cut-off near Dirac points*. For the solution of the equation

$$(\mathcal{L}_h(S_h) - z)u_h = f_h,$$

we split $u_h = u_h^{(+)} + u_h^{(-)}$, where

$$u_h^{(\pm)} = \mathcal{F}_{disc,h}^{-1}(\chi^{(\pm)}(h\eta)\widehat{u}_h(\eta)), \quad f_h^{(\pm)} = \mathcal{F}_{disc,h}^{-1}(\chi^{(\pm)}(h\eta)\widehat{f}_h(\eta)),$$

which satisfy

$$(\mathcal{L}_h(S_h) - z)u_h^{(\pm)} = f_h^{(\pm)}.$$

We also introduce the *Gauge transformation* $\mathcal{G}^{(\pm)}$.

$$(\mathcal{G}^{(\pm)}a)(n) = e^{ihn\cdot d_h^{(\pm)}}a(n) = e^{in\cdot d_1^{(\pm)}}a(n), \quad a \in L^2(\mathbf{Z}_h^2).$$

One can then show that $\widetilde{u}_h$ behaves as follows.

Theorem 5.2

$$\widetilde{u}_h \simeq e^{ix\cdot d_h^{(+)}}\widetilde{v}^{(+)} + e^{ix\cdot d_h^{(-)}}\widetilde{v}^{(-)},$$

where $v^{(\pm)}$ is a solution to the 2-dim. massless Dirac equation.[2]

Let us give a sketch of the proof of Theorem 5.2. We put

$$q(\eta) = 1 + e^{i\eta_1} + e^{i\eta_2}.$$

[2]For the topology of this expansion, see Theorem 6.1.

Then,

$$\Big(\mathcal{L}_h(e^{ih(\xi+d_h^{(\pm)}}) - z\Big)^{-1} =$$

$$\frac{1}{P_h^{(\pm)}(\xi)-z^2}\begin{pmatrix} 0 & q(h(\xi+d_h^{(\pm)})) \\ q(-h(\xi+d_h^{(\pm)})) & 0 \end{pmatrix}.$$

We take $\psi^{(\pm)}(\eta)\in C_0^\infty(\mathbf{R}^d)$ and put

$$f_h(x) = (\frac{h}{2\pi})^{d/2}\int_{\mathbf{R}^d} e^{ix\cdot\eta}\left(\psi^{(+)}(\eta-d_h^{(+)}) + \psi^{(-)}(\eta-d_h^{(-)})\right)d\eta.$$

Let $v_h^{(\pm)} = v_h^{(\pm)}(E+i0)$ for $E>0$. Then, we have for $\epsilon>0$

$$\|\widetilde{v}_h^{(\pm)}\|_{-1/2-\epsilon} \leq C\|f\|_{m,s},$$

$$\|p_-(D_x)\widetilde{v}_h^{(\pm)}\|_{-1/2+\epsilon} \leq C\|f\|_{m,s}, \quad p_-\in\mathcal{P}_-,$$

where $\|\cdot\|_{m,s}$ denotes the weighted Sobolev norm:

$$\|f\|_{m,s} = \sum_{|\alpha|\leq m}\|\partial^\alpha f\|_s.$$

Let $u_h = u_h(E+i0) = \mathcal{G}^{(+)}v^{(+)} + \mathcal{G}^{(-)}v^{(-)}$. Noting that

$$\widehat{\mathcal{G}^{(\pm)}v^{(\pm)}} = \widehat{v}^{(\pm)}(\xi - d_h^{(\pm)}),$$

we have

$$\widetilde{u}_h = e^{ix\cdot d_h^{(+)}}\widetilde{v}_h^{(+)} + e^{ix\cdot d_h^{(-)}}\widetilde{v}_h^{(-)}.$$

We then see that $v_h^{(\pm)}\to v^{(\pm)}$, hence $\widetilde{u}_h$ behaves like

$$\widetilde{u}_h \simeq e^{ix\cdot d_h^{(+)}}\widetilde{v}^{(+)} + e^{ix\cdot d_h^{(-)}}\widetilde{v}^{(-)}.$$

We show that $\widetilde{v}^{(\pm)}$ are solutions to massless Dirac equations. We consider the case of $v_h^{(+)}$, and make the chang of variables

$$\eta_1 = \xi_1 + \frac{2\pi}{3h}, \quad \eta_2 = \xi_2 - \frac{2\pi}{3h},$$

to obtain

$$\begin{aligned} 1+e^{ih\eta_1}+e^{ih\eta_2} &= e^{2\pi i/3}(e^{ih\xi_1}-1) + e^{-2\pi i/3}(e^{ih\xi_2}-1) \\ &\sim -hi\frac{\xi_1+\xi_2}{2} - h\frac{\sqrt{3}(\xi_1-\xi_2)}{2} \end{aligned}$$

as $h\to 0$. We put

$$\zeta_1 = \frac{\sqrt{3}}{6}(\xi_1-\xi_2), \quad \zeta_2 = -\frac{1}{6}(\xi_1+\xi_2).$$

