Scattering on graphs and one-dimensional approximations to \( N \)-dimensional Schrödinger operators

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In the present article we develop the spectral analysis of Schrödinger operators on lattice-type graphs. For the basic example of a cubic periodic graph the problem is reduced to the spectral analysis of certain regular differential operators on a fundamental star-like subgraph with a selfadjoint condition at the central node and quasiperiodic conditions at the boundary vertices. Using an explicit expression for the resolvent of lattice-type operator we develop in the second section appropriate Lippmann–Schwinger techniques for the perturbed periodic operator and construct the corresponding scattering matrix. It serves as a base for the approximation of the multi-dimensional Schrödinger operator by a one-dimensional operator on the graph: in the third section of the paper for given \( N \)-dimensional Schrödinger operators with rapidly decreasing potential we construct a lattice-type operator on a cubic graph embedded into \( \mathbb{R}^N \) and show that the original \( N \)-dimensional scattering problem can be approximated in a proper sense by the corresponding scattering problem for the perturbed lattice operator. © 2001 American Institute of Physics. [DOI: 10.1063/1.1347395]

I. INTRODUCTION

Modern interest in spectral properties of Schrödinger operators on graphs and corresponding scattering problems arises from the natural expectation that a dense lattice may serve as a natural approximation for the corresponding solid body. This basic idea is intensely exploited when constructing approximate solutions of partial differential equations on zero-dimensional meshes.\(^1\)

From a geometrical point of view, graphs are one-dimensional objects, but they have new interesting properties, which distinguish one-dimensional Schrödinger operators on graphs from one-dimensional Schrödinger operators on finite and infinite intervals. One property is the absence of a “global” solution of the Cauchy problem. Still we may describe the whole set of solutions of the corresponding homogeneous differential equation on a graph as a spline of solutions of local Cauchy problems for ordinary differential equations on edges. But now the whole structure of the finite-dimensional subspace of solutions of the homogeneous equation depends on the topology of the graph. Hence we see that Schrödinger operators on graphs have interesting mathematical structures which take an intermediate position between ordinary and partial differential equations. On the other hand, this makes them a useful tool for mathematical modeling and for a study of real physical systems, like nanowires, thin waveguides and networks. This is the reason of recent

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interest in differential operators on graphs, both for pure mathematics\textsuperscript{2–12} and applications.\textsuperscript{13–18}

In the present article we study cubic lattice type graphs in \( \mathbb{R}^N \). Lattice type graphs are periodic infinite graphs with no infinite edges. Our main objective is to study the possibility of an approximation of high-dimensional Schrödinger dynamics by corresponding dynamics on lattice-type graphs. One-dimensional geometry of graphs makes the spectral analysis and solution of scattering problems essentially less difficult than in high-dimensional systems. On the other hand, the partial discretization of the problem obtained by replacing the differential equation on the multi-dimensional space by the corresponding problem for an ordinary differential operator on the lattice-type graph, may serve not only for the aims of computing with use of the corresponding one-dimensional (or, generally, multi-dimensional) meshes viewed as approximations of domains of the original space, but also for qualitative modeling of spectral properties of the original multi-dimensional Schrödinger operator. This modeling is more natural, due to the continuous nature of graphs, compared with discrete zero-dimension lattice approximations of high-dimensional domains\textsuperscript{19,20} normally used for the construction of approximate solutions of partial differential equations.

The article is organized as follows. In Sec. II we consider the Schrödinger operator on a periodic cubic lattice graph in \( \mathbb{R}^N \). We would like to notice that we generalize results of Exner, who studied\textsuperscript{9} the Schrödinger operator on a cubic lattice type graph in \( \mathbb{R}^2 \). We derive the dispersion equation and explicit expressions for Bloch waves, for the resolvent kernel and obtain the Krein’s formula for the finitely perturbed periodic lattice. In Sec. III we consider the Schrödinger operator \( H = -\Delta + V(X) \) in Euclidean space \( \mathbb{R}^N \) supplied with the cubic lattice-type graph \( \Gamma \) with edges of the length \( 2a \). For given \( H \) we construct a family of Schrödinger operators \( L^{(a)} \) on \( \Gamma \) which have the following property: the restrictions of the solutions of the equation \( H\psi = \lambda \psi + F \) onto the lattice \( \Gamma \) are asymptotically close to the solutions of the equation \( L^{(a)}\psi = \lambda u + F \) when \( a \to 0 \). We construct an effective equation for the resolvent of the operator \( L^{(a)} \) and prove that it is of the Hilbert–Schmidt type, thus allowing for a straightforward numerical solution by iterative methods. Finally we compare the scattering matrix for the operators \( L^{(a)} \) on the graph \( \Gamma \) with the scattering matrix of the original \( N \)-dimensional operator \( H \).

II. ONE-BODY PROBLEM ON CUBIC LATTICE-TYPE GRAPHS

A. Periodic cubic graph in \( \mathbb{R}^N \)

In this section we consider a periodic cubic graph \( \Gamma \) in Euclidean space \( \mathbb{R}^N \). We assume that the edges of the graph are parallel to the vectors of a fixed orthogonal and normalized basis \( \{e_i\}, i=1,2,\ldots,N \). If each edge of the graph has length \( 2a \), then the whole graph may be produced by shifts of a fragment \( \Omega_a \) of the graph \( \Gamma \) (see Fig. 1) which is called a fundamental subgraph (the fundamental domain of the subgroup of all translations in the basic directions by distances multiple of \( 2a \)):

\[
\Omega_a := \{-a < x_s < a, \; s=1,2,\ldots,N\}.
\]

Denoting by \( \mu \) the Lebesgue measure on \( \Gamma \) we may consider the Hilbert Space \( \mathcal{H} = L_2(\Gamma) \) of all square-integrable functions on \( \Gamma \). It is clear that \( \mathcal{H} \) may be interpreted as an orthogonal sum of a countable number of copies of \( L_2(\Omega_a) \):

\[
\mathcal{H} = L_2(\Gamma) = l_2(\mathbb{Z}^2; L_2(\Omega_a)).
\]

In accordance with the last decomposition any function \( u(X) \in \mathcal{H} \) may be represented as a function of two variables: the discrete variable \( m \) which numerates the tiles \( \Omega_{a,m} \) of all discrete translations (multiple to \( 2a \)) of the fundamental subgraph \( \Omega_a \), and the inner coordinate \( x \) which defines the position of the point inside the given tile:

\[
u(X) = u(x,m), \quad X = 2a \sum_{i=1}^N m_i e_i + x,
\]
We introduce the differential operator $L_g$ acting in the Hilbert space $H$ on smooth functions as a second order differentiation in basic direction $e_i$ on each edge parallel to $e_i$.

$$L_g u = -\frac{d^2 u}{dx^2}.$$ 

One may easily check that this operator is symmetric on the domain of all smooth functions with compact support submitted to the following boundary condition at each node $m_1, m_2, \ldots, m_N$:

$$u(m \pm 0 e_i) = u(m \pm 0 e_k) := u(m), \quad 1 \leq i, k \leq N,$$

$$\sum_{i=1}^{N} \left[ \frac{du}{dx_i} (m + 0 e_i) - \frac{du}{dx_i} (m - 0 e_i) \right] := [u'](m) = \gamma(m) u(m),$$

where $\gamma(m) = \gamma(m)$. One may also easily check, using the strong subordination condition and embedding theorems, that for each bounded sequence $\gamma(m)$ the closure of the operator $L_\gamma$ is a self-adjoint operator in $H$ defined on the orthogonal sum of the Sobolev spaces $W^2_2$ on the edges submitted to the above boundary condition (1) at the nodes of the lattice. Our next aim is to explore the spectral structure of $L_\gamma$ in the simplest case when the function $\gamma$ is constant: $\gamma(m) = \gamma$. We do it for general $N$, but for the convenience of the reader we supply some figures for the simplest nontrivial case $N = 2$. In this case the infinite graph $\Gamma$ is represented by a square lattice of nodes each one connected with four neighbors (see Fig. 1). The internode distance is $2a$. This graph can be represented in the form $\Gamma = \{e_i\}_{i=1}^{N}$ where the fundamental subgraph $\Omega_a$ shown in Fig. 1 is a union of four branches $(0, \pm a e_i) = \Omega_a^{i, \pm}$ with a common origin. In this case the total number of edges attached to each node is equal to $2N = 4$. 

FIG. 1. Cubic lattice type graph $\Gamma_a$ and its fundamental subgraph $\Omega_a$ in $\mathbb{R}^2$. 

$$x = \{x_i\}_{i=1}^{N}, \quad -a < x_i < a; \quad m = \{m_i\}_{i=1}^{N} \in \mathbb{Z}^N.$$
The periodic self-adjoint operator $L_\gamma$ is singular. Following Gelfand’s approach\textsuperscript{21} we reduce the construction of the spectral decomposition for it to an analysis of the regular Sturm–Liouville problem for the operator $L_\gamma$ on the fundamental subgraph $\Omega_a$:

\[ L_\gamma^p := -\frac{d^2}{dx^2} \Xi_\lambda^p = \lambda \Xi_\lambda^p, \]

with the boundary condition (1) at the node and special quasiperiodic conditions at the ends of branches of $\Omega_a^p$ fixed by the vector parameter $P = (p_1, p_2, \ldots, p_s, \ldots, p_N)$. We call this vector parameter varying on $N$-dimensional torus $T_N$ a quasimomentum and write down the boundary conditions as

\[ \Xi_\lambda^p(m + a_x e_x) = e^{ip_s} \Xi_\lambda^p(m - a_x e_x), \quad -\pi < p_s < \pi, \quad s = 1, 2, 3, \ldots, N. \]

The operator $L_\gamma$ may be represented as

\[ L_\gamma = \int_{\mathbb{R}^N} \otimes L_\gamma^p d^N P, \]

which reduces the spectral analysis of operator $L_\gamma$ to the spectral analysis of the operators $L_\gamma^p$.

