Relativistic Schrödinger Equation with a Scalar Potential

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Abstract

We discover that it is possible to write a Schrödinger equation for a relativistic point particle experiencing a scalar potential, and that if the potential is weak, the equation can be approximated with a series. We find a paradox that according to the equation the effect from the potential is non-local.

It is well known that one possible attempt to describe a relativistic quantum particle is the relativistic Schrödinger equation

$$i\hbar\partial_t\psi(t,\mathbf{x}) \;=\; \sqrt{(mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}\psi(t,\mathbf{x}),$$

although there seems to be a consensus that this equation should be rejected [1]. I myself believe that this relativistic Schrödinger equation is valid, and consequently I'm also interested in studying related ideas further. One obvious deficiency in this relativistic Schrödinger equation is that it only describes non-interacting particles moving freely in three dimensional space. Eventually, in theoretical physics we are supposed to be interested in theories of interactions too. An obvious question arises that how should the relativistic Schrödinger equation be upgraded to handle interactions? There exists several different types of interactions in the world of physics, and it might be a good idea to not try to solve them all in a one swift move. We have to start from somewhere, and the simplest possible interaction perhaps is the interaction of a point particle with a background scalar field $U(t,\mathbf{x})$. When we say that the scalar field $U(t,\mathbf{x})$ is on the background, it means that we don't worry about why it is there or what has caused it. We just assume that this field is present for some outside reason. Then the question that we'll be interested in is that what happens to a particle whose motion is dictated by this background scalar field $U(t,\mathbf{x})$. The Hamiltonian for a non-relativistic particle that interacts with a potential $U(t,\mathbf{x})$ is well known to be.

$$H(t,\mathbf{x},\mathbf{p}) \;=\; \frac{\|\mathbf{p}\|^2}{2m} \;+\; U(t,\mathbf{x}). \tag{1}$$

In a non-relativistic setting we are usually not concerned about the transformation properties of $U(t,\mathbf{x})$, but let's now emphasize that we assume

$U(t,\mathbf{x})$ to be pointwisely scalar. For the relativistic theory we replace the Hamiltonian (1) with a new Hamiltonian

$$H(t,\mathbf{x},\mathbf{p}) \;=\; \sqrt{(U(t,\mathbf{x})+mc^2)^2+c^2\|\mathbf{p}\|^2}. \tag{2}$$

Most people who see this for the first time are probably puzzled by the potential term $U(t,\mathbf{x})$ being under the square root and the square operations besides the mass term. One observation that should be made is that if we calculate the Taylor series of this Hamiltonian with respect to the quantity $\frac{1}{c^2}$, and then ignore all the terms proportional to $\frac{1}{c^2},\frac{1}{c^4},\frac{1}{c^6},\ldots$, and also ignore the mass term mc^2, what remains is the non-relativistic Hamiltonian (1), so on the face of it this Hamiltonian (2) isn't entirely out of question. Hamiltonian equations of motion implied by (2) are

$$\dot{\mathbf{x}}(t) \;=\; \nabla_{\mathbf{p}}H(t,\mathbf{x}(t),\mathbf{p}(t)) \;=\; \frac{c^2\mathbf{p}(t)}{\sqrt{(U(t,\mathbf{x}(t))+mc^2)^2+c^2\|\mathbf{p}(t)\|^2}}$$

and

$$\begin{aligned}\dot{\mathbf{p}}(t) &= -\nabla_{\mathbf{x}}H(t,\mathbf{x}(t),\mathbf{p}(t))\\ &= -\frac{U(t,\mathbf{x}(t))+mc^2}{\sqrt{(U(t,\mathbf{x}(t))+mc^2)^2+c^2\|\mathbf{p}(t)\|^2}}\nabla_{\mathbf{x}}U(t,\mathbf{x}(t)).\end{aligned}$$

We encounter a challenge that it's not immediately obvious whether these equations of motion are Lorentz invariant. It is possible to show that these equation of motion are equivalent with the equation

$$D_\tau p^\mu(t(\tau)) \;=\; \partial^\mu U\big(t(\tau),\mathbf{x}(t(\tau))\big).$$

Here τ is the proper time experienced by the particle, and $p^\mu(t)$ is a quantity defined as

$$p^\mu(t) \;=\; \Big(\frac{\frac{1}{c}U(t,\mathbf{x}(t))+mc}{\sqrt{1-\frac{\|\dot{\mathbf{x}}(t)\|^2}{c^2}}},\;\frac{\big(\frac{1}{c^2}U(t,\mathbf{x}(t))+m\big)\dot{\mathbf{x}}(t)}{\sqrt{1-\frac{\|\dot{\mathbf{x}}(t)\|^2}{c^2}}}\Big)^\mu.$$

This $p^\mu(t)$ is not exactly the same as an ordinary four-momentum, but since we have assumed that $U(t,\mathbf{x})$ is a scalar, we see that our $p^\mu(t)$ transforms as a four-vector. This means that the equation $D_\tau p^\mu = \partial^\mu U$ is a kind of equation that can easily be seen to be Lorentz invariant. If one fact is that the Hamiltonian equations of motion are equivalent with the equation $D_\tau p^\mu = \partial^\mu U$, and another fact is that the equation $D_\tau p^\mu = \partial^\mu U$ can be seen to be Lorentz invariant, we can deduce that the Hamiltonian equations of motion are Lorentz invariant too. We can then also conclude that the Hamiltonian function defined in Equation (2) is fine.

Some people might be interested in a Hamiltonian

$$H(t,\mathbf{x},\mathbf{p}) \;=\; \sqrt{(mc^2)^2+c^2\|\mathbf{p}\|^2} \;+\; U(t,\mathbf{x}). \tag{3}$$

The problem with this Hamiltonian is that if we assume $U(t, \mathbf{x})$ to be pointwisely scalar, then the Hamiltonian equations of motion implied by (3) are not Lorentz invariant.

This was a kind of thing that once the Hamiltonian (2) had been written down by someone, from there on it is a mechanical calculation to check that the time evolution implied by it is Lorentz invariant. After this lesson, people might still be interested to know that how did someone invent the Hamiltonian (2) in the first place? It is not obvious how attempts to modify the non-relativistic Hamiltonian (1) or attempts to fix the flawed Hamiltonian (3) would lead to (2) via some argument. There is no need to keep the origin of the Hamiltonian (2) secret, so we can go through the story here. One of the topics we are interested in in theoretical physics is a real scalar Klein-Gordon field. When studying a real scalar Klein-Gordon field, we learn that if it isn't interacting with anything, its dynamics are dictated by the Lagrangian density $\mathcal{L} = \frac{1}{2}((\partial_\mu\phi)(\partial^\mu\phi) - m^2\phi^2)$ [2]. (The parameter m here is different from the particle's mass used earlier.) Then, suppose that ρ^μ describes some mass or charge density, and that we want the Klein-Gordon field to interact with this mass or charge density. In Lagrangian formalism this interaction should be implemented by adding some interaction term to the Lagrangian. By experimenting with partial differential equations it is possible to discover that an interaction term $-\phi\rho^0$ is interesting. For example, it is possible to derive the famous Yukawa potential out of the Lagrangian density $\mathcal{L}$ and the interaction term $-\phi\rho^0$. However, there is a principle that Lagrangian density should always be pointwisely scalar, and the interaction term $-\phi\rho^0$ is not pointwisely scalar. Then a question arises that what is the simplest possible interaction term that is a scalar, and simultaneously resembles the old term $-\phi\rho^0$ as much as possible? The obvious answer is a new interaction term $-\phi\sqrt{\rho_\mu\rho^\mu}$. Then, suppose we have constructed a model where a collection of relativistic particles interact via a real scalar Klein-Gordon field and the interaction term $-\phi\sqrt{\rho_\mu\rho^\mu}$. Suppose we extract one of the particles as a subject of interest, and consider everything else as a background. When we substitute the four-current of the one particle with Dirac delta function into the interaction term $-\phi\sqrt{\rho_\mu\rho^\mu}$, and denote $U \propto \phi$, we find that the dynamics of the particle are dictated by a Lagrangian function

$$L(t, \mathbf{x}, \dot{\mathbf{x}}) \;=\; -\big(U(t, \mathbf{x}) + mc^2\big)\sqrt{1 - \frac{\|\dot{\mathbf{x}}\|^2}{c^2}}. \tag{4}$$

Again, if we calculate the Taylor series of this Lagrangian with respect to the quantity $\frac{1}{c^2}$, and then ignore all the terms proportional to $\frac{1}{c^2}, \frac{1}{c^4}, \frac{1}{c^6}, \ldots$, and also ignore the mass term mc^2, what remains is the well-known non-relativistic Lagrangian, so on the face of it this Lagrangian (4) isn't entirely out of question. If we solve the Hamiltonian that is equivalent with the Lagrangian (4), the answer turns out to be the Hamiltonian (2).

The electric potential, often denoted as ϕ or A^0, is not pointwisely scalar, so the model we are now studying here should not be used to model electromagnetism.