Then, we have

$$-\frac{1}{3h}(1+e^{ih\eta_1}+e^{ih\eta_2}) \sim \zeta_1 - i\zeta_2.$$

We put

$$y_1 = \sqrt{3}(x_1 - x_2), \quad y_2 = -3(x_1 + x_2).$$

Then, the map $(x, \eta) \to (y, \zeta)$ is symplectic. We then have

$$-\frac{1}{3h}(1+e^{ih\eta_1}+e^{ih\eta_2}) \sim \zeta_1 - i\zeta_2,$$

as $h \to 0$. Similarly,

$$-\frac{1}{3h}(1+e^{-ih\eta_1}+e^{-ih\eta_2}) \sim \zeta_1 + i\zeta_2.$$

We have thus obtained

$$\mathcal{L}_h(e^{ih(\xi+h_d)}) \sim \begin{pmatrix} 0 & \zeta_1 - i\zeta_2 \\ \zeta_1 + i\zeta_2 & 0 \end{pmatrix} = \zeta_1\sigma_1 + \zeta_2\sigma_2,$$

where σ_1, σ_2 are Pauli spin matrices. Therefore, $v^{(+)}$ satisfies

$$\Big(\sigma_1 \frac{1}{i}\frac{\partial}{\partial y_1} + \sigma_2 \frac{1}{i}\frac{\partial}{\partial y_2} - E\Big)v^{(+)} = g^{(+)}.$$

Similarly, $v^{(-)}$ satisfies

$$\Big(-\sigma_1 \frac{1}{i}\frac{\partial}{\partial y_1} + \sigma_2 \frac{1}{i}\frac{\partial}{\partial y_2} - E\Big)v^{(-)} = g^{(-)}.$$

5.3.3 Derivation of Schrödinger equations. We expand the hexagonal lattice system near the bottom of the spectrum. To deal with the case near the lowest energy, we should consider

$$-\frac{1}{3h^2}\begin{pmatrix} 0 & 1+S_{h,1}^*+S_{h,2}^* \\ 1+S_{h,1}+S_{h,2} & 0 \end{pmatrix}.$$

Here, note that we take $\nu = 2$ in h^ν, while in the previous case $\nu = 1$.

The reference energy is $E_0 = -h^2/2$, and we consider the Hamiltonian

$$\mathcal{L}_h(e^{-ih\eta}) = -\frac{1}{3h^2}\begin{pmatrix} -3 & 1+e^{ih\eta_1}+e^{ih\eta_2} \\ 1+e^{-ih\eta_1}+e^{-ih\eta_2} & -3 \end{pmatrix}.$$

Then, the characteristic roots are

$$\lambda_h^{(\pm)}(\eta) = \frac{3 \pm \sqrt{3+2b_2(h\eta)}}{3h^2}.$$

The minimum is attained only at $\eta = 0$, and $\lambda_h^{(-)}(\eta)$ has a Taylor expansion

$$\lambda_h^{(-)}(\eta) = \frac{1}{9}\left(\eta_1^2 - \eta_1\eta_2 + \eta_2^2\right) + O(h^2).$$

Arguing in the same way as in the case of square lattice, we obtain the following theorem.

Theorem 5.3 *The solution of the Schrödinger equation on the hexagonal lattice*

$$(\mathcal{L}_h(S_h) + V_{disc,h} - z)u_h = f_h$$

converges to that for the continuum Schrödinger equation

$$\Big(- \frac{1}{9}(\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_1 \partial x_2} + \frac{\partial^2}{\partial x_2^2}) + V(x) - z\Big)u = f.$$

§6 General formulation I

The arguments in the previous section can be generalized so that we can deal with the following lattices:

Square, Triangluar, Hexagonal, ladder of square lattices, graphite.

We consider the symbol $\mathcal{L}_h(z)$ of $-\Delta_{\mathbf{\Gamma}_h}^{(h)}$. For $\eta \in \mathbf{R}^d$, let

$$\lambda_{1,h}(\eta) \leq \cdots \leq \lambda_{s,h}(\eta)$$

be the characteristic roots of $\mathcal{L}_h(e^{-ih\eta})$. We restrict ourselves to two cases: (1) a simpe root, (2) double roots.