\textit{Lemma 1:} For any quasimomentum $P$ the spectrum $\sigma_\gamma^p$ of the operator $L_\gamma^p$ is real, discrete and bounded from below. It has multiplicity one for almost all $P$. The eigenvalues $\lambda = k^2$ may be calculated as the roots of the transcendental equation,

\[ \sum_{s=1}^{N} \cos p_s + \frac{\gamma \sin 2ka}{2k} = N \cos 2ka. \]

The components of the eigenfunctions on the branches of the fundamental subgraph may be constructed in the form

\[ \Xi_\lambda^p = \sum_{s=1}^{N} \otimes \Xi_\lambda^{p_s}, \quad \Xi_\lambda^{p_s}(x_s) = \frac{G_\lambda^{p_s}(x_s, 0)}{G_\lambda^{0}(0, 0)}, \quad s = 1, 2, 3, \ldots, N, \]

where $G_\lambda^{p_s}(x, y)$ is the Green’s function of the one-dimensional quasiperiodic problem [integral kernel of the resolvent $(L_\gamma^p - \lambda)^{-1}$] on the s-branch $\Omega_s$ of the fundamental subgraph $-a < x_s < a$. Then

\[ G_\lambda^{0}(0,0) = \frac{\sin ka}{2k(\cos p - \cos 2ka)}, \]

\[ \Xi_\lambda^{p_s}(x_s) = \frac{e^{-ip_s/2}}{2 \sin ka} \left[ e^{-ik(x + a/2)} \sin \left( \frac{ka - p}{2} \right) + e^{ik(x + a/2)} \sin \left( \frac{ka + p}{2} \right) \right], \quad -a < x_s < 0, \]

\[ \Xi_\lambda^{p_s}(x_s) = \frac{e^{ip_s/2}}{2 \sin ka} \left[ e^{-ik(x - a/2)} \sin \left( \frac{ka + p}{2} \right) + e^{ik(x - a/2)} \sin \left( \frac{ka - p}{2} \right) \right], \quad 0 < x_s < a. \]

The normalizing coefficients $\rho_\lambda^p = \int \Xi_\lambda^p(x) |^2 d\mu$ of the eigenfunctions $\Xi_\lambda^{p_s}(x_s)$, $s = 1, 2, \ldots, N$ are calculated as

\[ \rho_\lambda^p = 2Na + \gamma \frac{ka \cos 2ka - \sin 2ka}{2ak^2 \sin 2ka}, \]
and are positive on the spectrum $\sigma_P^\gamma$ of the regular periodic problem. The spectral resolution and the Green’s function of the regular quasiperiodic problem are represented by the spectral series converging in $L_2$ for $x \neq y$:

$$
\sum_\lambda \Xi_\lambda^P(x) (\Xi_\lambda^P, f) \frac{1}{\rho_\lambda} = f(x),
$$

$$
G_\lambda^P(x,y) = \sum_\lambda \frac{\Xi_\lambda^P(x) \Xi_\lambda^P(y)}{\lambda(P) - \lambda} \frac{1}{\rho_\lambda}.
$$

**Proof:** Consider the following ratio of Green’s functions of the quasiperiodic problem on the $s$-branch of the fundamental subgraph:

$$
\Xi_{\lambda}^p(x) = \frac{G_\lambda^P(x,0)}{G_\lambda^P(0,0)}, \quad s = 1, 2, 3, \ldots, N.
$$

Then the quasiperiodicity condition is automatically fulfilled, and the boundary condition at the node is fulfilled for values of the spectral parameter $\lambda$ which satisfy the dispersion equation we derive now. Note that $\Xi_{\lambda}^p(0) = 1$ and the jump-condition $G_\lambda^P(+0,0) - G_\lambda^P(-0,0) = -1$ is fulfilled at the pole 0. Then the dispersion equation for $\Xi_{\lambda}^P := \Sigma_\gamma \Xi_{\lambda}^P$ has the form

$$
\sum_{s=1}^N \frac{1}{G_{\lambda}^P(0,0)} + \gamma = 0.
$$

At the value $m=0$ we calculate the expression for the Green’s function $G_\lambda^P$ in explicit form:

$$
G_\lambda^P(x,y) = \sum_{l=-\infty}^{\infty} e^{-ipf} e^{ik|x-y+2a|} \frac{1}{2ik} = \frac{e^{ik|x-y|}}{2ik} + \frac{1}{2ik} \frac{e^{i(2ka-p)}}{1-e^{i(2ka-p)}} e^{ik(x-y)} + \frac{1}{2ik} \frac{e^{i(ka+p)}}{1-e^{i(ka+p)}} e^{ik(y-x)}, \quad k^2 = \lambda,
$$

which implies $G_\lambda^P(0,0) = \sin 2ka/2k(\cos p - \cos 2ka)$. Then the dispersion equation acquires the form

$$
\sum_{s=1}^N \cos p_s + \frac{\gamma \sin 2ka}{2k} = N \cos 2ka, \quad k^2 = \lambda.
$$

The solutions $\lambda$ of this equation give the spectrum $\sigma_P^\gamma$ of the regular spectral problem on the fundamental subgraph with the quasiperiodic boundary condition (2). The spectrum $\sigma_P^\gamma$ depends on the quasimomentum $P = (p_1, p_2, \ldots, p_N)$. Hence due to the general spectral properties of the periodic problems\(^{21}\) the spectrum $\sigma_\gamma$ of the periodic operator on the whole space is calculated as a union of all $\sigma_P^\gamma$,

$$
\sigma_\gamma = \bigcup_{P \in T^*} \sigma_P^\gamma.
$$

The restrictions of the eigenfunctions of the periodic problem from the whole lattice (Bloch-functions) onto the fundamental subgraph are calculated as eigenfunctions of the regular quasiperiodic spectral problem with all possible quasimomenta. It is easy to check that each $s$-component of it on the $s$-branch $-a < x_s < a$ of the fundamental subgraph may be calculated as
\[ \Xi^p_{\lambda}(x_s) = \frac{\cos p_s - \cos(2ka)}{\sin 2ka} 2kG_{x_s}(x_s, 0), \quad s = 1, 2, 3, \ldots, N, \quad \lambda = k^2, \quad (8) \]

and then may be continued on the whole graph via the quasiperiodicity condition (2).

To calculate the spectral density of the periodic problem we need the normalizing coefficients of the Bloch waves for the regular problem with fixed \( P = (p_1, p_2, \ldots, p_N) \) on the fundamental subgraph centered at \( m = 0 \). According to the previous analysis, the \( x \)-component of the Bloch wave \( \Xi^p_{\lambda}(x) \) is presented for \( x = x_s \) as the ratio

\[ \Xi^p_{\lambda}(x_s) = \frac{G^p_{\lambda}(x_s, 0)}{G^p_{\lambda}(0, 0)} = \frac{e^{ik|x|} + \frac{1}{2ik} e^{i(2ka-p)/2} + \frac{1}{4k} e^{i(2ka+p)/2} - e^{-ik|x|}}{G^p_{\lambda}(0, 0)}, \quad p = p_s. \quad (9) \]

For \( x < 0 \), that is on the branch \( \Omega_a^- \) of the fundamental subgraph, the numerator of the Bloch wave (9) may be represented as

\[ G^p_{\lambda}(x, 0) = \frac{1}{2ik} \left[ e^{-ik|x|} + \frac{1}{2} e^{-i(2ka-p)/2} + \frac{1}{2} e^{i(2ka+p)/2} \right] + \frac{1}{4k} \left[ e^{-ik(x+a)} \sin \left( \frac{2ka-p}{2} \right) + e^{ik(x+a)} \sin \left( \frac{2ka+p}{2} \right) \right], \quad x < 0. \]

The same numerator on the complementary branch \( \Omega_a^+ \) (for \( x > 0 \)) is given by the formula

\[ G^p_{\lambda}(x, 0) = \frac{e^{ik|x|}}{4k} \left[ e^{-ik(x-a)} \sin \left( \frac{2ka+p}{2} \right) + e^{ik(x-a)} \sin \left( \frac{2ka-p}{2} \right) \right], \quad x > 0. \]

The normalizing coefficient \( \int_\Omega |\Xi^p|^2 \, dx \) of the Bloch-wave is calculated as a sum of integrals of the squares of all components of the Bloch-wave over all branches \( \Omega_x^\pm \) of the fundamental subgraph \( \Omega_a^\pm \):

\[ \sum_{s=1}^{N} \left[ J^s_- + J^s_+ \right], \quad \sum_{s=1}^{N} \left[ \frac{J^s_- + J^s_+}{|G^p_{\lambda}(0, 0)|^2} \right], \quad \sum_{s=1}^{N} \left[ \frac{J^s_- + J^s_+}{G^p_{\lambda}(0, 0)} \right]. \]

where \( J^s_\pm = \int_{\Omega_x^\pm} |G^p_{\lambda}(x, 0)|^2 \, dx \). These integrals are positive and they are represented by the formula

\[ J^s_\pm = \frac{a}{4k^4 \cos p - \cos 2ka} \left[ \sin^2 \left( \frac{2ka-p}{2} \right) + \sin^2 \left( \frac{2ka+p}{2} \right) \right] + 2 \sin \left( \frac{2ka+p}{2} \right) \sin \left( \frac{2ka-p}{2} \right) \sin \frac{2ka}{2ka}, \quad p = p_s. \]

Summing the result over all branches and using the dispersion equation (3) we obtain for the integral over the fundamental subgraph:
\[ \int_{\Omega_{u}} |\Xi_{\lambda}^{p}|^{2} \, dx = 2Na + \gamma \frac{2ka \cos 2ka - \sin 2ka}{2ak^{2} \sin 2ka} = \rho_{\lambda}^{p}. \]  

Hence the spectral expansion for the regular spectral problem on the fundamental subgraph with the quasiperiodic boundary conditions (2) has the form

\[ \sum_{\lambda} \Xi_{\lambda}^{p}(x) \Xi_{\lambda}^{p}(y) \frac{1}{\rho_{\lambda}^{p}} = \delta(x-y), \]

where the summation is over the spectrum \( \lambda \in \sigma_{\gamma}^{p} \) of the regular quasiperiodic problem. The expression for the square norm \( \rho_{\lambda}^{p} \) remains positive on the spectrum \( \sigma \) where the dispersion equation (3) is valid for \( -\pi < \rho_{\gamma} < \pi \). In particular we see that the norm of the Bloch-functions (4) for Kirchhoff’s (“zero-current”) boundary conditions \( \gamma = 0 \) is trivial, \( \rho_{\lambda}^{p} = 2aN \).

The spectral properties of the periodic operator \( L_{\gamma} \) on the whole graph \( \Gamma \) may be easily derived from the spectral properties of the regular operator \( L_{\gamma}^{p} \) on the fundamental subgraph. We already mentioned that \( \sigma_{\gamma} = \bigcup_{\rho} \sigma_{\gamma}^{p} \), and the eigenfunctions of the periodic problem (Bloch functions) may be obtained as the quasiperiodic continuation of the eigenfunctions \( \Xi_{\lambda}^{p} \) of the regular quasiperiodic problem. The spectral resolution for the periodic problem and the resolvent kernel may be obtained by averaging the corresponding expressions for the regular problem over the elementary cube of the dual lattice of quasimomenta \(-\pi < \rho_{\gamma} < \pi \), \( s = 1, 2, \ldots, N \):

\[ \frac{1}{(2\pi)^{N}} \int_{T} \sum_{\lambda \in \sigma_{\gamma}^{p}} \Xi_{\lambda}^{p}(x) \Xi_{\lambda}^{p}(y) \frac{1}{\rho_{\lambda}^{p}} \, d^{N}P = \delta(x-y). \]  

Each term of the series (12) above represents a spectral band of the periodic problem defined by corresponding branch \( \lambda(P) \) of the solution of the dispersion equation (3), \( P \in T^{N} \). The resolvent kernel \( G_{\gamma}^{z}(x,y) \) of the periodic problem [the integral kernel of the operator \( R_{\gamma,z} = (L_{\gamma} - z)^{-1} \)] may be represented now as a spectral integral:

\[ G_{\gamma}^{z}(x,y) = \frac{1}{(2\pi)^{N}} \int_{T} \sum_{\lambda \in \sigma_{\gamma}^{p}} \Xi_{\lambda}^{p}(x) \Xi_{\lambda}^{p}(y) \frac{d^{N}P}{\lambda(P) - z \rho_{\lambda}^{p}}. \]

**B. Perturbation in a finite number of nodes**

Consider now a perturbed periodic lattice with only finite number \( M < \infty \) of nodes \( (m_{1}, m_{2}, \ldots, m_{M}) \) affected. Actually we replace the standard boundary condition with \( \gamma(m) = \gamma \) [see the second condition in Eq. (1)] at the nodes \( m_{1}, m_{2}, \ldots, m_{M} \) by the local boundary condition

\[ [u'](m_{r}) = (\gamma + \beta_{r}) u(m_{r}), \quad r = 1, 2, \ldots, M, \]

with real \( \beta_{r} \). Our next aim is to construct the resolvent and scattered waves of the corresponding self-adjoint operator \( L_{\gamma} \beta \). We shall obtain both applying the Krein formula for generalized resolvents to our case. In fact we will rederive this remarkable formula in the present context; see also Refs. 24–26.