One of the axioms of Quantum Mechanics is that the time evolution of a wave function is given by a generic Schrödinger equation

$$i\hbar\partial_t\psi(t,x) \;=\; H(t,M_x,-i\hbar\nabla_x)\psi(t,x).$$

Here $H(t,M_x,-i\hbar\nabla_x)$ is a Hamiltonian operator that has been obtained by substituting $x \leftarrow M_x$ and $p \leftarrow -i\hbar\nabla_x$ into a classical Hamiltonian function $H(t,x,p)$. For example, if we substitute $U(t,\mathbf{x}) \leftarrow M_U$ and $\mathbf{p} \leftarrow -i\hbar\nabla_{\mathbf{x}}$ into the non-relativistic Hamiltonian (1), we obtain the famous non-relativistic Schrödinger equation

$$i\hbar\partial_t\psi(t,\mathbf{x}) \;=\; \Big(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{x}} \;+\; M_U\Big)\psi(t,\mathbf{x}).$$

Here M_U means a multiplication operator defined as

$$(M_U\psi)(t,\mathbf{x}) \;=\; U(t,\mathbf{x})\psi(t,\mathbf{x}).$$

Next, suppose we are interested in a quantum mechanical description of a relativistic particle whose motion is dictated by some scalar potential U. People, who don't take Special Relativity seriously, might make the mistake of substituting $U(t,\mathbf{x}) \leftarrow M_U$ and $\mathbf{p} \leftarrow -i\hbar\nabla_{\mathbf{x}}$ into Equation (3). Here we are going to avoid this mistake, and do the substitutions into Equation (2) instead. This gives us the equation

$$i\hbar\partial_t\psi(t,\mathbf{x}) \;=\; \sqrt{(M_U + mc^2)^2 - c^2\hbar^2\nabla^2_{\mathbf{x}}}\psi(t,\mathbf{x}),$$

that can be called *the relativistic Schrödinger equation of a point particle in a scalar potential*. Then we encounter the challenge that it's not obvious what the operator $\sqrt{(M_U + mc^2)^2 - c^2\hbar^2\nabla^2_{\mathbf{x}}}$ means. The presence of the multiplication operator M_U has a consequence that this operator cannot be defined simply by Fourier transforms like pseudo-differential operators often can. If our intention is to define this new operator presicely, the only guess that one can possibly come up with is that we must use the diagonalization of the operator $(M_U+mc^2)^2 - c^2\hbar^2\nabla^2_{\mathbf{x}}$. Suppose we have discovered a large collection of wave functions $\psi_1,\psi_2,\psi_3,\ldots$ and eigenenergies $E_1,E_2,E_3,\ldots$ that work in a such way that if

$$\psi(\mathbf{x}) \;=\; \sum_{n=1}^{\infty}\psi_n(\mathbf{x}),$$

then

$$\big((M_U+mc^2)^2 - c^2\hbar^2\nabla^2_{\mathbf{x}}\big)\psi(\mathbf{x}) \;=\; \sum_{n=1}^{\infty}E_n\psi_n(\mathbf{x}).$$

Then the answer to the question that what does the operator $\sqrt{(M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}$ mean, is that it means this:

$$\sqrt{(M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}\psi(\mathbf{x}) \;=\; \sum_{n=1}^{\infty} \sqrt{E_n}\psi_n(\mathbf{x}).$$

Then an obvious question arises that what if the potential U is of such kind that we don't know how to diagonalize the operator $(M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2$? An answer is that then we are in trouble and we are not getting a definition for the operator $\sqrt{(M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}$. Based on this obstacle some people might criticize this operator as useless. If one fact is that the operator can only be defined via a diagonalization of another operator, and another fact is that usually we don't know how to solve the diagonalization, then don't these facts imply that nothing can be done with the new operator? An answer to these doubts is that we can still try to approximate the operator

$$\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}$$

by using an assumption that ε is small. Now it hopefully looks like that our objective has been set sufficiently low, and it may actually be possible to achieve it. However, trying to use the assumption that ε is small turns out to not be an easy task either. If somebody was already thinking about using the well known Taylor series

$$\sqrt{1+z} \;=\; 1 + \frac{1}{2}z - \frac{1}{8}z^2 + \frac{1}{16}z^3 - \cdots$$

that we learn in calculus, we'll have to inform him or her that that would have worked hypothetically only if the operators M_U and $\nabla_{\mathbf{x}}^2$ had been commuting. The fact that M_U and $\nabla_{\mathbf{x}}^2$ don't commute implies difficulties into the attempts to write a series with respect to ε.

Let's try to approach this approximation task by first studying simpler problems, and then making an attempt to slowly return to the relativistic Schrödinger equation with a scalar potential via small steps. Suppose that $A \in \mathbb{C}^{N\times N}$ and $B \in \mathbb{C}^{N\times N}$ are some noncommuting matrices with some $N \in \{2, 3, 4, \ldots\}$. How could we approximate $\sqrt{A + \varepsilon B}$ under the assumption that ε is small? If we try an ansatz

$$\sqrt{A + \varepsilon B} \;=\; \sqrt{A} \;+\; \varepsilon C_1 \;+\; \varepsilon^2 C_2 \;+\; \varepsilon^3 C_3 \;+\; \varepsilon^4 C_4 \;+\; \cdots,$$

and multiply both sides of this equation with themselves, we see that the ansatz works if the equations

$$\begin{aligned} B &= \sqrt{A}C_1 + C_1\sqrt{A} \\ 0 &= \sqrt{A}C_2 + C_1^2 + C_2\sqrt{A} \\ 0 &= \sqrt{A}C_3 + C_1C_2 + C_2C_1 + C_3\sqrt{A} \\ 0 &= \sqrt{A}C_4 + C_1C_3 + C_2^2 + C_3C_1 + C_4\sqrt{A} \\ &\vdots \end{aligned}$$

can be made true. If A is an arbitrary matrix, solving C_1 looks very difficult. Let's ease the problem by assuming that A is diagonal. This assumption makes solving C_1 a lot easier, and then the answer is

$$(C_1)_{n,m} = \frac{B_{n,m}}{\sqrt{A_{n,n}} + \sqrt{A_{m,m}}}.$$

Here we have to assume that the square roots of the eigenvalues of A are of such kind that they don't cause division by zero. Once we have learnt that C_1 could be solved like this, we see that the rest of the matrices $C_2, C_3, C_4, \ldots$ can be solved similarly with recursive formulas

$$\begin{aligned} (C_2)_{n,m} &= -\frac{(C_1^2)_{n,m}}{\sqrt{A_{n,n}} + \sqrt{A_{m,m}}} \\ (C_3)_{n,m} &= -\frac{(C_1C_2)_{n,m} + (C_2C_1)_{n,m}}{\sqrt{A_{n,n}} + \sqrt{A_{m,m}}} \\ (C_4)_{n,m} &= -\frac{(C_1C_3)_{n,m} + (C_2^2)_{n,m} + (C_3C_1)_{n,m}}{\sqrt{A_{n,n}} + \sqrt{A_{m,m}}} \\ &\vdots \end{aligned}$$

Next, let's define a matrix $D^2 \in \mathbb{R}^{N\times N}$ by setting it as

$$D^2 = \begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 0 & 1 \\ 1 & -2 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 \\ 0 & 0 & 1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -2 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 1 & -2 \end{pmatrix}.$$

The intention is that we don't define matrix D at all, but instead only the matrix D^2 directly like this. Let's define a matrix $A \in \mathbb{R}^{N\times N}$ by setting it as

$$A = \mu I_{N\times N} - D^2,$$

where $\mu > 0$ is some positive constant. The reason for why we should be interested in A defined like this is that this A has some similarity with the operator $(mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2$. Let's define a matrix $B \in \mathbb{R}^{N\times N}$ by setting it as

$$B \;=\; \begin{pmatrix} B_1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & B_2 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & B_3 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & B_4 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & B_{N-1} & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & B_N \end{pmatrix},$$

where $B_n \in \mathbb{R}$ are some numbers for all $n \in \{1, 2, \ldots, N\}$. The reason for why we should be interested in B defined like this is that this B has some similarity with the operators M_U and $2mc^2 M_U + \varepsilon M_U^2$. If we learn how to approximate $\sqrt{A + \varepsilon B}$ with these A and B, the lesson could turn out to be useful for the approximation of the operator $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}$.

With these A and B we cannot use the above solved series for $\sqrt{A + \varepsilon B}$ directly, because now A isn't diagonal. If we diagonalize A, maybe we can then. Let's define a matrix $U \in \mathbb{C}^{N\times N}$ by setting it as

$$U_{n,m} \;=\; \frac{1}{\sqrt{N}} e^{-\frac{2\pi i(n-1)(m-1)}{N}}$$

for all $n, m \in \{1, 2, 3, \ldots, N\}$. Now this U is a unitary matrix that defines a discrete Fourier transform [3]. Using the definitions of D^2 and U we can calculate that

$$(D^2 U^\dagger)_{n,m} \;=\; \frac{1}{\sqrt{N}}\big(e^{\frac{2\pi i(m-1)(n-2)}{N}} \;-\; 2e^{\frac{2\pi i(m-1)(n-1)}{N}} \;+\; e^{\frac{2\pi i(m-1)n}{N}}\big)$$

for all $n, m \in \{1, 2, \ldots, N\}$. Using this, we can next calculate

$$\begin{aligned} (UD^2U^\dagger)_{n,m} \;&=\; \sum_{n'=1}^{N} U_{n,n'}(D^2U^\dagger)_{n',m} \\ =\; & \frac{1}{N}\sum_{n'=1}^{N} e^{-\frac{2\pi i(n-1)(n'-1)}{N}}\big(e^{\frac{2\pi i(m-1)(n'-2)}{N}} \;-\; 2e^{\frac{2\pi i(m-1)(n'-1)}{N}} \;+\; e^{\frac{2\pi i(m-1)n'}{N}}\big) \\ =\; & \frac{1}{N}\Big(e^{-\frac{2\pi i(m-1)}{N}} \;-\; 2 \;+\; e^{\frac{2\pi i(m-1)}{N}}\Big)\sum_{n'=0}^{N-1} e^{\frac{2\pi i(m-n)n'}{N}} \\ =\; & 2\Big(\cos\Big(\frac{2\pi(m-1)}{N}\Big) \;-\; 1\Big)\delta_{n,m}. \end{aligned}$$