We assume for some $1 \leq j \leq s$, there exists an h-independent open set $\mathcal{K}_0$ in $\mathbf{T}^d$ with the following properties.

(**B-1**) *On $\mathcal{K}_0$, $\lambda_j(e^{-i\eta}) \geq 0$, and there exists a unique $d_1 \in \mathcal{K}_0$ such that $\lambda_j(e^{-id_1}) = 0$.*

We next assume either the following (B-2-1) or (B-2-2):

(**B-2-1**) *There exist constants $\epsilon_1, \epsilon_2 > 0$ such that*

$$\lambda_{j-1}(e^{-i\eta}) < -\epsilon_1 < \lambda_j(e^{-i\eta}) < \epsilon_2 < \lambda_{j+1}(e^{-i\eta}), \quad \forall \eta \in \overline{\mathcal{K}_0}. \qquad (11)$$

(**B-2-2**) *$\lambda_{j-1}(e^{-i\eta}) = -\lambda_j(e^{-i\eta})$, and there exist constants $\epsilon_1, \epsilon_2 > 0$ such that*

$$\lambda_{j-2}(e^{-i\eta}) < -\epsilon_1 < \lambda_{j-1}(e^{-i\eta}) \leq \lambda_j(e^{-i\eta}) < \epsilon_2 < \lambda_{j+1}(e^{-i\eta}), \quad \forall \eta \in \overline{\mathcal{K}_0}. \qquad (12)$$

In both cases, we put

$$\mathcal{K} = \mathcal{K}_0 - d_1 = \{\eta - d_1\,;\, \eta \in \mathcal{K}_0\}, \tag{13}$$

$$P_h(\xi) = \lambda_{j,h}(\xi + d_h), \quad d_h = d_1/h, \tag{14}$$

and assume as follows.

(**B-3**) *For $0 \neq \xi \in \mathcal{K}/h$, the limit*

$$P_h(\xi) \to P(\xi), \tag{15}$$

together with all of its derivatives, exists as $h \to 0$, where $P(\xi)$ is C^∞ for $\xi \neq 0$, homogeneous of degree $\gamma > 0$ and

$$CP(\xi) \le P_h(\xi) \le C^{-1}P(\xi), \quad on \quad \mathcal{K}/h \tag{16}$$

for a constant $C > 0$.

Let $\Pi_h(\xi)$ be the eigenprojection associated with the eigenvalue $\lambda_{j,h}(\xi + d_h)$ for the case (B-2-1), and the sum of eigenprojections associated with $\lambda_{j-1,h}(\xi + d_h)$ and $\lambda_{j,h}(\xi + d_h)$ for the case (B-2-2). We assume:

(**B-4**) *For $0 \neq \xi \in \mathcal{K}/h$, there exists a projection $\Pi_0(\xi)$ such that*

$$\Pi_h(\xi) \to \Pi_0(\xi), \tag{17}$$

as $h \to 0$, together with all derivatives.

We then have the following theorem. We state only for the case (B-2-1).

Theorem 6.1 *Assume that $f \in H^{m,s}(\mathbf{R}^d)$ for some $s > d+1$ and $m > [d/2]+1$. Assume (B-1), (B-2-1), (B-3), (B-4) and (U-1). Let $u_h(n, E+i0)$ be an outgoing solution to the gauge transformed equation*

$$(-\mathcal{G}_h^*\Delta_{disc,h}\mathcal{G}_h - E)u_h = f_h \quad on \quad \mathbf{Z}^d,$$

where $f_h(n) = f(hn)$. We put $\widehat{u}_h(\xi, E+i0) = \mathcal{F}_{disc,h}u_h$, and

$$\widehat{v}_h(\xi, E+i0) = \chi_d(h\xi)\Pi_h(\xi)\widehat{u}_h(\xi, E+i0). \tag{18}$$

$$\widetilde{v}_h(x, E+i0) = (\frac{h}{2\pi})^{d/2}\int_{\mathbf{T}_h^d} e^{ix\cdot\xi}\widehat{u}_h(\xi, E+i0)d\xi. \tag{19}$$

Then, there exists a strong limit

$$\lim_{h\to 0}\widetilde{v}_h(x, E+i\epsilon) = \widetilde{v}(x, E+i0) \quad in \quad L^{2,-1/2-\epsilon}(\mathbf{R}^d), \quad \epsilon > 0,$$

which is a unique outgoing solution to the Schrödinger equation

$$(P(D_x) - E)\widetilde{v} = g \quad on \quad \mathbf{R}^d,$$

where $(\mathcal{F}_{cont}g)(\xi) = \Pi_0(\xi)(\mathcal{F}_{cont}f)(\xi)$, and $\widetilde{v}$ satisfies the radiation condition

$$p_-(x, D_x)\widetilde{v} \in L^{2,-1/2+\epsilon}(\mathbf{R}^d), \quad p_- \in \mathcal{P}_-.$$