For given nodes \( m_{1}, m_{2}, m_{3}, \ldots, m_{M} \) consider the finite-dimensional Hilbert space \( \mathcal{E} \) of complex \( M \)-vectors \( U = (u_{1}, u_{2}, u_{3}, \ldots, u_{M}) \). Each continuous function \( u \) on the cubic lattice may generate a corresponding vector \( \vec{u} \) by the rule \( (\vec{u})_{s} = u(m_{s}), s = 1, 2, \ldots, M \). The scalar product in \( \mathcal{E} \) we denote as \( \langle \vec{u}, \vec{v} \rangle = \sum_{s=1}^{M} u_{s} v_{s} \). We need also a real scalar product in \( \mathcal{E} \) with complex conjugation absent on the second term. We denote it just by the angular brackets \( \langle \vec{u}, \vec{v} \rangle \) = \( \sum_{s=1}^{M} u_{s} v_{s} \). We also consider a finite-dimensional operator \( G_{\gamma}^{z} \) in \( \mathcal{E} \) defined by the matrix
The operator defined in $\mathcal{E}$ by the diagonal matrix $\text{diag}\{\beta_i\}$ will be denoted by

$B=\text{diag}\{\beta_i\}$.

**Theorem 1:** The resolvent kernel $G_h^\beta(x,y), x,y \in \Gamma$, of the operator $L_{\gamma\beta}$ is represented by the following Krein formula:

$$G_h^\beta(x,y) = G_h^\gamma(x,y) - \left( \frac{I}{I+BG_h^\gamma} \tilde{G}_h^\gamma(x) \right).$$

where $\tilde{G}_h^\gamma(x)$ is an $M$-dimensional vector-function with the components $G_h^\gamma(x,m_s), s = 1,2,\ldots,M$. The spectrum of the operator $L_{\gamma\beta}$ consists of an absolutely-continuous branch(es) which coincides with the (absolutely-continuous) spectrum $\sigma_\gamma$ of $L_{\gamma}$ and a finite number of eigenvalues in each spectral gap, which may be found from the dispersion equation $\det[I+BG_h^\gamma]=0$.

The scattered waves $\Phi_h^\beta$ which serve as eigenfunctions of the absolutely-continuous spectrum of the operator $L_{\gamma\beta}$ are parameterized by the quasimomenta $P$ of the initial Bloch-waves and may be constructed in analogy to the resolvent kernel:

$$\Phi_h^P = \Xi_h^P(x) - \left( \frac{I}{I+BG_h^\gamma} \tilde{\Xi}_h^P \right).$$

**Proof:** We begin with an auxiliary statement concerning the resolvent of the periodic problem.

Let us denote by $[\cdot]_m - \gamma I_m$ the following boundary value at the node $m$ for the function $u$ defined on the cubic graph:

$$([\cdot]_m - \gamma I_m)u = \sum_{i=1}^{N} \left[ \frac{du}{dx_i}(m+0e_i) - \frac{du}{dx_i}(m-0e_i) \right] - \gamma u(m).$$

Then for the resolvent kernel $G_h^\gamma(x,s)$ the following statement is true:

$$([\cdot]_m - \gamma I_m)G_h^\gamma(x,s) = -\delta_{ms}.$$  \hspace{1cm} (16)

Indeed, let us introduce the delta-function $\delta(x-m)$ attached to the node $m$ of the cubic graph. It may be represented as a sum of delta-functions constructed on the one-dimensional branches of the fundamental subgraph as

$$\delta(x-m) = \frac{1}{N} \sum_{i=1}^{N} \delta(x_i - m_i),$$

since both left and right parts define the same functional on the class of all continuous functions on the graph. This means that the periodic operator $L_{\gamma}$ may be represented as

$$L_{\gamma} = -\frac{d^2}{dx^2} + \gamma \sum_m \delta(x-m),$$

and the Green’s function $G_h^\gamma(x,s)$ which satisfies the equation

$$\frac{d^2}{dx^2}G_h^\gamma(x,n) + \gamma \sum_m \delta(x-m)G_h^\gamma(x,n) = \lambda G_h^\gamma(x,n) + \delta(x-n),$$

may be integrated on a small subgraph $\Omega_{e,m} = (-e<x_i<2am_i, e \ll 1)$ which gives the following result due to (27):
The left side of the last formula coincides with \((\mathcal{L} - \lambda I) G^\gamma_{\lambda}(x, n)\), as announced. It is clear that the statement is true for any bounded sequence \(\gamma(n)\) depending on \(n\) as well.

To prove the first relation (15) we consider the Ansatz for the resolvent kernel of the perturbed periodic operator in the form

\[
G^\gamma_{\lambda}(x, y) = G^\lambda_{\lambda}(x, y) + \sum_{i=1}^{M} A_i G^\lambda_{\lambda}(x, m_i). \tag{19}
\]

Then applying the operation \((\mathcal{L} - \lambda I)\) to the ansatz \(G^\gamma_{\lambda}(x, m_i)\) we obtain the vector \(-\delta_{rr} - \sum_{i=1}^{M} A_i \delta_{rt} \in \mathcal{E}_.\) On the other hand if the boundary condition (14) for \(G^\gamma_{\lambda}(x, m_i)\) is fulfilled, then this vector must coincide with the vector \(\beta_i G^\lambda_{\lambda}(m_r, m_i) + \sum_{i=1}^{M} G^\lambda_{\lambda}(m_r, m_i) A_i\). This gives a finite-dimensional equation for \(A_i, \ t=1, 2, \ldots, N.

\[
-(I + B_G) \tilde{A} = \tilde{G}_\lambda.
\]

If the operator \(I + B_G\) is invertible, then the vector \(\tilde{A}\) of coefficients \(A_i\) may be obtained as

\[
\tilde{A} = \frac{I}{I + B_G} \tilde{G}_\lambda,
\]

which gives the first relation (15). The second relation (16) may be obtained in a similar way by using the ansatz

\[
\Phi^\rho_{\lambda}(x) = \Xi^\rho_{\lambda}(x) + \sum_{i=1}^{M} A_i G^\lambda_{\lambda}(x, m_i).
\]

\[
\square
\]

III. APPROXIMATION OF N-DIMENSIONAL SCHRO"DINGER DYNAMICS BY DYNAMICS ON CUBIC GRAPH

A. Approximation theorems

We have seen above that quantum systems on the corresponding embedded graphs inherit some basic spectral features from relevant systems on bulk space. On the other hand, the less the dimension of mesh we are using for approximation of the multi-dimensional problem, the easier the corresponding computing; see the article\(^20\) by McCormic. At the same time the analysis for one-dimensional graphs may be developed in terms of solutions of corresponding Cauchy problems for ordinary differential equations on the edges of the graph, which is almost as simple to solve with the use of modern computers as discrete equations. But the continuous nature of ordinary differential equations allows us to observe high-energy phenomena in a most natural form. In particular one may derive the realistic asymptotic formulas, e.g., for a description of the scattering processes. This is our motivation for analyzing Schrödinger dynamics in \(N\)-dimensional space in terms of the corresponding dynamics on one-dimensional cubic graphs filling the whole space \(\mathbb{R}^N\).

Let us consider a Schrödinger operator in \(\mathbb{R}^N\),

\[
H = -\Delta + V(X), \quad X \in \mathbb{R}^N, \tag{20}
\]

with a continuous, rapidly decreasing potential \(V(X) \in L_2(\mathbb{R}^N) \cap C(\mathbb{R}^N)\). For any \(a > 0\) we can discretize the space \(\mathbb{R}^N\) representing it as a tiling...
where the coefficient in the measure
notations:
the subgroup of the shift group forming the tiling above. Indeed, when using the following
component
of the same orthogonal and normalized basis
$X_m$
where the tile
$vectors of a standard orthogonal and normalized basis $H_2$
sense that the graph
origin. The structure of this lattice is obviously compatible with the tiling introduced above in the
that the graph $\Gamma_a$ can be naturally embedded in the space $R^N$ as a cubic lattice with the step
2a so that the fundamental subgraph of it forms the boundary of the fundamental domain $K_a$ of the
subgroup of the shift group forming the tiling above. Indeed, when using the following
notations:
x is a point of the fundamental subgraph of $\Omega_a = \bigcup_{j=1}^{N} [-ae_j, ae_j] = \bigcup_{j=1}^{N} \Omega_a^j$;
$X$ is a point of the graph $\Gamma_a$: $X = 2am + x$, $m \in Z^N$;
$X_m = 2am$ is the $m$-th node of the cubic lattice with the edge 2a.
Together with the space $R^N$ we consider a graph $\Gamma_a$ which has the structure of a cubic lattice:
$\Gamma_a = \Omega_a \times Z^N$,
where $\Omega_a$ is a union of $N$ pairwise orthogonal edges $[-ae_i, ae_i]$ directed along the basic vector
of the same orthogonal and normalized basis $\{e_i\}_{i=1}^{N}$ and having only one common point at the
origin. The structure of this lattice is obviously compatible with the tiling introduced above in the
sense that the graph $\Gamma_a$ can be naturally embedded in the space $R^N$ as a cubic lattice with the step
2a so that the fundamental subgraph of it forms the boundary of the fundamental domain $K_a$ of the
subgroup of the shift group forming the tiling above. Indeed, when using the following
notations:
x is a point of the fundamental subgraph of $\Omega_a = \bigcup_{j=1}^{N} [-ae_j, ae_j] = \bigcup_{j=1}^{N} \Omega_a^j$;
$X$ is a point of the graph $\Gamma_a$: $X = 2am + x$, $m \in Z^N$;
$X_m = 2am$ is the $m$-th node of the graph $\Gamma_a$;
x$_j$ is a point of the interval $\Omega_a^j = [-ae_j, ae_j]$ (the $j$-edge of the fundamental subgraph $\Omega_a^j \subset \Gamma_a$),
we describe the natural embedding of the graph $\Gamma_a$ into $R^N$ as an identification of points $X_m$ and
$X_m$ and a realization of the edges of the graph as intervals parallel to coordinate axes in $R^N$
connected to the orthogonal basis $\{e_i\}_{i=1}^{N}$. In particular the fundamental subgraph $\Omega_a$ is then
embedded into the cube $K_a$ such that each $j$-axis of this cube $\{X: X_i = 0, l \neq j\}$ corresponds to the
component $\Omega_a^j$ of the fundamental subgraph and $x_j = x_j$.
One can consider the Hilbert space $H_a$ of functions on the graph $\Gamma_a$:
$H_a = L^2(\Gamma_a, \nu dX) = L^2(Z^N, L^2(\Omega_a, \nu dx)) = L^2\left(Z^N \sum_{j=1}^{N} \oplus L^2([-a, a], \nu dx_j)\right)$,
where the coefficient in the measure
$\nu = (2a)^{N-1}/N$
(21)
is chosen in order to preserve the measure under the embedding described above:
$\int_{K_a} d^N x = \nu \int_{\Omega_a} dx$.
(22)
The Laplace operator on the graph is given as
$L_0^{(a)} = -N \sum_{m \in Z^N} \sum_{j=1}^{N} \oplus \partial^2_{x_j} = -N \frac{d^2}{dx^2}$,
(23)
in the Hilbert space $H_a$ with the domain $D^{(a)}$ described as a linear variety,
\[
L^{(\alpha)} = L_0^{(\alpha)} + q_\alpha(X),
\]
with the (generalized) potential \( q_\alpha(X) = q_\alpha(x,m) \) which will be specified later.