We see that U diagonalizes D^2. Since identity matrix remains as a diagonal matrix in any transform, U diagonalizes A too, and

$$(UAU^\dagger)_{n,m} \;=\; \Big(\mu \;+\; 2 \;-\; 2\cos\Big(\frac{2\pi(m-1)}{N}\Big)\Big)\delta_{n,m}.$$

Equation

$$B \;=\; \sqrt{A}C_1 \;+\; C_1\sqrt{A}$$

is equivalent with the equation

$$UBU^\dagger \;=\; (U\sqrt{A}U^\dagger)(UC_1U^\dagger) \;+\; (UC_1U^\dagger)(U\sqrt{A}U^\dagger).$$

It could be a good idea to spend few seconds thinking about whether the equation $(U\sqrt{A}U^\dagger)_{n,m} = \sqrt{(UAU^\dagger)_{n,m}}$ is true or not. We can assume that $\sqrt{A}$ has been defined in a such way that first we wrote A in terms of its eigenvectors and eigenvalues, and then we modified that representation by putting square roots on the eigenvalues. With this definition of $\sqrt{A}$ the answer is that the equation is true. This means that we can avoid using $\sqrt{A}$ in the solution formula for $UC_1U^\dagger$, and write it as

$$(UC_1U^\dagger)_{n,m} \;=\; \frac{(UBU^\dagger)_{n,m}}{\sqrt{(UAU^\dagger)_{n,n}} + \sqrt{(UAU^\dagger)_{m,m}}}.$$

This specifies C_1 too, and the solution formula for C_1 is

$$\begin{aligned}(C_1)_{n,m} \;&=\; \sum_{n',m'=1}^{N} (U^\dagger)_{n,n'} \frac{(UBU^\dagger)_{n',m'}}{\sqrt{(UAU^\dagger)_{n',n'}} + \sqrt{(UAU^\dagger)_{m',m'}}} U_{m',m} \\ &= \frac{1}{N^2} \sum_{n',m'=1}^{N} \frac{e^{\frac{2\pi i((n'-1)(n-1)-(m'-1)(m-1))}{N}} \sum\limits_{j=1}^{N} e^{\frac{2\pi i(m'-n')(j-1)}{N}} B_{j,j}}{\sqrt{\mu + 2 - 2\cos\big(\frac{2\pi(n'-1)}{N}\big)} + \sqrt{\mu + 2 - 2\cos\big(\frac{2\pi(m'-1)}{N}\big)}}.\end{aligned}$$

At one point we are eventually going to be interested in the limit $N \to \infty$. There is a problem that now the most significant Fourier modes are at the beginning $\{0, 1, 2, \ldots\}$ and at the end $\{\ldots, N-2, N-1\}$ of the index set, and we don't want half of the relevant Fourier modes to vanish in the limit $N \to \infty$. Let's assume that N is even, and use the formula

$$\begin{aligned}\sum_{n',m'=1}^{N} \;&=\; \sum_{n'=1}^{\frac{N}{2}} \sum_{m'=1}^{\frac{N}{2}} + \sum_{n'=1}^{\frac{N}{2}} \sum_{m'=\frac{N}{2}+1}^{N} + \sum_{n'=\frac{N}{2}+1}^{N} \sum_{m'=1}^{\frac{N}{2}} + \sum_{n'=\frac{N}{2}+1}^{N} \sum_{m'=\frac{N}{2}+1}^{N} \\ &= \sum_{n'=1}^{\frac{N}{2}} \sum_{m'=1}^{\frac{N}{2}} + \sum_{n'=1}^{\frac{N}{2}} \sum_{m'=-\frac{N}{2}+1}^{0} + \sum_{n'=-\frac{N}{2}+1}^{0} \sum_{m'=1}^{\frac{N}{2}} + \sum_{n'=-\frac{N}{2}+1}^{0} \sum_{m'=-\frac{N}{2}+1}^{0}\end{aligned}$$

to rearrange the sums into a form

$$\begin{aligned}&(C_1)_{n,m} \\ &= \frac{1}{N^2} \sum_{n',m'=-\frac{N}{2}+1}^{\frac{N}{2}} \frac{e^{\frac{2\pi i((n'-1)(n-1)-(m'-1)(m-1))}{N}} \sum\limits_{j=1}^{N} e^{\frac{2\pi i(m'-n')(j-1)}{N}} B_{j,j}}{\sqrt{\mu + 2 - 2\cos\big(\frac{2\pi(n'-1)}{N}\big)} + \sqrt{\mu + 2 - 2\cos\big(\frac{2\pi(m'-1)}{N}\big)}}.\end{aligned}$$

This way the most significant Fourier modes are at the center $\{\ldots,-2,-1,0,1,2,\ldots\}$ of the index set.

Let's start modifying this solution formula for C_1 into a direction where it can become more useful for infinite dimensional situations. Let $L>0$ be some parameter, whose purpose is to define intervals $[0,L]$ and $\big[-\frac{L}{2},\frac{L}{2}\big]$. Let's denote $\Delta x=\frac{L}{N}$, and let's replace the previous matrix A with a new matrix A by setting it as

$$A \;=\; \mu I_{N\times N} \;-\; \frac{1}{\Delta x^2}D^2.$$

The old eigenvalues get replaced with new eigenvalues

$$(UAU^\dagger)_{n,m} \;=\; \Big(\mu \;+\; \frac{1}{\Delta x^2}\Big(2 \;-\; 2\cos\Big(\frac{2\pi(m-1)}{N}\Big)\Big)\Big)\delta_{n,m}.$$

Then the previous matrix C_1 gets replaced with a new matrix C_1

$$(C_1)_{n,m} \;=\; \frac{1}{N^2}\sum_{n',m'=-\frac{N}{2}+1}^{\frac{N}{2}} \frac{e^{\frac{2\pi i((n'-1)(n-1)-(m'-1)(m-1))}{N}}\sum\limits_{j=1}^{N}e^{\frac{2\pi i(m'-n')(j-1)}{N}}B_{j,j}}{\sqrt{\mu+\frac{1}{\Delta x^2}\big(2-2\cos\big(\frac{2\pi(n'-1)}{N}\big)\big)}+\sqrt{\mu+\frac{1}{\Delta x^2}\big(2-2\cos\big(\frac{2\pi(m'-1)}{N}\big)\big)}}.$$

Let's define a new function $b:[0,L]\to\mathbb{R}$ by setting its values as $b(x')\approx B_{j,j}$, where $x'\approx\frac{jL}{N}$. We can then replace the sum with respect to j with an integral with respect to x', and we get an approximation

$$\begin{aligned}(C_1)_{n,m} \;&\approx\; \frac{1}{N^2}\sum_{n',m'=-\frac{N}{2}+1}^{\frac{N}{2}} \frac{e^{\frac{2\pi i((n'-1)(n-1)-(m'-1)(m-1))}{N}}\big(\frac{1}{\Delta x}\int\limits_0^L e^{\frac{2\pi i(m'-n')x'}{L}}b(x')dx'\big)}{\sqrt{\mu+\frac{1}{\Delta x^2}\big(2-2\cos\big(\frac{2\pi(n'-1)}{N}\big)\big)}+\sqrt{\mu+\frac{1}{\Delta x^2}\big(2-2\cos\big(\frac{2\pi(m'-1)}{N}\big)\big)}}\\ &\approx\; \frac{\Delta x}{L^2}\sum_{n',m'=-\frac{N}{2}+1}^{\frac{N}{2}} \frac{e^{\frac{2\pi i((n'-1)(n-1)-(m'-1)(m-1))}{N}}\int\limits_0^L e^{\frac{2\pi i(m'-n')x'}{L}}b(x')dx'}{\sqrt{\mu+\frac{1}{\Delta x^2}\big(2-2\cos\big(\frac{2\pi(n'-1)}{N}\big)\big)}+\sqrt{\mu+\frac{1}{\Delta x^2}\big(2-2\cos\big(\frac{2\pi(m'-1)}{N}\big)\big)}}.\end{aligned}$$

Taking the limit of the denominator looks easy. If we take limits $N \to \infty$ and $\Delta x \to 0$ in a such way that L remains constant, we get

$$\lim_{\substack{N\to\infty \\ \Delta x\to 0}} \frac{1}{\Delta x^2}\Big(2 \;-\; 2\cos\Big(\frac{2\pi(n'-1)}{N}\Big)\Big) \;=\; \frac{4\pi^2(n'-1)^2}{L^2}.$$

The limit of the numerator looks peculiar, because it seems to produce trivial e^0. We can solve this issue by denoting $x \approx \frac{nL}{N}$ and $y \approx \frac{mL}{N}$, and taking the limit $N \to \infty$ in a such way that x and y remain constant. It is approriate to simultaneously replace the notation $(C_1)_{n,m}$ with $c_1(x,y)$.