§7 General formulation II

Let us consider the case where the characteristic root $\lambda_{j,h}(\xi)$ has a unique global minimum. Assume that

(**C-1**) *On* $\mathbf{T}^d$, $\lambda_j(e^{-i\eta}) \geq 0$, *and there exists a unique* $d_1 \in \mathbf{T}^d$ *such that* $\lambda_j(e^{-id_1}) = 0$.

(**C-2**) *There exist constants* $\epsilon_1, \epsilon_2 > 0$ *such that*

$$\lambda_{j-1}(e^{-i\eta}) < -\epsilon_1 < \lambda_j(e^{-i\eta}) < \epsilon_2 < \lambda_{j+1}(e^{-i\eta}), \quad \forall \eta \in \mathbf{T}^d. \tag{20}$$

(**C-3**) *Letting* $P_h(\xi)$ *be*

$$P_h(\xi) = \lambda_{j,h}(\xi + d_h), \quad d_h = d_1/h, \tag{21}$$

we assume that $P_h(\xi) \to P(\xi)$ *on* $\mathbf{T}^d$, *where*

$$P(\xi) = \sum_{|\alpha|=2m} a_\alpha \xi^\alpha, \tag{22}$$

m *being a positive integer.*

(**C-4**) *The eigenvector associated with* $\lambda_j(e^{-\eta})$ *does not depend on* η.

Under these additional assumptions, one can add a scalar potential $V(x)$ to $-\Delta_{\Gamma_h}$. Assume that

(**V-2**) $V(x) \in H_0^s(\mathbf{R}^d)$ *for some* $s > d/2$.

We finally assume the uniqueness of solutions to the Schrödinger equation.

(**U-2**) *The solution of the equation*

$$(P(D_x) + V(x) - E)u = f \in \mathcal{B} \tag{23}$$

satisfying $u \in \mathcal{B}^*$ *and the radiation condition is unique.*

Theorem 7.1 *Assume that* $f \in H^{m,s}(\mathbf{R}^d)$ *for some* $s > d+1$ *and* $m > [d/2] + 1$. *Assume (C-1), (C-2), (C-3), (C-4) and (U-2). Let* $z \notin \mathbf{R}$, *and* $u_h(n, z)$ *be an* L^2*-solution of the equation*

$$(-\mathcal{G}_h^* \Delta_{disc,h} \mathcal{G}_h + V_{disc,h} - z)u_h = f_h \quad on \quad \mathbf{Z}^d,$$

where $f_h(n) = f(hn)$. *Then, there exist a strong limit*

$$\lim_{h \to 0} \widetilde{u}_h(x, z) = \widetilde{u}(x, z) \quad in \quad L^{2,-s}(\mathbf{R}^d), \quad 0 < s < 1/2.$$

The convergence is locally uniform on $\mathbf{R}^d$. *Moreover,* u *satisfies*

$$u = \Pi_0 u, \quad (P(D_x) + V(x) - z)u = \Pi_0 f. \tag{24}$$

§8 Complex energy

In the above arguments, we used Rellich type uniqueness theorem. For this, we need the unique continuation theorem for the Helmholtz equation on the lattice. However, Kagome lattice, Subdivision of square lattice do not have this unique continuation property. For this case, by considering the complex energy, our theorem still holds:

Theorem 8.1 *Assume that $f \in H^{m,s}(\mathbf{R}^d)$ for some $s > d+1$ and $m > [d/2]+1$. Assume (C-1), (C-2), (C-3), (C-4) and (U-2). Let $z \notin \mathbf{R}$, and $u_h(n,z)$ be an L^2-solution of the equation*

$$(-\mathcal{G}_h^* \Delta_{disc,h} \mathcal{G}_h + V_{disc,h} - z) u_h = f_h \quad on \quad \mathbf{Z}^d,$$

where $f_h(n) = f(hn)$. Then, there exist a strong limit

$$\lim_{h \to 0} \widetilde{u}_h(x,z) = \widetilde{u}(x,z) \quad in \quad L^{2,-s}(\mathbf{R}^d), \quad 0 < s < 1/2.$$

The convergence is locally uniform on $\mathbf{R}^d$. Moreover, u satisfies

$$u = \Pi_0 u, \quad (P(D_x) + V(x) - z)u = \Pi_0 f. \tag{25}$$

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