It is obvious that general elements of the basic Hilbert space \( L_2(\mathbb{R}^N) \) of all square-integrable functions on \( \mathbb{R}^N \) cannot be restricted onto the embedded one-dimensional graph as square-integrable functions. In fact we need even more. The restrictions of functions on \( \mathbb{R}^N \) to the lattice \( \Gamma_a \) should be in a proper sense twice differentiable. Exact additional conditions of the smoothness of elements of the original Hilbert space \( L_2(\mathbb{R}^N) \) may be easily derived from Sobolev’s embedding theorems, but for the moment we just consider the trivial class \( W^2_2(\mathbb{R}^N) \), \( 2l > N \) which consists of continuous \( (\text{Lip}_{1/2} + 1) \) Lipshitz-functions in \( \mathbb{R}^N \) and the class

\[
\mathcal{F} := W^2_2(\mathbb{R}^N), \quad 2l - N > 4,
\]

which gives after restriction onto the one-dimensional lattice \( \Gamma_a \) functions in \( C^{2 + (1/l + 1)}(\Gamma_a) \). Below we prove two preparatory statements which will be summarized later in form of the theorem on approximations announced above.

**Lemma 2:** For any function \( u \in W^2_2(\mathbb{R}^N) \), \( 2l > N \) its restriction \( u_a \) onto the graph \( \Gamma_a \) belongs to \( L_2(\Gamma_a) \cap \text{Lip}_{2l - N/2}(\Gamma_a) \), and the modulo of continuity,

\[
\omega_X^a(\delta) := \sup_{|K| \leq \delta} |u(X + K) - u(X)|,
\]

of the function \( u \) at the point \( X \in \mathbb{R}^N \) is a square-integrable function of \( X \) in \( \mathbb{R}^N \) for any \( \delta \ll 1 \):

\[
\int_{\mathbb{R}^N} \omega_X^a(\delta)^2 \, dX^N \leq C \delta^{2(l+1)} \|u\|_{W^2_2}^2.
\]

The restriction operator \( u \rightarrow u_a \) is asymptotically isometric for \( a \rightarrow 0 \):

\[
\left| \int_{\mathbb{R}^N} |u|^2 \, dX^N - \int_{\Gamma_a} |u_a|^2(X) \, v \, dX \right| \leq a C_0 \left( \int_{\mathbb{R}^N} |u|^2 \, dX^N + \int_{\mathbb{R}^N} |\nabla u|^2 \, dX^N \right)

+ a^2 \left( a + \frac{1}{a} \right) C_1 \int_{\mathbb{R}^N} |\nabla u|^2 \, dX^N.
\]

Similarly, there is a constant \( C < \infty \), such that for any functions \( u, v \in W^2_2(\mathbb{R}^N) \), \( 2l > N \), and its restrictions \( u_a, v_a \) onto the graph \( \Gamma_a \),

\[
\left| \int_{\mathbb{R}^N} u \bar{v} \, dX^N - \int_{\Gamma_a} u_a \bar{v}_a \, v \, dX \right| \leq a C \left( \|u\|_{W^2_2}^2 + \|v\|_{W^2_2}^2 \right).
\]

**Proof:** We begin with the proof of the second statement. Note first of all that in the case \( 2l > N \) the function \( u \in W^2_2 \) in the unit cube \( K_1 \) may be estimated as

\[
\sup_{K_1} |u|^2 \leq C_0 \int_{K_1} |u|^2 \, dX^N + C_1 \int_{K_1} |\nabla u|^2 \, dX^N,
\]
and the increment of $u$ on any direct path $(x, x')$ in the unit cube the following estimate holds with some absolute constants $C_1,C_2$: 

$$|u(x) - u(x')|^2 \leq \left[ \int_{(x,x')} |\nabla u|^2 (s) \, ds \right]^2 \leq C_0 \int_{K_a} |\nabla u|^2 \, dx^N + C_1 \int_{K_a} |\nabla' u|^2 \, dx^N.$$ 

By scaling this gives 

$$\sup_{x \in K_a} |u|^2 \leq C_0 (2a)^{-N} \int_{K_a} |u|^2 \, dx^N + (2a)^{2l-N} C_1 \int_{K_a} |\nabla'u|^2 \, dx^N,$$

$$\sup_{x,x' \in K_a} |u(x) - u(x')|^2 \leq C_0 (2a)^{2l-N} \int_{K_a} |\nabla u|^2 \, dx^N + (2a)^{2l-N} C_1 \int_{K_a} |\nabla'u|^2 \, dx^N.$$

Hence for the real function $u$ the estimate for the increment of $u^2$ for $u \in W^l_2(K_a)$ along any direct path $(x, x')$, in $K_a$ may be reduced to an estimation of the product 

$$|u^2(x) - u^2(x')| = |u(x) + u(x')||u(x) - u(x')|,$$

which may be transformed with use of Cauchy’s inequality to the form 

$$|u^2(x) - u^2(x')| \leq \left( \frac{a}{N} \right)^{l-N} C_0 \int_{K_a} (|u|^2 + |\nabla u|^2) \, dx^N + (2a)^{2l-N} \left( 2a + \frac{1}{2a} \right) C_1 \int_{K_a} |\nabla'u|^2 \, dx^N.$$

Having $j$ fixed somehow we choose the point $x' = x'$ on $\Omega_x$ and then integrate over $K_a$ and sum over all $j$ and over the tiling $K_{\Gamma_a}$. Then redefining we obtain the estimate for the integral over Lebesgue measure $\mu$ on the lattice $\Gamma$:

$$\left| \int_{\mathbb{R}^N} |u|^2 \, dx^N - \frac{(2a)^{N-1}}{N} \int_{\Gamma_a} |u|^2 \, dx \right| \leq \left[ \frac{(2a)^{N-1}}{N} C_0 \int_{\mathbb{R}^N} (|u|^2 + |\nabla u|^2) \, dx^N + (2a)^{2l-N} \right.$$

$$\times \left( 2a + \frac{1}{2a} \right) C_1 \int_{K_a} |\nabla'u|^2 \, dx^N \right].$$

To obtain a similar estimate for complex-valued functions one may derive it separately for real and imaginary parts of them, and then add both parts. The final result for the estimation of the scalar product $\langle u, v \rangle$ is obtained with use of the polarization identity.

Using the assertion proved above we may reduce the verification of the first statement of the lemma to the proof of the corresponding fact in $\mathbb{R}^N$. This may be easily derived for rapidly decreasing smooth functions. The increment of the function $u(X)$ may be estimated in the usual way:

$$u(X+K) - u(X) = \frac{1}{(2\pi)^{N/2}} \int_{\mathbb{R}^N} e^{iP^X(-1+e^{PK})} \left( 1 + P^2 \right)^{l/2} u(P)(1 + P^2)^{l/2} \, dP^N.$$ 

Denoting the Fourier transform by $F$ we may rewrite the last expression in the form 

$$u(X+K) - u(X) = F^{-1}A(K,*)F(1 + D^2)^{l/2}u(X),$$

where $A$ is the pseudo-differential operator with the symbol 

$$A(K,P) = \frac{e^{iPK}}{(1 + P^2)^{l/2}}.$$
and $D^2$ is the Laplace operator in $L_0^n(R^N)$. Using the uniform estimate $|A(K, P)| \leq C \delta^{|l|+l}$ for the symbol in the ball $|K| \leq \delta$ and the unitarity of the Fourier-transform in $L_2^n(R^N)$ we see that for any continuous function $K(X)$, $|K(X)| \leq \delta$ we may estimate $\int_{R^N}|u(X + K(X) - u(X)|^2 dX$ by the product $C \delta^{2l+|l|} \|u\|^2_{L_2^n(R^N)}$. The function $K(X)$ may be chosen such that

$$|u(X + K(X) - u(X)| = \sup_{|X| \leq \delta}|u(X + K(X) - u(X)| = \omega_X^0(\delta).$$

This gives the first statement of the lemma.

Lemma 2 permits us to substitute the pre-Hilbert space of all $W^l_2$-smooth, $2l > N$, square-integrable functions in $R^N$ by the pre-Hilbert space of Lipschitz–continuous functions on the cubic graph. We need one more step to substitute the Laplace operator on $R^N$ by the Laplace on the cubic lattice, $-\Delta \rightarrow L_0^n$.

Define the classes

$$F_0 := W^l_2(R^N); \quad F_2 := W^{l+2}_2(R^N).$$

Then the following statement may be considered as a motivation for the substitution of the Laplace operator $-\Delta$ on the graph.

**Lemma 3:** The restriction $u_a$ of any function $u \in F_2$ onto the graph $\Gamma_a$,

$$u_a(x) = u(X), \quad \text{if} \quad X = X \in \Gamma_a,$$

in $C^2 + (2l - N)(2l - N + 2)(\Gamma_a) \cap L_2(\Gamma_a)$ exists and the diagram

$$\begin{array}{ccc}
  u & \text{differentiation} & \quad -\Delta u \\
  \downarrow \text{restriction} & \quad & \quad \text{restriction} \downarrow \\
  u_a & \text{differentiation} & \quad L_0^a u_a \leftrightarrow -\Delta u|_a
\end{array}$$

is “almost commutative” in the following weak sense: for any test-function $\varphi \in W^l_2(\Gamma_a)$ the weak deviation of $L_0^a u_a$ from $-\Delta u|_a$ for small $a$ may be estimated as

$$\left| \int_{\Gamma_a} (L_0^a u_a + \Delta u|_a) \varphi \, dx \right| \leq C_a^{1/|l|+1},$$

where $C$ is a constant depending on $\|u\|_{W^{l+2}_2(R^N)}, \|\varphi\|_{W^l_2(\Gamma_a)}^2$.