With these preparations the limit $N \to \infty$ gives us a formula

$$\lim_{N\to\infty} c_1(x,y) \;\approx\; \frac{\Delta x}{L^2} \sum_{n',m'=-\infty}^{\infty} \frac{e^{\frac{2\pi i((n'-1)x-(m'-1)y)}{L}} \int\limits_0^L e^{\frac{2\pi i(m'-n')x'}{L}} b(x')dx'}{\sqrt{\mu + \frac{4\pi^2(n'-1)^2}{L^2}} + \sqrt{\mu + \frac{4\pi^2(m'-1)^2}{L^2}}}$$

$$= \frac{\Delta x}{L^2} \sum_{n',m'=-\infty}^{\infty} \frac{e^{\frac{2\pi i(n'x-m'y)}{L}} \int\limits_0^L e^{\frac{2\pi i(m'-n')x'}{L}} b(x')dx'}{\sqrt{\mu + \frac{4\pi^2(n')^2}{L^2}} + \sqrt{\mu + \frac{4\pi^2(m')^2}{L^2}}}.$$

Strictly speaking, the limit should have been $\lim\limits_{N\to\infty} c_1(x,y) \;=\; 0$, because $\Delta x \to 0$, but we can probably agree that it makes sense to leave Δx in the limit expression like this. The quantity $c_1(x,y)$ was derived in a such way that when we use $c_1(x,y)$ as a matrix in a matrix multiplication, firstly we should be using ordinary sums where y gets summed over an infinite number of points. Then the factor Δx makes this sum turn into an integral, and Δx becomes the dx (or dy) symbol.

If we assume that our calculations don't have mistakes, next it would make sense to proceed into studying the limit $L \to \infty$. However, since it's not fully certain whether these ideas are still working after the limit $N \to \infty$, it might be a good idea so check how the new operator with fixed L seems to be working with some redundant calculation.

We should specify what convention we use for Fourier transforms of the functions of the form $f : [0,L] \to \mathbb{C}$. Let's decide that we use the convention

$$\hat{f}(k) \;=\; \frac{1}{L}\int\limits_0^L e^{-\frac{2\pi i k x}{L}} f(x)dx \qquad \text{and} \qquad f(x) \;=\; \sum_{k=-\infty}^{\infty} e^{\frac{2\pi i k x}{L}} \hat{f}(k).$$

The effects of the operators $\mu - D_x^2$ and $\sqrt{\mu - D_x^2}$ on a function $f : [0,L] \to \mathbb{C}$ can then be written as

$$(\mu - D_x^2)f(x) \;=\; \sum_{k=-\infty}^{\infty} \Big(\mu + \frac{4\pi^2 k^2}{L^2}\Big) e^{\frac{2\pi i k x}{L}} \hat{f}(k)$$

and

$$\sqrt{\mu - D_x^2} f(x) \;=\; \sum_{k=-\infty}^{\infty} \sqrt{\mu + \frac{4\pi^2 k^2}{L^2}}\, e^{\frac{2\pi i k x}{L}} \hat{f}(k).$$

Let's define an operator $\mathcal{B}$ with the formula

$$(\mathcal{B}f)(x) \;=\; b(x) f(x).$$

The question that we are now interested in is that do we now know how to approximate the operator $\sqrt{\mu - D_x^2 + \varepsilon\mathcal{B}}$? Let's define an operator $\mathcal{O}$ with the formula

$$\begin{aligned}(\mathcal{O}f)(x) \;&=\; \sqrt{\mu - D_x^2} f(x) \\ &+\; \frac{\varepsilon}{L^2} \int_0^L \Big(\sum_{n,m=-\infty}^{\infty} \frac{e^{\frac{2\pi i (nx - my)}{L}} \int_0^L e^{\frac{2\pi i (m-n) x'}{L}} b(x') dx'}{\sqrt{\mu + \frac{4\pi^2 n^2}{L^2}} + \sqrt{\mu + \frac{4\pi^2 m^2}{L^2}}} \Big) f(y) dy.\end{aligned}$$

Now we have a reason to hope that the approximation

$$\mathcal{O}^2 \;=\; \mu - D_x^2 \;+\; \varepsilon\mathcal{B} \;+\; O(\varepsilon^2)$$

should be true. Is it possible to verify this with some calculation? In attempt to keep our formulas under some control, for a moment, let's denote

$$r(n,m,x,y) \;=\; e^{\frac{2\pi i (nx - my)}{L}} \int_0^L e^{\frac{2\pi i (m-n) x'}{L}} b(x') dx'$$

and

$$s(n,m) \;=\; \sqrt{\mu + \frac{4\pi^2 n^2}{L^2}} + \sqrt{\mu + \frac{4\pi^2 m^2}{L^2}}.$$

Now the effect of the operator $\mathcal{O}$ can be written as

$$(\mathcal{O}f)(x) \;=\; \sqrt{\mu - D_x^2} f(x) \;+\; \frac{\varepsilon}{L^2} \int_0^L \sum_{n,m=-\infty}^{\infty} \frac{r(n,m,x,y)}{s(n,m)} f(y) dy.$$

The effect of the operator $\mathcal{O}^2$ is then

$$\begin{aligned}(\mathcal{O}^2 f)(x) \;&=\; (\mu - D_x^2) f(x) \\ &+\; \frac{\varepsilon}{L^2} \Big(\sqrt{\mu - D_x^2} \int_0^L \sum_{n,m=-\infty}^{\infty} \frac{r(n,m,x,y)}{s(n,m)} f(y) dy \\ &+\; \int_0^L \sum_{n,m=-\infty}^{\infty} \frac{r(n,m,x,y)}{s(n,m)} \sqrt{\mu - D_y^2} f(y) dy \Big) \;+\; O(\varepsilon^2).\end{aligned}$$

The latter term proportional to $\frac{\varepsilon}{L^2}$ can be written as

$$\begin{aligned}
&\int_0^L \sum_{n,m=-\infty}^{\infty} \frac{r(n,m,x,y)}{s(n,m)}\Big(\sum_{k=-\infty}^{\infty}\sqrt{\mu+\frac{4\pi^2k^2}{L^2}}\,e^{\frac{2\pi iky}{L}}\hat{f}(k)\Big)dy\\
&= \int_0^L \sum_{n,m=-\infty}^{\infty} \frac{r(n,m,x,y)}{s(n,m)}\Big(\sum_{k=-\infty}^{\infty}\sqrt{\mu+\frac{4\pi^2k^2}{L^2}}\,e^{\frac{2\pi iky}{L}}\Big(\frac{1}{L}\int_0^L e^{-\frac{2\pi ikx''}{L}}f(x'')dx''\Big)\Big)dy.
\end{aligned}$$

The former term proportional to $\frac{\varepsilon}{L^2}$ is trickier, and it might be a good idea to define some temporary Fourier coefficients as

$$\hat{a}(k) \;=\; \frac{1}{L}\int_0^L e^{-\frac{2\pi ikx''}{L}}\Big(\int_0^L \sum_{n,m=-\infty}^{\infty}\frac{r(n,m,x'',y)}{s(n,m)}f(y)dy\Big)dx'',$$

and then conclude that the former term can be written as

$$\begin{aligned}
&\sqrt{\mu-D_x^2}\int_0^L \sum_{n,m=-\infty}^{\infty}\frac{r(n,m,x,y)}{s(n,m)}f(y)dy\\
&= \sum_{k=-\infty}^{\infty}\sqrt{\mu+\frac{4\pi^2k^2}{L^2}}\,e^{\frac{2\pi ikx}{L}}\hat{a}(k)\\
&= \sum_{k=-\infty}^{\infty}\sqrt{\mu+\frac{4\pi^2k^2}{L^2}}\,e^{\frac{2\pi ikx}{L}}\Big(\frac{1}{L}\int_0^L e^{-\frac{2\pi ikx''}{L}}\Big(\int_0^L \sum_{n,m=-\infty}^{\infty}\frac{r(n,m,x'',y)}{s(n,m)}f(y)dy\Big)dx''\Big).
\end{aligned}$$

In both terms we used parameter x'' to define the Fourier transform that was needed for the implementation of the pseudo-differential operator. If we add the two terms, and take as much common factors as possible, we get

$$\begin{aligned}
&\frac{1}{L}\sum_{k,n,m=-\infty}^{\infty}\int_0^L dy\int_0^L dx''\,\sqrt{\mu+\frac{4\pi^2k^2}{L^2}}\,e^{-\frac{2\pi ikx''}{L}}\\
&\Big(e^{\frac{2\pi ikx}{L}}\frac{r(n,m,x'',y)}{s(n,m)}f(y)\;+\;e^{\frac{2\pi iky}{L}}\frac{r(n,m,x,y)}{s(n,m)}f(x'')\Big)\\
&= \frac{1}{L}\sum_{k,n,m=-\infty}^{\infty}\int_0^L dy\int_0^L dx''\,\sqrt{\mu+\frac{4\pi^2k^2}{L^2}}\,e^{-\frac{2\pi ikx''}{L}}\frac{e^{-\frac{2\pi imy}{L}}}{\sqrt{\mu+\frac{4\pi^2n^2}{L^2}}+\sqrt{\mu+\frac{4\pi^2m^2}{L^2}}}\\
&\Big(\int_0^L e^{\frac{2\pi i(m-n)x'}{L}}b(x')dx'\Big)\Big(e^{\frac{2\pi ikx}{L}}e^{\frac{2\pi inx''}{L}}f(y)\;+\;e^{\frac{2\pi iky}{L}}e^{\frac{2\pi inx}{L}}f(x'')\Big).
\end{aligned}$$