**Proof:** Due to Lemma 2 it is sufficient to derive the required estimate on the fundamental subgraph and then sum it over the whole tiling. If we denote by $u_0(m), u_a(m), u_d(m)$, respectively, the values of the function $u$ and the values of its first derivatives with respect to $x_s, x_t$ and second derivatives with respect to $x_s, x_t$ at the node $m$, we may write down the Taylor formula on the tile $\Omega_{a,m}$ for the function $u$,

$$u(2am + x) = u_0(m) + \sum_s u_s(m)x_s + \frac{1}{2} \sum_{s,t} u_{st}(m)x_s x_t + O(\omega^a_m(|x|)),$$

and for the restriction $u_a$ of $u$ onto the lattice $\Gamma_a, x \in \Omega^x_{a}$:

$$u_a(2am + x) = u_0(m) + u_s(m)x_s + \frac{1}{2} u_{st}(m)x_s^2 + O(\omega^a_m(|x|)).$$
A straightforward calculation of the multi-dimensional Laplace on \( u \) gives on the tile \( \Omega_m \):

\[
\Delta u = \sum_i u_i(x) + O(\omega_m^\Delta(|x|)),
\]

(26)

where \( \omega_m(\delta) \) stands for the modulo of continuity of the function \( f \) on the tile \( \Omega_m \). The application of the lattice Laplace \( L_{s}^a \) to the branch \( \Omega_{a,m}^s \) of the tile \( \Omega_{a,m} \) gives

\[
L_{s}^a u = Nu_s + O(\omega_m^a(|x|)).
\]

(27)

It is clear that the last two expressions (26), (27) have a lot in common: the restriction of the first of them onto the branch \( \Omega_{a,m}^s \) gives \( \sum u_s(x) + O(\omega_m^s(|x|)) \), hence integrating over \( \Omega_{a,m} \) with the test-function \( \varphi \) we obtain

\[
\varphi(2am + x) = \varphi(2am) + O(\omega_m^s(|x|)).
\]

Summing over \( s = 1,2,\ldots,N \) and \( m \) results in

\[
\left| \int_{\Gamma_a} (-\Delta u)(x) \varphi \nu v \, dx \right| \leq C \sum_m \left( \left( \int_{\Omega_{a,m}} |\varphi|^2 \nu v \, dx \right)^{1/2} \left( \int_{\Omega_{a,m}} |\omega_m^{D^2u}(x)|^2 \, dx \right)^{1/2} + \left( \int_{\Omega_{a,m}} |\omega_m^x(x)|^2 \nu v \, dx \right)^{1/2} \left( \int_{\Omega_{a,m}} |D^2u|^2 \, dx \right)^{1/2} + \left( \int_{\Omega_{a,m}} |\omega_m^{D^2u}(x)|^2 \nu v \, dx \right)^{1/2} \left( \int_{\Omega_{a,m}} |\omega_m^x(x)|^2 \, dx \right)^{1/2} \right),
\]

where \( C \) is an absolute constant and \( |D^2u|^2, |\omega_m^{D^2u}|^2 \) stay for sums of squares of second derivatives and of the moduli of continuity of them, respectively. The integrals of the squares of the moduli of continuity may be estimated via the mean-value theorem as

\[
\int_{\Omega_{a,m}} |\omega_m^{D^2u}(x)|^2 \nu v \, dx \leq (2a)^N |\omega_m^x(2a)|^2,
\]

and hence

\[
\sum_m \int_{\Omega_{a,m}} |\omega_m^{D^2u}(x)|^2 \nu v \, dx \leq \sum_m (2a)^N |\omega_m^x(2a)|^2,
\]

which coincides with an integral sum for the integral \( \int_{\Gamma_a} |\omega_m^{x}(2a)|^2 \nu v \, dx \). Using the local estimate for \( X \in \Omega_{a,m} \),

\[
\omega_m^x(2a) \leq \omega_{x}^x(4a),
\]

we may substitute the integral sum by the integral \( \int_{\Gamma_a} |\omega_{x}^x(4a)|^2 \nu v \, dx \) and estimate it using Lemma 2. These steps give the announced estimate with some constant \( C \) depending on \( \|u\|_{W^{2/2}(\Gamma_a)}\), \( \|\varphi\|_{W^{2/2}(\Gamma_a)} \).

Consider a pair of differential equations,

\[
-\Delta u + V(x)u = \lambda u + F,
\]

\[
L_{s}^a u + q(x) u = \lambda u + F_a,
\]
with nonhomogeneous terms $F \in W^2_2(R^N)$ and with $F_a = F|_{\Gamma_a}$. To approximate the multidimensional dynamics in $R^N$ by the corresponding one-dimensional dynamics on the graph $\Gamma_a$ we have to compare the resolvents of corresponding Schrödinger operators. For given continuous potential $V(X)$ in $R^N$ [see Eq. (20)], we have to construct a potential $g_a(X)$ (continuous, singular or generalized) on the graph $\Gamma_a$ [see Eq. (24)] so that following diagram:

\[
\begin{array}{c}
\text{solution} \\
\downarrow \text{approximation} \\
L_0^{(a)} u + q(x)u := L^{(a)}u = \lambda u + F|_{\Gamma_a} \rightarrow u(X) \rightarrow_{a \rightarrow 0} \partial \mathcal{H}|_{\Gamma_a}
\end{array}
\]

is "approximately commutative" in a sense similar to one of the diagrams discussed in Lemma 3. Now the exact meaning of the diagram (28) is clarified by the following.

**Theorem 2:** Let $H = -\Delta + V(X)$ be a Schrödinger operator in $L_2(R^N)$ with a real uniformly bounded square-integrable and continuous potential $V(X)$. Consider the family of lattice-type graphs $\Gamma_a$ naturally embedded into $R^N$ as described above and the family $\{L^{(a)}\}$ of operators (each acting in its own space $\mathcal{H}_a$) given by Eq. (24) with the generalized delta-functional potentials, $q_a(X) = (2N\nu)^{-1} \sum_{m \in Z^N} \delta(x - x_m) \int_{K_a} V(x + 2am)d^Nx$. (29)

Then for any pair of test functions $Y(X) \in F_2, \Psi(X) \in F_2$ and the restrictions $\psi^{(a)}(X), \psi^{(a)}$ onto the graph $\Gamma_a$ the following weak approximation property is valid when $a \rightarrow 0$:

\[
|\langle HY, \Psi \rangle_{L_2(R^N)} - \langle L^{(a)}u^{(a)}, \psi^{(a)} \rangle_{\mathcal{H}_a}| \leq \mathcal{C}a^{1/4} \|Y\|_{W_2^1(R^N)} \|\Psi\|_{W_2^1(R^N)}.
\]

**Proof:** First let us notice that the choice of the (generalized) potential $q_a(x)$ is not unique; however, the one given leads to an essential simplification.

The comparison of the bilinear forms of the differential operator parts $\Delta$ and $L^{(a)}$ was done in Lemma 3. It remains to compare the parts which contain the potentials. Using Taylor expansions for the test functions $Y$ and $\Psi$, we have for instance,

\[
Y(x, m) = \nu^{(a)}(2am) + \frac{2}{\nu^{(a)}(2am)} \sum_{n=1}^{2} \sum_{\nu=1}^{n} \frac{\partial^n Y(x, m)}{n!} \frac{x^\nu}{n!} + O(\omega_m^\nu Y(2a)).
\]

where the symbolic notations for a high-order differential are used. Therefore we may obtain the approximate formula for the bilinear term with the potential

\[
\langle HY, \Psi \rangle_{L_2(R^N)} = \sum_{m \in Z^N} \int_{K_a} V(x + 2am)Y(x + 2am)\Psi(x + m)d^Nx
\]

\[
= \sum_{m \in Z^N} \langle \nu^{(a)}(2am), \psi^{(a)} \rangle(2am) \int_{K_a} V(x + m)d^Nx + a^{1/4} \|Y\|_{W_2^1(R^N)} \|\Psi\|_{W_2^1(R^N)}.
\]

Due to the continuity of the restrictions $\nu, \psi$ we may approximate the potential $V(X)$ by the combination $q_a(X)$ of delta functions on the lattice $\Gamma_a$ attached to the points $2am$ [see Eq. (29)]. Using the bracket notations for functionals on continuous functions we have
\[ u^{(a)}(2am) \overline{u^{(a)}}(2am) = \int_{\Gamma_a} \delta(X-2am)u^{(a)}(X)\overline{u^{(a)}}(X)dX = \nu^{-1}\langle \delta(X-X_M)u^{(a)}(X),\overline{u^{(a)}}(X) \rangle_{\mathcal{H}_a}, \]

hence

\[ \langle V(X)Y,\Psi \rangle_{L_2(\mathbb{R}^N)} = \nu^{-1} \sum_{m \in \mathbb{Z}^N} \langle \delta(X-X_m)u^{(a)},\overline{u^{(a)}} \rangle_{\mathcal{H}_a} \int_{K_a} V(x+m)dX \]

\[ + O(a^{1/1+1/4}[\|Y\|_{L_2(\mathbb{R}^N)}][\|Y\|_{L_2(\mathbb{R}^N)}]) \]

\[ = \langle q_a(X)u^{(a)},\overline{u^{(a)}} \rangle_{\mathcal{H}_a} + O(a^{1/1+1/4}[\|Y\|_{L_2(\mathbb{R}^N)}][\|Y\|_{L_2(\mathbb{R}^N)}]). \quad (31) \]

Using Lemma 3 and Eq. (30) concludes the proof of the theorem.

We see now that the family of the operators \( L^{(a)} \) on the graphs \( \Gamma_a \) approximates in the weak sense the \( N \)-dimensional Schrödinger operator \( H \) when \( a \to 0 \). This result will now lead to the desired interpretation of the ‘‘weak commutativity’’ of the diagram (28).

**Definition 1:** The function \( \mathcal{U} \in \mathcal{F}_2 \) is called a weak solution of the equation

\[ -\Delta \mathcal{U} + V \mathcal{U} = \lambda \mathcal{U} + F, \quad F \in \mathcal{F}, \quad (32) \]

if for all test-functions \( \Psi \in \mathcal{F}_0 \) the following equation holds:

\[ \langle (-\Delta + V - \lambda)\mathcal{U},\Psi \rangle_{L_2(\mathbb{R}^N)} = \langle F,\Psi \rangle_{L_2(\mathbb{R}^N)}. \]

**Definition 2:** The function \( u \in W_2^1(\Gamma_a) \) is called a weak solution of the equation solution,

\[ L_0^{(a)}u + q_au = \lambda u + f, \quad (33) \]

if for all restrictions \( \psi \) of the test-functions \( \Psi \in \mathcal{F}_0 \) onto the lattice \( \Gamma_a \) the following equation holds:

\[ \langle (H_0^{(a)} + q - \lambda)u,\psi \rangle_{\mathcal{H}_a} = \langle f,\psi \rangle_{\mathcal{H}_a}, \]

for all functions \( \psi \in \mathcal{H}_a \).

The following theorem is valid.

**Theorem 3:** If \( \mathcal{U} \) is a weak solution of Eq. (32), then its restriction \( \mathcal{U}|_{\Gamma_a} \) to the graph \( \Gamma_a \) is approximated by a weak solution of Eq. (33) with \( f = F|_{\Gamma_a} \) in the following sense:

\[ \langle (L_0^{(a)} + q_\Gamma^{(a)})\mathcal{U}|_{\Gamma_a},\psi \rangle_{\mathcal{H}_a} - \langle F|_{\Gamma_a},\psi \rangle_{\mathcal{H}_a} \to 0, \quad \text{if} \quad a \to 0, \quad (34) \]

for any \( \psi \in \mathcal{H}_a \), where \( q_\Gamma(x) \) is given by Eq. (29).