It is not obvious how the calculation should continue from here. At this point people who have some experience with Fourier analysis probably assume that the sums and integrals should be carried out in a such order that the new inner operation would produce some delta functions. However, now none of the just encountered sums or integrals can be used directly to produce any delta functions. Let's cancel the action of taking the common factors, and handle the two terms separately again for a moment. We keep the former term as it is, but in the latter term we swap the parameters x'' and y. If we take as much common factors as possible after this swap of parameters, we get

$$\frac{1}{L}\sum_{k,n,m=-\infty}^{\infty}\int_0^L dy\int_0^L dx''\,\frac{\sqrt{\mu+\frac{4\pi^2k^2}{L^2}}}{\sqrt{\mu+\frac{4\pi^2n^2}{L^2}}+\sqrt{\mu+\frac{4\pi^2m^2}{L^2}}}\Big(\int_0^L e^{\frac{2\pi i(m-n)x'}{L}}b(x')dx'\Big)$$
$$\Big(e^{-\frac{2\pi ikx''}{L}}e^{\frac{2\pi ikx}{L}}e^{\frac{2\pi i(nx''-my)}{L}}\;+\;e^{-\frac{2\pi iky}{L}}e^{\frac{2\pi ikx''}{L}}e^{\frac{2\pi i(nx-mx'')}{L}}\Big)f(y).$$

Now it is possible to integrate with respect to the parameter x'', and produce some Kronecker deltas with the formulas

$$\int_0^L e^{\frac{2\pi i(n-k)x''}{L}}dx''\;=\;L\delta_{n,k}\qquad\text{and}\qquad\int_0^L e^{\frac{2\pi i(k-m)x''}{L}}dx''\;=\;L\delta_{k,m}.$$

After this step, the expression starts to simplify trivially:

$$\sum_{k,m,n=-\infty}^{\infty}\int_0^L dy\frac{\sqrt{\mu+\frac{4\pi^2k^2}{L^2}}}{\sqrt{\mu+\frac{4\pi^2n^2}{L^2}}+\sqrt{\mu+\frac{4\pi^2m^2}{L^2}}}\Big(\int_0^L e^{\frac{2\pi i(m-n)x'}{L}}b(x')dx'\Big)$$
$$\Big(e^{\frac{2\pi ikx}{L}}e^{-\frac{2\pi imy}{L}}\delta_{n,k}\;+\;e^{-\frac{2\pi iky}{L}}e^{\frac{2\pi inx}{L}}\delta_{k,m}\Big)f(y)$$
$$=\;\sum_{m,n=-\infty}^{\infty}\int_0^L dy\;\frac{1}{\sqrt{\mu+\frac{4\pi^2n^2}{L^2}}+\sqrt{\mu+\frac{4\pi^2m^2}{L^2}}}\Big(\int_0^L e^{\frac{2\pi i(m-n)x'}{L}}b(x')dx'\Big)$$
$$\Big(e^{\frac{2\pi inx}{L}}e^{-\frac{2\pi imy}{L}}\sqrt{\mu+\frac{4\pi^2n^2}{L^2}}\;+\;e^{-\frac{2\pi imy}{L}}e^{\frac{2\pi inx}{L}}\sqrt{\mu+\frac{4\pi^2m^2}{L^2}}\Big)f(y)$$
$$=\;\sum_{m,n=-\infty}^{\infty}\int_0^L dy\;\Big(\int_0^L e^{\frac{2\pi i(m-n)x'}{L}}b(x')dx'\Big)e^{\frac{2\pi inx}{L}}e^{-\frac{2\pi imy}{L}}f(y)$$
$$=\;\int_0^L dy\int_0^L dx'\;\underbrace{\Big(\sum_{m=-\infty}^{\infty}e^{\frac{2\pi im(x'-y)}{L}}\Big)}_{=L\delta(x'-y)}\underbrace{\Big(\sum_{n=-\infty}^{\infty}e^{\frac{2\pi in(x-x')}{L}}\Big)}_{=L\delta(x-x')}b(x')f(y)$$
$$=\;L^2b(x)f(x)$$

From here we see that the relation $\mathcal{O}^2 = \mu - D_x^2 + \varepsilon\mathcal{B} + O(\varepsilon^2)$ is true. We can conclude that the relation

$$\mathcal{O} \;=\; \sqrt{\mu - D_x^2 \;+\; \varepsilon\mathcal{B}} \;+\; O(\varepsilon^2)$$

is true too, and we have now successfully approximated the operator $\sqrt{\mu - D_x^2 + \varepsilon\mathcal{B}}$. Having seen how the trick of swapping the parameters x'' and y was needed at one step, we now know that the calculation could be simplified a little bit. We could have decided in the beginning of the calculation that the effect of the operator $\mathcal{O}^2$ is

$$\begin{aligned}(\mathcal{O}^2 f)(x) \;&=\; (\mu - D_x^2)f(x)\\ &\quad+\; \frac{\varepsilon}{L^2}\Big(\sqrt{\mu - D_x^2}\int\limits_0^L \sum_{n,m=-\infty}^{\infty} \frac{r(n,m,x,y)}{s(n,m)} f(y)dy\\ &\qquad+\; \int\limits_0^L \sum_{n,m=-\infty}^{\infty} \frac{r(n,m,x,x'')}{s(n,m)} \sqrt{\mu - D_{x''}^2} f(x'')dx''\Big) \;+\; O(\varepsilon^2).\end{aligned}$$

In the former term we should use parameter x'' in the integral that defines the Fourier transform for the implementation of the pseudo-differential operator $\sqrt{\mu - D_x^2}$, and in the latter term we should use parameter y in the integral that defines the Fourier transform for the implementation of the pseudo-differential operator $\sqrt{\mu - D_{x''}^2}$. It would not have been possible to know in advance that these choices of notation lead to the smoothest possible calculation, but now we know this.

Let's start modifying this formula for $\sqrt{\mu - D_x^2 + \varepsilon\mathcal{B}}$ into a direction where it will become possible to study the limit $L \to \infty$. There is an issue that the relevant contributions to the Fourier integrals are now coming from the end points of the interval $[0, L]$. We don't want half of the relevant contributions to vanish in the limit $L \to \infty$, so we replace the previous input function f with a new input function of the form

$$f : \Big[-\frac{L}{2}, \frac{L}{2}\Big] \to \mathbb{C}.$$

Our convention for Fourier transforms will be

$$\hat{f}(k) \;=\; \frac{1}{L}\int\limits_{-\frac{L}{2}}^{\frac{L}{2}} e^{-\frac{2\pi i k x}{L}} f(x)dx \qquad \text{and} \qquad f(x) \;=\; \sum_{k=-\infty}^{\infty} e^{\frac{2\pi i k x}{L}} \hat{f}(k).$$

We assume that function b also is of the form

$$b : \Big[-\frac{L}{2}, \frac{L}{2}\Big] \to \mathbb{C},$$

and the operator $\mathcal{B}$ is again defined as $(\mathcal{B}f)(x) = b(x)f(x)$. We define an operator $\mathcal{O}$ with the formula

$$\begin{aligned}(\mathcal{O}f)(x) \;&=\; \sqrt{\mu - D_x^2}f(x) \\ &+\; \frac{\varepsilon}{L^2}\int\limits_{-\frac{L}{2}}^{\frac{L}{2}}\Big(\sum_{n,m=-\infty}^{\infty}\frac{e^{\frac{2\pi i(nx-my)}{L}}\int\limits_{-\frac{L}{2}}^{\frac{L}{2}} e^{\frac{2\pi i(m-n)x'}{L}}b(x')dx'}{\sqrt{\mu+\frac{4\pi^2n^2}{L^2}}+\sqrt{\mu+\frac{4\pi^2m^2}{L^2}}}\Big)f(y)dy.\end{aligned}$$

If we denote $\xi_1 \approx \frac{n}{L}$, $\xi_2 \approx \frac{m}{L}$ and $\Delta\xi = \frac{1}{L}$, the operator $\mathcal{O}$ can be expressed as being approximately

$$\begin{aligned}(\mathcal{O}f)(x) \;&\approx\; \sqrt{\mu - D_x^2}f(x) \\ &+\; \varepsilon\int\limits_{-\frac{L}{2}}^{\frac{L}{2}}\Big(\int\limits_{\mathbb{R}^2}d^2\xi\;\frac{e^{2\pi i(\xi_1x-\xi_2y)}\int\limits_{-\frac{L}{2}}^{\frac{L}{2}} e^{2\pi i(\xi_2-\xi_1)x'}b(x')dx'}{\sqrt{\mu+4\pi^2\xi_1^2}+\sqrt{\mu+4\pi^2\xi_2^2}}\Big)f(y)dy.\end{aligned}$$

The approximation should become precise in the limit $L \to \infty$, so by taking this limit we obtain a new operator

$$\begin{aligned}(\mathcal{O}f)(x) \;&=\; \sqrt{\mu - D_x^2}f(x) \\ &+\; \varepsilon\int\limits_{-\infty}^{\infty}\Big(\int\limits_{\mathbb{R}^2}d^2\xi\;\frac{e^{2\pi i(\xi_1x-\xi_2y)}\int\limits_{-\infty}^{\infty} e^{2\pi i(\xi_2-\xi_1)x'}b(x')dx'}{\sqrt{\mu+4\pi^2\xi_1^2}+\sqrt{\mu+4\pi^2\xi_2^2}}\Big)f(y)dy.\end{aligned}$$