**Proof:** The class \( \mathcal{F}_2 \) of test functions is dense in the space \( L_2(\mathbb{R}^N) \), therefore we can restrict our consideration to the case \( \mathcal{U} \in \mathcal{F}_2 \). Applying Theorem 2 we have

\[ \langle \mathcal{U},\Psi \rangle_{L_2(\mathbb{R}^N)} = \langle \mathcal{U}|_{\Gamma_a},\Psi|_{\Gamma_a} \rangle_{\mathcal{H}_a} + O(a^{1/1+1/4}[\|\mathcal{U}\|_{L_2(\mathbb{R}^N)}][\|\mathcal{U}\|_{L_2(\mathbb{R}^N)}]). \]

Following the pattern of the proof of Theorem 2 one can see that

\[ \langle \mathcal{U},\Psi \rangle_{L_2(\mathbb{R}^N)} = \langle \mathcal{U}|_{\Gamma_a},\Psi|_{\Gamma_a} \rangle_{\mathcal{H}_a} + O(a^{1/1+1/4}[\|\mathcal{U}\|_{L_2(\mathbb{R}^N)}][\|\mathcal{U}\|_{L_2(\mathbb{R}^N)}]); \]

\[ \langle F,\Psi \rangle_{L_2(\mathbb{R}^N)} = \langle F|_{\Gamma_a},\Psi|_{\Gamma_a} \rangle_{\mathcal{H}_a} + O(a^{1/1+1/4}[\|F\|_{L_2(\mathbb{R}^N)}][\|F\|_{L_2(\mathbb{R}^N)}]); \]
for any $\mathcal{U} \in \mathcal{F}_2, \Psi, F \in \mathcal{F}_0$. The function $\mathcal{U} \in \mathcal{F}_2 \subset \mathcal{F}_0$ is a weak solution of Eq. (32), and the restriction $\mathcal{F}_0|_{\Gamma_0}$ of the class $\mathcal{F}_0$ to the graph $\Gamma_0$ is dense in the space $\mathcal{H}_a$; therefore formula (34) is true.

The last statement confirms the “approximate commutativity” of diagram (28) in the weak sense when $a \to 0$, thus motivating the study of the operators $L^{(a)}$.

**B. Analysis of operators $L^{(a)}$**

Due to the specific (delta-functional) perturbation, the easiest way to investigate the operators $H^{(a)}$ is to use the Lippmann–Schwinger equation for the resolvents,

$$R(z) = R_0(z) - R_0(z) q_a R(z),$$  \hspace{1cm} (35)

where we omit index $a$ and use the notations

$$R_0(z) = (L_0^{(a)} - z)^{-1};$$

$$R(z) = (L^{(a)} - z)^{-1} = (L_0^{(a)} + q_a(X) - z)^{-1}. \hspace{1cm} (36)$$

The unperturbed resolvent $R_0(z)$ was constructed in Sec. II A through its kernel (the Green’s function) $G_0(x, y)$ [see Eq. (13)]. The case under consideration is given by $\gamma = 0$ (Kirchhoff's condition). In this case we see from Eq. (3) that the spectrum of the unperturbed operator $L_0^{(a)}$ being the union of spectra of fiber the operators $L_0^{(a)} P$, $P \in T^N$, is absolutely continuous and fills the positive semiaxis. Indeed, $-1 \leq (1/N) \sum_{j=1}^{N} \cos p_j \leq 1$ for all $P = \{p_j\}_{j=1}^{N} \in T^N$, and $(1/N) \sum_{j=1}^{N} \cos p_j$ takes all values in the interval $[-1, 1]$ when $P$ varies on $T^N$. Therefore, solutions $k$ of Eq. (3) in case $\gamma = 0$ fill the whole real axis after integration over $T^N$, and the spectrum $\sigma_0 \ni \lambda = k^2$ of the operator $L_0^{(a)}$ fills the positive semiaxis.

The kernel of the unperturbed resolvent (the Green’s function) constructed in Sec. II A has a tensor structure. We denote its tensor elements as $R_{m,n}^{(0)j'}(x, x', z)$. $1 \leq j, j' \leq N$, $m, m' \in Z^N$. Tensor elements of the local perturbation $q_a(X)$ given by Eq. (29) are

$$q_{m,n}^{j,j'}(x, x') = \nu^{-2} V_m S_{mn} \delta_{jj'} \delta(x') \delta(x), \hspace{1cm} (37)$$

where

$$V_m = \int_{K_0} V(\tilde{X}, m) d^N\tilde{X}. \hspace{1cm} (38)$$

Therefore the Lippmann–Schwinger equation (35) for the tensor elements of the perturbed resolvent takes the form

$$R_{m,n}^{jj'}(x, x', z) = R_{m,n}^{(0)j'}(x, x', z) - \sum_{n \in Z^N} V_n \sum_{l=1}^{N} R_{m,n}^{(0)jl}(x, 0, z) R_{nl}^{jj'}(0, x', z), \hspace{1cm} (39)$$

which for $x = 0$ implies

$$R_{m,n}^{jj'}(0, x', z) = R_{m,n}^{(0)j'}(0, x', z) - \sum_{n \in Z^N} V_p \sum_{l=1}^{N} R_{m,n}^{(0)jl}(0, 0, z) R_{nl}^{jj'}(0, x', z). \hspace{1cm} (40)$$

Let us show that the elements $R^{(0)jl}_{mn}(0, 0, z)$ do not depend on $j, l$. Indeed, let $R^{(a)}_0(z) = (L_0^{(a)} P - z)^{-1}$ be the resolvent of the fiber operator $L^{(a)}_0 P$. Using the spectral decomposition a tensor element of its kernel can be constructed in terms of the eigenfunctions [see Eq. (13)]:
\[ r^{(0)ij}_{P}(x, x', z) = \sum_{n=-\infty}^{\infty} \frac{\Xi^{p}_{Nk^{2}_{n}(P)}(x) \Xi^{p}_{Nk^{2}_{n}(P)}(x')}{Nk^{2}_{n}(P) - z}, \]

where \( Nk^{2}_{n}(P) \) are the eigenvalues of the operator \( L^{(a)}_{P} \). One can check by straightforward calculations that in our case (\( \gamma = 0 \)) the eigenfunctions have the form

\[
\Xi^{p}_{Nk^{2}_{n}(P)}(x) = \begin{cases} 
(Na \nu)^{-1/2} [\cos k_{n}x + \alpha_{\pm}^{-} \sin k_{n}x], & -a \leq x < 0, \\
(Na \nu)^{-1/2} [\cos k_{n}x - \alpha_{\pm}^{+} \sin k_{n}x], & 0 < x \leq a,
\end{cases}
\]

(41)

where

\[
\alpha_{\pm}^{-} = \frac{e^{\pm ipl} - \cos 2k_{n}a}{\cos 2k_{n}a}.
\]

Using Eq. (41), we have

\[
r^{(0)ij}_{P}(0, 0, z) = \frac{1}{2 \nu \alpha (2 \pi)^{N}} \sum_{n=-\infty}^{\infty} \frac{1}{Nk^{2}_{n}(P) - z},
\]

where \( k_{n}(P) \) are the solutions of Eq. (3) with \( \gamma = 0 \). Therefore we can see for any \( j, l = 1, 2, \ldots, N \)

\[
A_{mn}(z) = R^{(0)ij}_{mn}(0, 0, z)
\]

\[
= \frac{1}{(2 \pi)^{N}} \int_{\mathcal{T}^{N}} e^{i(m - n \mathbf{P}) \mathbf{d} \mathbf{N}}
\]

\[
= \frac{1}{2 \nu \alpha (2 \pi)^{N}} \int_{\mathcal{T}^{N}} e^{i(m - n \mathbf{P})} \sum_{n=-\infty}^{\infty} \frac{d^{N} \Theta}{Nk^{2}_{n}(\Theta) - z}.
\]

(42)

From Eqs. (39), (40), (42) we have

\[
R^{ij}_{mm'}(0, x', z) = R^{(0)ij}_{mm'}(0, x', z) - \sum_{n \in \mathbb{Z}^{N}} A_{mn}(z) V_{n} \sum_{l=1}^{N} R^{ij}_{nm}(0, x', z).
\]

(43)

Summation over \( j = 1, 2, \ldots, N \) gives

\[
\sum_{j=1}^{N} R^{ij}_{mm'}(0, x', z) = \sum_{j=1}^{N} R^{(0)ij}_{mm'}(0, x', z) - N \sum_{n \in \mathbb{Z}^{N}} A_{mn}(z) V_{n} \sum_{j=1}^{N} R^{ij}_{nm}(0, x', z).
\]

(44)

One can also check that \( \sum_{j=1}^{N} R^{(0)ij}_{mm'}(0, x, z) \) does not depend on index \( l \). Indeed, using Eq. (13) we have

\[
\sum_{j=1}^{N} R^{(0)ij}_{mm'}(0, x, z) = \sum_{j=1}^{N} \int_{\mathcal{T}^{N}} d^{N} P e^{i(m - m' \mathbf{P})} \sum_{n=-\infty}^{\infty} \frac{\Xi^{p}_{Nk^{2}_{n}(P)}(0) \Xi^{p}_{Nk^{2}_{n}(P)}(x)}{Nk^{2}_{n}(P) - z}.
\]

Therefore, using Eq. (41) we get

\[
\sum_{j=1}^{N} R^{(0)ij}_{mm'}(0, x, z) = \frac{1}{\nu \alpha} \int_{\mathcal{T}^{N}} d^{N} P e^{i(m - m' \mathbf{P})} \sum_{n=-\infty}^{\infty} \frac{1}{Nk^{2}_{n}(P) - z} (\cos k_{n}(P)x + \alpha_{\pm}(P) \sin k_{n}(P)x).
\]
The only possible dependence on $l$ is given through the coefficients $\alpha_l^\pm$ defined in Eq. (41). Therefore, the only $l$-dependent contribution to the latter expression is given by

$$\frac{1}{\nu a} \int d^N P e^{z i p (e^{i (m-n').P})} \sum_{n=-\infty}^{\infty} \frac{\sin k_n(P)x}{N k_n^2(P)-z}.$$  

From Eq. (3) at $\gamma=0$ we see that $k_n^2(P)$ is invariant with respect to every permutation of indices $P=(p_1, p_2, \ldots, p_N) \rightarrow P'=(p_1, p_{i_1}, \ldots, p_{i_N})$. Therefore the same is true for the function $\sum_{n=-\infty}^{\infty} \sin k_n(P)x/Nk_n^2(P)-z$. Hence, the latter integral actually does not depend on $l$, and the same is true for $\sum_{j=1}^{N} R^{(0)j'}_{mm'}(0, x, z)$. Therefore we can introduce the notation

$$G^{(0)}_{mm'}(x, z) = \sum_{j=1}^{N} R^{(0)j'}_{mm'}(0, x, z),$$

and from Eq. (44) see that

$$G_{mm'}(x, z) = \sum_{j=1}^{N} R^{j'}_{mm'}(0, x, z)$$

does not depend on $l$ as well. Eq. (40) implies

$$G_{mm'}(x, z) = G^{(0)}_{mm'}(x, z) - N \sum_{n \in \mathbb{Z}^N} A_{nn'}(z) V_{n} G_{mm'}(x, z).$$  

Combining Eqs. (39), (40), (43), (44) we can express the tensor elements of the perturbed resolvent in terms of solutions of Eq. (45):

$$R^{j'}_{mm'}(x, x', z) = R^{(0)j'}_{mm'}(x, x', z) - \sum_{n \in \mathbb{Z}^N} V_{n} \sum_{l=1}^{N} R^{(0)l}_{mm'}(x, 0, z) \times \left( R^{(0)l'}_{mm'}(0, x', z) - \sum_{n' \in \mathbb{Z}^N} A_{nn'}(z) V_{n} G_{nn'}(x', z) \right).$$  

Therefore, the construction of the resolvent of the operator $L^{(a)}$ is reduced to the solution of the effective tensor equation (45). Let us notice that $x$ and $z$ play the role of parameters in this effective equation. We omit the parameter $x$ in the further notations and rewrite the effective equation (45) in the tensor form

$$G(z) = G^{(0)}(z) - N A(z) \hat{V} G,$$  

where tensor elements of the tensors $G(z)$, $G^{(0)}(z)$ and $A(z)$ are $G_{mm'}(x, z)$, $G^{(0)}_{mm'}(x, z)$ and $A_{mm'}(z)$, respectively; $\hat{V}$ stands for a diagonal tensor with the elements $V_m$.