Based on the way this operator looks we can tell that it the most apparently has something to do with the convention that $f : \mathbb{R} \to \mathbb{C}$ and its Fourier transform $\hat{f} : \mathbb{R} \to \mathbb{C}$ are related according to the relations

$$\hat{f}(\xi) \;=\; \int\limits_{-\infty}^{\infty} e^{-2\pi i\xi x}f(x)dx \qquad \text{and} \qquad f(x) \;=\; \int\limits_{-\infty}^{\infty} e^{2\pi i\xi x}\hat{f}(\xi)d\xi.$$

However, in Quantum Mechanics we usually prefer to use the convention

$$\hat{\psi}(k) \;=\; \int\limits_{-\infty}^{\infty} e^{-\frac{i}{\hbar}kx}\psi(x)dx \qquad \text{and} \qquad \psi(x) \;=\; \frac{1}{2\pi\hbar}\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}kx}\hat{\psi}(k)dk.$$

We should figure out how to modify the operator $\mathcal{O}$ so that it would become compatible with this convention from Quantum Mechanics. By denoting

$k_1 = 2\pi\xi_1$ and $k_2 = 2\pi\xi_2$ the previous operator can equivalently be expressed as

$$\begin{aligned}(\mathcal{O}f)(x) \;&=\; \sqrt{\mu - D_x^2}f(x)\\ &+\; \varepsilon\int\limits_{-\infty}^{\infty}\Big(\frac{1}{(2\pi)^2}\int\limits_{\mathbb{R}^2} d^2k\,\frac{e^{i(k_1x-k_2y)}\int\limits_{-\infty}^{\infty} e^{i(k_2-k_1)x'}b(x')dx'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2}}\Big)f(y)dy.\end{aligned}$$

We should make some further adjustment to get the Planck's constant right. Let's define a new scaled parameter $\mathcal{X} = \hbar x$, and new functions $\overline{f}$ and $\overline{b}$ according to the relations $\overline{f}(\mathcal{X}) = f(x)$ and $\overline{b}(\mathcal{X}) = b(x)$. The operator $\sqrt{\mu - D_x^2}$ is the same as $\sqrt{\mu - \hbar^2 D_{\mathcal{X}}^2}$, and the operator $\sqrt{\mu - D_x^2 + \varepsilon\mathcal{B}}$ is the same as $\sqrt{\mu - \hbar^2 D_{\mathcal{X}}^2 + \varepsilon\mathcal{B}}$. Therefore we can approximate this new operator with the same old formula, and with a change of integration variables according to relations $\mathcal{Y} = \hbar y$ and $\mathcal{X}' = \hbar x'$ the old formula can be transformed into the form

$$\begin{aligned}(\mathcal{O}\overline{f})(\mathcal{X}) \;&=\; \sqrt{\mu - \hbar^2 D_{\mathcal{X}}^2}\,\overline{f}(\mathcal{X})\\ &+\; \frac{\varepsilon}{(2\pi\hbar)^2}\int\limits_{-\infty}^{\infty}\Big(\int\limits_{\mathbb{R}^2} d^2k\,\frac{e^{\frac{i}{\hbar}(k_1\mathcal{X}-k_2\mathcal{Y})}\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_1)\mathcal{X}'}\overline{b}(\mathcal{X}')d\mathcal{X}'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2}}\Big)\overline{f}(\mathcal{Y})d\mathcal{Y}.\end{aligned}$$

We can then forget the old f and b, and carry out a new change of notation by removing the bars from the notations $\overline{f}$ and $\overline{b}$, and again restoring the ordinary looking parameters x, x' and y. Let's summarize the result we obtained after all these small steps: Firstly, we are interested in the operator $\sqrt{\mu - \hbar^2 D_x^2}$ that can be applied on wave functions of the form $\psi : \mathbb{R} \to \mathbb{C}$. This operator can be defined by the formula

$$\begin{aligned}\sqrt{\mu - \hbar^2 D_x^2}\psi(x) \;&=\; \frac{1}{2\pi\hbar}\int\limits_{-\infty}^{\infty}\sqrt{\mu + k^2}e^{\frac{i}{\hbar}kx}\hat{\psi}(k)dk\\ &=\; \frac{1}{2\pi\hbar}\int\limits_{-\infty}^{\infty}\sqrt{\mu + k^2}e^{\frac{i}{\hbar}kx}\Big(\int\limits_{-\infty}^{\infty} e^{-\frac{i}{\hbar}kx'}\psi(x')dx'\Big)dk.\end{aligned}$$

We assume that $b : \mathbb{R} \to \mathbb{R}$ is some function, and define an operator $\mathcal{B}$ by the formula $(\mathcal{B}\psi)(x) = b(x)\psi(x)$. Then we become interested in approximating the operator $\sqrt{\mu - \hbar^2 D_x^2 + \varepsilon\mathcal{B}}$. The answer to this is that if we define an operator $\mathcal{O}$ by the formula

$$\begin{aligned}(\mathcal{O}\psi)(x) \;&=\; \sqrt{\mu - \hbar^2 D_x^2}\psi(x) \\ &+\; \frac{\varepsilon}{(2\pi\hbar)^2}\int\limits_{-\infty}^{\infty}\Big(\int\limits_{\mathbb{R}^2} d^2k\; \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_1)x'}b(x')dx'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2}}\Big)\psi(y)dy,\end{aligned}$$

then the approximation $\mathcal{O} = \sqrt{\mu - \hbar^2 D_x^2 + \varepsilon\mathcal{B}} + O(\varepsilon^2)$ is true. Since we are human beings who sometimes do mistakes, it is not immediately fully certain whether this claim is true. We leave it as a voluntary exercise for the reader to check with a redundant calculation that if $\mathcal{O}$ is defined as above, then equation $\mathcal{O}^2 = \mu - \hbar^2 D_x^2 + \varepsilon\mathcal{B} + O(\varepsilon^2)$ is true. In order to survive this task the reader should remember the earlier lesson about how the parameters x'' and y should be used. With the correct choice of notation for the integration variables the calculation should work similarly as the earlier calculation we elaborated. The main difference turns out to be that the earlier Kronecker and Dirac delta formulas get replaced with the scaled Dirac delta formulas

$$\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k-k')x}dx \;=\; 2\pi\hbar\delta(k-k') \quad\text{and}\quad \int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}k(x-x')}dk \;=\; 2\pi\hbar\delta(x-x').$$

It is possible to formulate the operator $\mathcal{O}$ we are now speaking about in several different ways. One way is that we express the operator as

$$(\mathcal{O}\psi)(x) \;=\; \sqrt{\mu - \hbar^2 D_x^2}\psi(x) \;+\; \varepsilon\int\limits_{-\infty}^{\infty} c_1(x,y)\psi(y)dy,$$

where we denote

$$c_1(x,y) \;=\; \frac{1}{(2\pi\hbar)^2}\int\limits_{\mathbb{R}^2} d^2k\; \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_1)x'}b(x')dx'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2}}.$$

We can say both positive and negative about this way. A positive comment is that if somebody likes the way the matrix multiplication looks, then it's nice that we made this operation using $c_1(x,y)$ look like a generalization of the matrix multiplication. The negative side to the quantity $c_1(x,y)$ is that it's not obvious whether the integrals that define it converge. The quantities $\sqrt{\mu+k_1^2}$ and $\sqrt{\mu+k_2^2}$ in denominator make the integrand approach zero in the limits $k_1 \to \pm\infty$ and $k_2 \to \pm\infty$. This convergence to zero is so slow that it alone doesn't make the integrals converge absolutely. The integrand seems to have quite a lot of oscillation behavior to it, so maybe the integrals do converge after all. Eventually we are going to be interested in upgrading this one dimensional example situation into a three dimensional situation, where the denominator will have expressions $\sqrt{\mu + \|\mathbf{k}_1\|^2}$ and $\sqrt{\mu + \|\mathbf{k}_2\|^2}$, and the integrals will be over the space $\mathbb{R}^3$. In three dimensional situation the integrand's convergence to zero in the limits $\|\mathbf{k}_1\| \to \infty$ and $\|\mathbf{k}_2\| \to \infty$ is going to be so slow that the integrals will not be converging with certainty according to any reasonable standard. Since we can foresee some trouble in the three dimensional situation, we can conclude that already in the one dimensional situation the quantity $c_1(x,y)$ is slightly suspicious, and maybe at the edge of not making sense. It is also possible to express the operator $\mathcal{O}$ with a formula

$$\begin{aligned}(\mathcal{O}\psi)(x) \;&=\; \sqrt{\mu - \hbar^2 D_x^2}\psi(x) \\ &+\; \frac{\varepsilon}{(2\pi\hbar)^2}\int\limits_{-\infty}^{\infty}\Big(\int\limits_{-\infty}^{\infty}\frac{e^{\frac{i}{\hbar}k_1 x}\hat{b}(k_1 - k_2)}{\sqrt{\mu + k_1^2} + \sqrt{\mu + k_2^2}}dk_1\Big)\hat{\psi}(k_2)dk_2.\end{aligned}$$

Now the convergence looks a lot better. We can assume that the Fourier transforms $\hat{b}$ and $\hat{\psi}$ are well-defined. We can assume that $\hat{b}(k)$ converges to zero in the limits $k \to \pm\infty$ sufficiently fast to make the integral with respect to k_1 converge. We can assume that $\hat{\psi}(k)$ converges to zero in the limits $k \to \pm\infty$ sufficiently fast to make the integral with respect to k_2 converge. If the convergence of the integrals is important to someone, this latter careful ordering of the integrals is probably the right way. However, it is questionable whether the convergence is the most important thing at this point. Next, we are going to be interested in the task of generalizing the higher order terms of the matrix approximation into the infinite dimensional setting of interest, and in my opinion the most important thing will be to accomplish this efficiently with the smallest possible effort. So next we are going to ignore the convergence issues for a moment, but at the same time we should be keeping in mind that eventually we might want to reorder the intergals to make them converge.