We can formulate the above result in the form of the following.

**Lemma 4:** The tensor elements of the resolvent $R(Z) = (L^{(a)}_0+q(X)-z)^{-1}$ are given by Eq. (46), where the tensor $G(z)$ is the solution of the equation (47).

In order to study properties of the equation (47) we need the following technical result.

**Lemma 5:** The function

$$\tau_z(P) = \sum_{n=-\infty}^{\infty} \frac{1}{Nk_n^2(P)-z}$$

has bounded derivatives $\partial_{p_1}^{N} \ldots \partial_{p_N} \tau_z(P)$ on $T^N$ for all $z \in \mathbb{C}\setminus \mathbb{R}$. 


The function \(\text{Arccos}(m^6 z)\) can be bounded in the closed interval \((-1,1)\) for any \(z\in \mathbb{C}\setminus \mathbb{R}_{+}\) and can have poles of the order not higher than \(1-(\mu^2)^{N+1/2}\) in the points \(\mu=\pm 1\). However, due to the definition of function \(\mu(P)\) if \(\mu=\pm 1\) then \(p_j=\pm 1\) for all \(j=1,1,\ldots,d\), thus \(p_j=1\) for all \(j=1,2,\ldots,N\). Therefore the function \(\Pi^N_{j=1} \sin p_j\) has zeros of the order \((1-\mu^2)^N\) in these points. Consequently, the functions \([\partial^N\chi^N_z(\mu(P))/\partial \mu^n] \Pi^N_{j=1} \sin \theta_j\) are bounded in the closed interval \([-1,1]\) for any \(n\in \mathbb{Z}\) and \(\chi^N_z(\mu(P)) = O(n^2) (1+o(1))\).

One can also check that
\[
\frac{\partial^N \chi^N_z(\mu(P))}{\partial \mu^n} = O(n^2) (1+o(1)),
\]
when \( n \to \pm \infty \) for all \( P \in \mathbf{T}^N \), \( z \in \mathbf{C} \setminus \mathbf{R}_+ \). Hence the series (49) converges.

The following statement is true.

**Theorem 4:** For any potential \( V(X) \in L_2(\mathbf{R}^N) \cap C(\mathbf{R}^N) \) the operator \( A(z) \hat{V} \) is a Hilbert–Schmidt operator in the space \( L_2(\mathbf{Z}^N) \) for all \( z \in \mathbf{C} \setminus \mathbf{R}_+ \) if the tensor elements \( A_{mn}(z) \) are given by Eq. (42) and \( \hat{V} \) is the diagonal tensor with elements \( V_m = \int_{K_a} V(\hat{X}, m)d^N\hat{X}, \ m \in \mathbf{Z}^N \).

**Proof:** It suffices to prove that

\[
\sum_{m, n} |(A(z) \hat{V})_{mn}|^2 < \infty. \tag{52}
\]

We have

\[
\sum_{m, n} |(A(z) \hat{V})_{mn}|^2 = (Na(2\pi)^N)^{-2} \sum_{m, n} \left| \int_{\mathbf{T}^N} e^{i(m-n \cdot P)} \tau_z(P)d^N P \int_{K_a} V(\hat{X}, P)d^N \hat{X} \right|^2
\]

\[
= (Na(2\pi)^N)^{-2} \sum_{q} \left| \int_{\mathbf{T}^N} e^{i(q \cdot P)} \tau_z(P)d^N P \sum_{n} \int_{K_a} V(\hat{X}, n)d^N \hat{X} \right|^2. \tag{53}
\]

First, using the Hölder inequality we estimate

\[
\sum_{n} \left| \int_{K_a} V(\hat{X}, n)d^N \hat{X} \right|^2 \leq (2a)^N \sum_{n} |V(\hat{X}, n)|^2 d^N \hat{X}
\]

\[
= (2a)^N \int_{\mathbf{R}^N} |V(X)|^2 d^N X
\]

\[
= (2a)^N \|V(X)\|_{L_2(\mathbf{R}^N)}^2 < \infty. \tag{54}
\]

Next, using Lemma 5 we can integrate by parts and get the estimation

\[
\sum_{n} \left| \int_{\mathbf{T}^N} e^{i(n \cdot P)} \tau_z(P)d^N P \right|^2
\]

\[
= \int_{\mathbf{T}^N} \tau_z(P)d^N P + \sum_{n_1, n_2, \ldots, n_N \neq 0} \left| \frac{1}{\Pi_{j=1}^N n_j} \int_{0}^{2\pi} dp_1 \cdots \int_{0}^{2\pi} dp_N \partial_{n_1}^{P_1} \partial_{n_2}^{P_2} \cdots \partial_{n_N}^{P_N} \tau_z(P) \prod_{j=1}^N e^{-in_j P} \right|^2
\]

\[
\leq \int_{\mathbf{T}^N} \tau_z(P)d^N P + \left( \int_{\mathbf{T}^N} \partial_{n_1}^{P_1} \partial_{n_2}^{P_2} \cdots \partial_{n_N}^{P_N} \tau_z(P)|d^N P \right)^2 \sum_{n_1, n_2, \ldots, n_N \neq 0} \frac{1}{\Pi_{j=1}^N n_j^2}
\]

\[
= \int_{\mathbf{T}^N} \tau_z(P)d^N P + \left( \frac{\pi}{3} \right)^N \left( \int_{\mathbf{T}^N} \partial_{n_1}^{P_1} \partial_{n_2}^{P_2} \cdots \partial_{n_N}^{P_N} \tau_z(P)|d^N P \right)^2 < \infty. \tag{55}
\]

Combining Eqs. (53)–(55) and Lemma 5 we get the proof.

This theorem allows us to use iteration methods in order to find the solutions of Eq. (48) and construct the resolvent of the operator \( L^{(a)} \).

**C. Scattering matrix**

In order to discuss scattering for the pair of operators \( L^{(a)}_0 \) and \( L^{(a)} \) it is enough to impose the condition\(^28\)

\[
\left| \int_{\Omega_a} q(x + 2a m)dx \right| \leq \frac{C}{1 + |m|^{2+a}}, \ a > 0.
\]

By construction it is equivalent to the following condition on the potential \( V(X) \):
\[
\left| \int_{K_m} V(x + 2am) \, dx \right| \leq \frac{C}{1 + |m|^{2+\epsilon}}.
\]

Under this condition we will calculate the scattering matrix for the pair of operators \( L^{(a)}_0, L^{(a)} \).

We start with the equation for the \( T \)-matrix:

\[
T(z) = q_a - q_a R_0(z) T(z),
\]

which can be solved in the same manner as the Lippmann–Schwinger equation (35) for the resolvent. Indeed, substituting Eq. (29) into Eq. (56) we have for the tensor elements of the kernel of the \( T \)-matrix,

\[
T^{ij'}_{mm'}(x,x',z) = \nu^{-2} V_m \delta(x) C^{ij'}_{mm'}(x',z),
\]

where

\[
C^{ij'}_{mm'}(x,z) = \nu^{-2} \delta(x-x') \delta_{mm'} \delta_{jj'} - \sum_n \sum_l \int_0^a dy R^{(0)j'l}(0,y,z) T^{ij'}_{mm'}(y,x,z).
\]

Hence \( C^{ij'}_{mm'}(x,z) \) obeys the following equation:

\[
C^{ij'}_{mm'}(x,z) = \nu^{-2} \delta(x) \delta_{mm'} \delta_{jj'} - \sum_n \sum_l V_n R^{(0)j'l}(0,0,z) C^{ij'}_{mm'}(x,z).
\]

Using the fact that the coefficients \( R^{(0)j'l}(0,0,z) \) do not depend on indices \( j,l \), we denote

\[
J^{j'}_{mm'}(x,z) = \sum_{j=1}^{2N} C^{(0)j'l}(x,z)
\]

and get

\[
Q^{j'}_{mm'}(x,z) = \delta(x) \delta_{mm'} - N \sum_n A_{mm'} V_p Q^{j'}_{mm'}(x,z).
\]

This equation shows that \( J^{j'}_{mm'}(x,z) \) does not depend on the index \( l \). Therefore it can be omitted and we get the equation

\[
\sum_n (\delta_{mm'} + N A_{mm'} V_p) J^{j'}_{nn'}(x,z) = \nu^{-2} \delta(x) \delta_{mm'},
\]

or in tensor form,

\[
(I + N A(z) \hat{V}) J(x,z) = \nu^{-2} \delta(x) I.
\]

By Eqs. (56)–(60) tensor elements of the \( T \)-matrix can be expressed in terms of the solution of Eq. (62) as

\[
T^{ij'}_{mm'}(x,x',z) = \nu^{-2} \delta(x) \delta(x') V_m \left( \delta_{mm'} \delta_{jj'} - \sum_n A_{nn'}(z) V_n (I + N A(z) \hat{V})^{-1}_{nn'} \right) \delta_{mm'}.
\]

Introducing the notation
we can write down the latter formula as

\begin{equation}
\mathcal{D}(z) = A(z) \hat{V}(I + N A(z))^{-1},
\end{equation}

we can write down the latter formula as

\begin{equation} 
T_{i\j}^{m\n}(x,x',z) = \nu^{-2} \delta(x) \delta(x') V_{m}(\delta_{m\n} \delta_{ij} - D_{m\n}(z)).
\end{equation}

Knowing the kernel of the \( T \)-matrix we can construct the scattering matrix in the standard way. In order to construct the scattering matrix for a fixed energy, let us define the isoenergetic surface \( T_{\lambda} \subset T^{N} \) for any fixed energy \( \lambda > 0 \) as follows. The set of all possible quasimomenta \( P \) for the fixed energy \( \lambda \):

\begin{equation}
\mathcal{T}_{\lambda} = \{ P \in T^{N}; \mu(P) = \cos 2a \sqrt{\lambda/N} \},
\end{equation}

where \( \mu(P) = (1/N) \sum_{j=1}^{N} \cos \phi_{j} \). Isoenergetic surfaces in case \( N=2 \) are shown in Fig. 2. Due to Eq. (3) with \( \gamma=0 \) for a fixed energy \( \lambda = Nk_{n}^{2}(P) \) we have \( \cos 2ak_{n}(P) = \mu(P) \). Let us fix some energy \( \lambda > 0 \) and suppose that \( P, P' \in T_{\lambda} \). The corresponding unit vectors are denoted by \( \hat{P}, \hat{P}' \).
The corresponding wave functions of the unperturbed Hamiltonian $L_0^{(a)}$ given by Eq. (23) we denote by $\Xi^\ell_{\lambda}, \Xi^{\ell'}_{\lambda}$. We can calculate the kernel of the scattering operator in the unperturbed representation as

$$S_{\lambda}(P,P') = \delta(\hat{P} - \hat{P}') - 2\pi i \langle T(\lambda + i0) \Xi^\ell_{\lambda}, \Xi^{\ell'}_{\lambda} \rangle_{H_\lambda}.$$

For fixed energy $\lambda = Nk_n^2(P)$ we can write

$$S_{nn'}(P,P') = \delta_{nn'} \left[ \delta(\hat{P} - \hat{P}') - 2\pi i \delta(\mu(P) - \mu(P')) \right] \frac{2\pi i}{a\nu} \sum_m V_m e^{-i(P-P',m)}$$

$$+ \frac{2\pi i N}{a\nu} \sum_m V_m e^{-i(P,m)} \sum_{mm'} D_{nn'm} \langle Nk_n^2(P) + i0 \rangle e^{i(P',m')} \right], \quad (65)$$

This leads to the following statement.

Theorem 5: Under the condition of the existence of the scattering matrix for the pair of operators $L_0^{(a)}, L_0^{(a)} + q_a$, its matrix elements $S_{nn'}(P,P')$ for fixed energy $\lambda = Nk_n^2(P)$ are given by the following formula:

$$S_{nn'}(P,P') = \delta_{nn'} \left[ \delta(\hat{P} - \hat{P}') - 2\pi i \delta(\mu(P) - \mu(P')) \right] \frac{2\pi i}{a\nu} \sum_m V_m e^{-i(P-P',m)}$$

$$+ \frac{2\pi i N}{a\nu} \sum_m V_m e^{-i(P,m)} \sum_{mm'} D_{nn'm} \langle Nk_n^2(P) + i0 \rangle e^{i(P',m')} \right], \quad (66)$$

where $D_{nn'm}(z)$ are the tensor elements of the tensor $D(z)$ given by Eq. (64).

The proof is obvious by substituting Eqs. (41), (64) into Eq. (65).

A natural question appears. Is the above constructed scattering matrix for the system on the graph $\Gamma_a$ related to the scattering matrix associated with the original $N$-dimensional Schrödinger dynamics? In order to clarify this question one has to construct the “representative” of the plane wave $e^{i(Q,X)}$; $Q,X \in \mathbb{R}^N$, on the graph $\Gamma_a$, observe its scattering under the evolution on $\Gamma_a$, and, finally, associate the resulting scattered waves in $\Gamma_a$ with scattered waves in $\mathbb{R}^N$.

We propose the following procedure. As the main aim in the description of scattering processes is to obtain the angular distribution of the scattered wave given the incoming plane wave, we have to establish a correspondence between the direction of the propagation of the plane wave $e^{i(Q,X)}$ and of its $\Gamma_a$-“representative.” In this context, the correspondence between the angle $\hat{Q} = Q/|Q|$ and the direction of the wave propagation in $\Gamma_a$ should be kept intact. The following steps meet this requirement.

1. Given the $\mathbb{R}^N$-plane wave $e^{i(Q,X)}$ we calculate the quasimomentum $P_Q = 2aQ \bmod 2\pi$.
2. We calculate the function $\mu(P_Q) = (1/N) \sum_{j=1}^N \cos(P_{Q,j}) = (1/N) \sum_{j=1}^N \cos 2aQ_j$.
3. Given the $\mathbb{R}^N$-dynamics energy $E = |Q|^2$, we introduce the value $\mu_Q = \cos 2aQ$. Then, for any quasimomentum $P \in T_Q$ on the isoenergetic surface $T_Q = \{P; \mu(P) = \mu_Q\}$ (see Fig. 3) we have the correspondence between the $\mathbb{R}^N$-energy and the $\Gamma_a$-energy.
4. We find the intersection point $\bar{P}_Q = \bar{T}_Q \cap \Lambda_Q$. The quasimomentum $\bar{P}_Q$ corresponds to the $\Gamma_a$-energy equal to $|Q|^2$ (because $\bar{P}_Q \in \bar{T}_Q$), if the number of the mode $n = :|Q|^2 = Nk^2_n(\bar{P}_Q)$ is chosen properly (see step 5). On the other hand, it corresponds to the same direction of the wave propagation as the $\mathbb{R}^N$-plane wave $e^{i(Q,X)}$ (because $\bar{T}_Q \in \Lambda_Q$).
(5) Given the $\mathbb{R}^N$-dynamics energy $E = |Q|^2$, we calculate the number of the mode of the corresponding wave function in $\Gamma_a$:

$$n_Q = \left\lfloor \frac{2a}{\pi |Q|} \right\rfloor .$$

(6) We take the corresponding eigenfunction $\Xi_{Nk_n^2}^P(x)$ of the fiber Hamiltonian $L_0^{(a)}\tilde{P}_Q$ and consider the function

$$\Xi_{Nk_n^2}^P(x)e^{i(m,\tilde{P}_Q)} ,$$

as the "representative" of the $\mathbb{R}^N$-plane wave $e^{i(Q,X)}$ on the graph $\Gamma_a$. By construction, this wave propagates in the same direction as $e^{i(Q,X)}$ and has the same $\Gamma_a$-energy $Nk_n^2(\tilde{P}_Q) = |Q|^2$ as the $\mathbb{R}^N$-energy of the plane wave $e^{i(Q,X)}$.

(7) We consider the scattering of the wave (67) in the graph $\Gamma_a$:

$$S \Xi_{Nk_n^2}^P(x)e^{i(m,\tilde{P}_Q)} \rightarrow \int_{\tilde{T}_Q} S_{n_Q^2}^P(\tilde{P}_Q^\prime, \tilde{P}_Q) \Xi_{Nk_n^2}^P(x)e^{i(m,\tilde{P}_Q^\prime)} d\tilde{P}_Q^\prime .$$

The scattered wave thus obtained is a composition of the waves $\Xi_{Nk_n^2}^P(x)e^{i(m,\tilde{P}_Q^\prime)}$, $\tilde{P}_Q^\prime \in \tilde{T}_Q$ (see Fig. 3).
(8) For every $\vec{P}'_Q \in \mathcal{T}_Q$ we calculate the momentum $Q' = \vec{P}'_Q (\|Q\|/\|\vec{P}'_Q\|)$ (see Fig. 3) and construct the $\mathbb{R}^N$-plane wave $e^{i(Q',X)}$. It propagates in the same direction as the $\Gamma_a$-wave $\Xi_{Nk^n_{Q}}(x)e^{i(m,\vec{P}'_Q)}$ and has the energy $|Q'|^2 = |Q|^2$.

(9) We define the action of the approximate scattering matrix for the $\mathbb{R}^N$-dynamics as
\[
S_{a}^{approx} : e^{i(Q,X)} \rightarrow \int_{\mathcal{T}_Q} S_{a}^{n} e^{i(Q'Q')} e^{i(|Q'|^2 - |Q|^2)} d\vec{P}'_Q. \tag{68}
\]

This 9-step procedure is necessary. Indeed, a simple restriction of the plane wave $e^{i(Q,X)}$ to the graph $\Gamma_a$,

\[
e^{i(Q,X)}|_{\Gamma_a} = v_Q(x) e^{i2a(m,P_Q)}, \tag{69}
\]

where $P_Q = 2aQ (\text{mod } 2\pi)$, i.e., $(P_Q)_{l} = 2a(l)(\text{mod } 2\pi), \ l = 1,2,\ldots,N,$ and $v_Q(x) = e^{iQx}$, brings the following difficulty. Function (69) is associated with the quasimomentum $P_Q = 2aQ (\text{mod } 2\pi)$, but it corresponds to a wave packet containing components with different energies. Indeed, one can decompose the function $v_Q(x)$ defined on the fundamental subgraph $\Omega_a$ in terms of the eigenfunctions of the fiber Hamiltonian $L_0^{(a)}$:

\[
v_Q(x) = \sum_{n=0}^{\infty} c^n_{Q} \Xi_{Nk^n_{Q}}(x),
\]

where

\[
c^n_{Q} = (v_Q(x), \Xi_{Nk^n_{Q}})_{L^2(\Omega_a)},
\]

and Eq. (69) can be rewritten as

\[
e^{i(Q,X)}|_{\Gamma_a} = \sum_{n=0}^{\infty} c^n_{Q} \Xi_{Nk^n_{Q}}(x) e^{i2a(m,P_Q)}. \tag{70}
\]

This is a wave packet with the components all having the same quasimomentum $P_Q = 2aQ (\text{mod } 2\pi)$ but different energies $Nk^n_{Q}$. However, all these energies may be different from the energy $|Q|^2$ of the plane wave $e^{i(Q,X)}$ if the latter is considered in the frame of the original $N$-dimensional Schrödinger dynamics. Indeed, this energy equals

\[
|Q|^2 = \sum_{l=1}^{N} q_l^2, \tag{71}
\]

while the energies $Nk^n_{Q} \approx (\Theta_P)$ are determined by the equation

\[
\cos 2ak_n(P_Q) = \mu(P_Q) = \frac{1}{N} \sum_{l=1}^{N} \cos(P_Q)_l = \frac{1}{N} \sum_{l=1}^{N} \cos 2a(l),
\]

i.e.,

\[
Nk^n_{Q} = \frac{N}{4a} \left( (-1)^n \sum_{l=1}^{N} \cos 2a(l) + 2\pi \frac{n+1}{2} \right)^2. \tag{72}
\]

Obviously, the right hand sides of Eqs. (71) and (72) are different for almost all sets $\{q_l\}$. Therefore, if we have the same direction of the wave propagation in $\mathbb{R}^N$ and in $\Gamma_a$ [i.e., the quasimomentum $P = P_Q = 2aQ (\text{mod } 2\pi)$], we cannot, in the general case, have the corres-
dence of the energies. This is a manifestation of the fact that the relations between energy and momentum (quasimomentum) are not the same for the dynamics in $\mathbb{R}^N$ and in $\Gamma_a$. Therefore, if one takes the function (69) as the "representative" of the plane wave $e^{i(Q,X)}$, the scattering process in $\Gamma_a$ will not preserve the energy of the $\mathbb{R}^N$-dynamics. It makes it difficult to approximate in this way the $\mathbb{R}^N$-scattering process by the $\Gamma_a$-scattering process. This problem does not appear if one uses the 9-step procedure described above.

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