Where did the expression

$$\sum_{j=1}^{N} e^{\frac{2\pi i(m'-n')(j-1)}{N}} B_{j,j}$$

come from into the matrix approximation? This was first

$$\sum_{j,j'=1}^{N} e^{-\frac{2\pi i(n'-1)(j-1)}{N}} B_{j,j'} e^{\frac{2\pi i(m'-1)(j'-1)}{N}},$$

but then this simplified, since B is diagonal. Suppose we don't like the formula $(\mathcal{B}\psi)(x) = b(x)\psi(x)$, and want to use the formula

$$(\mathcal{B}\psi)(x) \;=\; \int\limits_{-\infty}^{\infty} B(x,y')\psi(y')dy'$$

with some $B(x,y')$ instead. Is this possible? The answer is yes: We can put $B(x,y') = b(x)\delta(x-y')$. We can then interpret the expression

$$\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_1)x'}b(x')dx'$$

as originally having been

$$\int\limits_{-\infty}^{\infty} dx' \int\limits_{-\infty}^{\infty} dy'\; e^{-\frac{i}{\hbar}k_1x'}B(x',y')e^{\frac{i}{\hbar}k_2y'},$$

but then having simplified.

Let's think about this: Does there exist a simple "rule of thumb" that could be used turn the matrix

$$(C_1)_{n,m} \;=\; \frac{1}{N^2}\sum_{n',m'=1}^{N} \frac{e^{\frac{2\pi i((n'-1)(n-1)-(m'-1)(m-1))}{N}} \sum\limits_{j,j'=1}^{N} e^{-\frac{2\pi i(n'-1)(j-1)}{N}} B_{j,j'} e^{\frac{2\pi i(m'-1)(j'-1)}{N}}}{\sqrt{\mu+2-2\cos\left(\frac{2\pi(n'-1)}{N}\right)}+\sqrt{\mu+2-2\cos\left(\frac{2\pi(m'-1)}{N}\right)}}$$

into a quantity

$$c_1(x,y) \;=\; \frac{1}{(2\pi\hbar)^2}\int\limits_{\mathbb{R}^2} d^2k\; \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)} \int\limits_{-\infty}^{\infty} dx' \int\limits_{-\infty}^{\infty} dy'\; e^{-\frac{i}{\hbar}k_1x'}B(x',y')e^{\frac{i}{\hbar}k_2y'}}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2}}?$$

The two expressions obviously are very similar. How about we just carry out the substitutions

$$\frac{2\pi(n'-1)(n-1)}{N} \;\leftarrow\; \frac{k_1x}{\hbar}, \qquad \frac{2\pi(m'-1)(m-1)}{N} \;\leftarrow\; \frac{k_2y}{\hbar},$$

$$\frac{2\pi(n'-1)(j-1)}{N} \;\leftarrow\; \frac{k_1x'}{\hbar}, \qquad \frac{2\pi(m'-1)(j'-1)}{N} \;\leftarrow\; \frac{k_2y'}{\hbar},$$

$$\sqrt{\mu+2-2\cos\left(\frac{2\pi(n'-1)}{N}\right)} \;\leftarrow\; \sqrt{\mu+k_1^2},$$

$$\sqrt{\mu+2-2\cos\left(\frac{2\pi(m'-1)}{N}\right)} \;\leftarrow\; \sqrt{\mu+k_2^2},$$

$$\frac{1}{N^2}\sum_{n',m'=1}^{N} \leftarrow \frac{1}{(2\pi\hbar)^2}\int_{\mathbb{R}^2} d^2k, \qquad \sum_{j,j'=1}^{N} \leftarrow \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dy'$$

and

$$B_{j,j'} \leftarrow B(x',y')?$$

Let's decide that we want to approximate the operator $\sqrt{\mu - \hbar^2 D_x^2 + \varepsilon\mathcal{B}}$ with a series

$$\sqrt{\mu - \hbar^2 D_x^2 + \varepsilon\mathcal{B}} \;=\; \sqrt{\mu - \hbar^2 D_x^2} \;+\; \varepsilon\mathcal{C}_1 \;+\; \varepsilon^2\mathcal{C}_2 \;+\; \varepsilon^3\mathcal{C}_3 \;+\; \varepsilon^4\mathcal{C}_4 \;+\; \cdots,$$

and that for all $n \in \{1,2,3,\ldots\}$ we want to express the operator $\mathcal{C}_n$ as

$$(\mathcal{C}_n\psi)(x) \;=\; \int_{-\infty}^{\infty} c_n(x,y)\psi(y)dy.$$

The question that we are then interested in is that how do we solve the quantities $c_n(x,y)$?

The equation that determines C_2 is

$$0 \;=\; \sqrt{A}C_2 \;+\; C_1^2 \;+\; C_2\sqrt{A}.$$

This is equivalent with

$$0 \;=\; (U\sqrt{A}U^\dagger)(UC_2U^\dagger) \;+\; UC_1^2U^\dagger \;+\; (UC_2U^\dagger)(U\sqrt{A}U^\dagger).$$

We can solve C_2 to be

$$(C_2)_{n,m} \;=\; -\sum_{n',m'=1}^{N}(U^\dagger)_{n,n'}\frac{(UC_1^2U^\dagger)_{n',m'}}{\sqrt{(UAU^\dagger)_{n',n'}} + \sqrt{(UAU^\dagger)_{m',m'}}}U_{m',m}$$

$$= -\frac{1}{N^2}\sum_{n',m'=1}^{N}\frac{e^{\frac{2\pi i((n'-1)(n-1)-(m'-1)(m-1))}{N}}\sum\limits_{j,j'=1}^{N} e^{-\frac{2\pi i(n'-1)(j-1)}{N}}(C_1^2)_{j,j'}e^{\frac{2\pi i(m'-1)(j'-1)}{N}}}{\sqrt{\mu+2-2\cos\left(\frac{2\pi(n'-1)}{N}\right)} + \sqrt{\mu+2-2\cos\left(\frac{2\pi(m'-1)}{N}\right)}}.$$

We can apply the above decided rule of thumb to this matrix otherwise except the matrix B must be replaced with something new. The operator $\mathcal{C}_1^2$ can be expressed as

$$(\mathcal{C}_1^2\psi)(x) \;=\; \int_{-\infty}^{\infty}\Big(\int_{-\infty}^{\infty} c_1(x,y')c_1(y',y)dy'\Big)\psi(y)dy.$$

Therefore we augment our rule of thumb with a new substitution

$$(C_1^2)_{j,j'} \;\leftarrow\; \int_{-\infty}^{\infty} c_1(x',y'')c_1(y'',y')dy'',$$

and then we are ready to turn the matrix C_2 into the quantity $c_2(x,y)$ by setting it as

$$
\begin{aligned}
&c_2(x,y) \;=\\
&-\frac{1}{(2\pi\hbar)^2}\int\limits_{\mathbb{R}^2} d^2k\;\frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}\int\limits_{-\infty}^{\infty}dx'\int\limits_{-\infty}^{\infty}dy'\;e^{-\frac{i}{\hbar}k_1x'}\Big(\int\limits_{-\infty}^{\infty}c_1(x',y'')c_1(y'',y')dy''\Big)e^{\frac{i}{\hbar}k_2y'}}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2}}.
\end{aligned}
$$

The equation that determines C_3 is

$$
0 \;=\; \sqrt{A}C_3 \;+\; C_1C_2 \;+\; C_2C_1 \;+\; C_3\sqrt{A}.
$$

This is equivalent with

$$
0 \;=\; (U\sqrt{A}U^\dagger)(UC_3U^\dagger) \;+\; UC_1C_2U^\dagger \;+\; UC_2C_1U^\dagger \;+\; (UC_3U^\dagger)(U\sqrt{A}U^\dagger).
$$

We can solve C_3 to be

$$
\begin{aligned}
(C_3)_{n,m} \;&=\; -\sum_{n',m'=1}^{N}(U^\dagger)_{n,n'}\frac{(UC_1C_2U^\dagger)_{n',m'}+(UC_2C_1U^\dagger)_{n',m'}}{\sqrt{(UAU^\dagger)_{n',n'}}+\sqrt{(UAU^\dagger)_{m',m'}}}U_{m',m}\\
&=\; -\frac{1}{N^2}\sum_{n',m'=1}^{N}\frac{e^{\frac{2\pi i((n'-1)(n-1)-(m'-1)(m-1))}{N}}}{\sqrt{\mu+2-2\cos\left(\frac{2\pi(n'-1)}{N}\right)}+\sqrt{\mu+2-2\cos\left(\frac{2\pi(m'-1)}{N}\right)}}\Bigg(\\
&\qquad\sum_{j,j'=1}^{N}e^{-\frac{2\pi i(n'-1)(j-1)}{N}}\big((C_1C_2)_{j,j'}+(C_2C_1)_{j,j'}\big)e^{\frac{2\pi i(m'-1)(j'-1)}{N}}\Bigg).
\end{aligned}
$$

Our rule of thumb turns this into a quantity

$$
\begin{aligned}
c_3(x,y) \;&=\; -\frac{1}{(2\pi\hbar)^2}\int\limits_{\mathbb{R}^2} d^2k\;\frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2}}\Bigg(\int\limits_{-\infty}^{\infty}dx'\int\limits_{-\infty}^{\infty}dy'\\
&\qquad e^{-\frac{i}{\hbar}k_1x'}\Bigg(\int\limits_{-\infty}^{\infty}\big(c_1(x',y'')c_2(y'',y')+c_2(x',y'')c_1(y'',y')\big)dy''\Bigg)e^{\frac{i}{\hbar}k_2y'}\Bigg).
\end{aligned}
$$

The equation that determines C_4 is

$$
0 \;=\; \sqrt{A}C_4 \;+\; C_1C_3 \;+\; C_2^2 \;+\; C_3C_1 \;+\; C_4\sqrt{A}.
$$

This is equivalent with

$$
\begin{aligned}
0 \;=\;& (U\sqrt{A}U^\dagger)(UC_4U^\dagger) \;+\; UC_1C_3U^\dagger \;+\; UC_2^2U^\dagger \;+\; UC_3C_1U^\dagger\\
&+\; (UC_4U^\dagger)(U\sqrt{A}U^\dagger).
\end{aligned}
$$

We can solve C_4 to be

$$\begin{aligned}
&(C_4)_{n,m} \;= \\
&-\sum_{n',m'=1}^{N} (U^\dagger)_{n,n'} \frac{(UC_1C_3U^\dagger)_{n',m'} + (UC_2^2U^\dagger)_{n',m'} + (UC_3C_1U^\dagger)_{n',m'}}{\sqrt{(UAU^\dagger)_{n',n'}} + \sqrt{(UAU^\dagger)_{m',m'}}} U_{m',m} \\
&= -\frac{1}{N^2} \sum_{n',m'=1}^{N} \frac{e^{\frac{2\pi i((n'-1)(n-1)-(m'-1)(m-1))}{N}}}{\sqrt{\mu+2-2\cos\big(\frac{2\pi(n'-1)}{N}\big)} + \sqrt{\mu+2-2\cos\big(\frac{2\pi(m'-1)}{N}\big)}} \Big(\\
&\quad \sum_{j,j'=1}^{N} e^{-\frac{2\pi i(n'-1)(j-1)}{N}} \big((C_1C_3)_{j,j'} + (C_2^2)_{j,j'} + (C_3C_1)_{j,j'}\big) e^{\frac{2\pi i(m'-1)(j'-1)}{N}} \Big).
\end{aligned}$$

Our rule of thumb turns this into a quantity

$$\begin{aligned}
c_4(x,y) \;=\; & -\frac{1}{(2\pi\hbar)^2} \int\limits_{\mathbb{R}^2} d^2k \; \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2}} \Big(\int\limits_{-\infty}^{\infty} dx' \int\limits_{-\infty}^{\infty} dy' \\
& e^{-\frac{i}{\hbar}k_1x'} \Big(\int\limits_{-\infty}^{\infty} \big(c_1(x',y'')c_3(y'',y') + c_2(x',y'')c_2(y'',y') \\
& \qquad + c_3(x',y'')c_1(y'',y')\big) dy'' \Big) e^{\frac{i}{\hbar}k_2y'} \Big).
\end{aligned}$$

Next, we should start substituting the solved quantities $c_1, c_2, c_3, \ldots$ into the formulas of the succeeding quantities. Initially this produces a lot of integrals, but in each term three of the integrals can be carried out to produce a delta function, and the expressions simplify quite a bit. The formula for $c_2(x,y)$ simplifies into a form

$$\begin{aligned}
c_2(x,y) \;=\; & -\frac{1}{(2\pi\hbar)^3} \int\limits_{\mathbb{R}^3} d^3k \; \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2}} \\
& \cdot \frac{\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_3-k_1)x'} b(x') dx'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_3^2}} \cdot \frac{\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_3)x'} b(x') dx'}{\sqrt{\mu+k_3^2}+\sqrt{\mu+k_2^2}}.
\end{aligned}$$

The formula for $c_3(x,y)$ can be written in a form

$$\begin{aligned}
c_3(x,y) \;=\; & \frac{1}{(2\pi\hbar)^4}\int\limits_{\mathbb{R}^4} d^4k \, \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}}{(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2})(\sqrt{\mu+k_2^2}+\sqrt{\mu+k_4^2})} \\
& \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_4-k_1)x'}b(x')dx'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_4^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_3-k_4)x'}b(x')dx'}{\sqrt{\mu+k_4^2}+\sqrt{\mu+k_3^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_3)x'}b(x')dx'}{\sqrt{\mu+k_3^2}+\sqrt{\mu+k_2^2}} \\
+ & \frac{1}{(2\pi\hbar)^4}\int\limits_{\mathbb{R}^4} d^4k \, \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}}{(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2})(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_3^2})} \\
& \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_4-k_1)x'}b(x')dx'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_4^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_3-k_4)x'}b(x')dx'}{\sqrt{\mu+k_4^2}+\sqrt{\mu+k_3^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_3)x'}b(x')dx'}{\sqrt{\mu+k_3^2}+\sqrt{\mu+k_2^2}} .
\end{aligned}$$

The formula for $c_4(x,y)$ can be written in a form

$$\begin{aligned}
c_4(x,y) \;=\; & -\frac{1}{(2\pi\hbar)^5}\int\limits_{\mathbb{R}^5} d^5k \, \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}}{(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2})(\sqrt{\mu+k_4^2}+\sqrt{\mu+k_2^2})(\sqrt{\mu+k_5^2}+\sqrt{\mu+k_2^2})} \\
& \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_5-k_1)x'}b(x')dx'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_5^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_4-k_5)x'}b(x')dx'}{\sqrt{\mu+k_5^2}+\sqrt{\mu+k_4^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_3-k_4)x'}b(x')dx'}{\sqrt{\mu+k_4^2}+\sqrt{\mu+k_3^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_3)x'}b(x')dx'}{\sqrt{\mu+k_3^2}+\sqrt{\mu+k_2^2}} \\
- & \frac{1}{(2\pi\hbar)^5}\int\limits_{\mathbb{R}^5} d^5k \, \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}}{(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2})(\sqrt{\mu+k_5^2}+\sqrt{\mu+k_3^2})(\sqrt{\mu+k_5^2}+\sqrt{\mu+k_2^2})} \\
& \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_5-k_1)x'}b(x')dx'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_5^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_4-k_5)x'}b(x')dx'}{\sqrt{\mu+k_5^2}+\sqrt{\mu+k_4^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_3-k_4)x'}b(x')dx'}{\sqrt{\mu+k_4^2}+\sqrt{\mu+k_3^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_3)x'}b(x')dx'}{\sqrt{\mu+k_3^2}+\sqrt{\mu+k_2^2}} \\
- & \frac{1}{(2\pi\hbar)^5}\int\limits_{\mathbb{R}^5} d^5k \, \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}}{(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2})(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_4^2})(\sqrt{\mu+k_4^2}+\sqrt{\mu+k_2^2})} \\
& \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_5-k_1)x'}b(x')dx'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_5^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_4-k_5)x'}b(x')dx'}{\sqrt{\mu+k_5^2}+\sqrt{\mu+k_4^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_3-k_4)x'}b(x')dx'}{\sqrt{\mu+k_4^2}+\sqrt{\mu+k_3^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_3)x'}b(x')dx'}{\sqrt{\mu+k_3^2}+\sqrt{\mu+k_2^2}} \\
- & \frac{1}{(2\pi\hbar)^5}\int\limits_{\mathbb{R}^5} d^5k \, \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}}{(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2})(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_3^2})(\sqrt{\mu+k_3^2}+\sqrt{\mu+k_5^2})} \\
& \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_5-k_1)x'}b(x')dx'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_5^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_4-k_5)x'}b(x')dx'}{\sqrt{\mu+k_5^2}+\sqrt{\mu+k_4^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_3-k_4)x'}b(x')dx'}{\sqrt{\mu+k_4^2}+\sqrt{\mu+k_3^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_3)x'}b(x')dx'}{\sqrt{\mu+k_3^2}+\sqrt{\mu+k_2^2}} \\
- & \frac{1}{(2\pi\hbar)^5}\int\limits_{\mathbb{R}^5} d^5k \, \frac{e^{\frac{i}{\hbar}(k_1x-k_2y)}}{(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_2^2})(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_3^2})(\sqrt{\mu+k_1^2}+\sqrt{\mu+k_4^2})} \\
& \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_5-k_1)x'}b(x')dx'}{\sqrt{\mu+k_1^2}+\sqrt{\mu+k_5^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_4-k_5)x'}b(x')dx'}{\sqrt{\mu+k_5^2}+\sqrt{\mu+k_4^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_3-k_4)x'}b(x')dx'}{\sqrt{\mu+k_4^2}+\sqrt{\mu+k_3^2}} \cdot \frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_2-k_3)x'}b(x')dx'}{\sqrt{\mu+k_3^2}+\sqrt{\mu+k_2^2}} .
\end{aligned}$$

Although this formula for $c_4(x, y)$ is big in the sense that it has a lot of symbols in it, it also has some simplicity to it. Clearly, a small number of element types just get repeated multiple times, and the formula could be compressed quite a bit with some special notations. These formulas might remind some people about the stories about Feynman diagrams, and a question arises that could some kind of Feynman diagrams even be useful here? According to the standard story the Feynman diagrams are supposed to describe processes where particles get created and annihilated. Here we are interested in a model where there is only one particle and one fixed background potential, so we probably shouldn't be speaking about Feynman diagrams. Nevertheless, some graphical representation of the formulas for the quantities $c_1, c_2, c_3, \ldots$ could be useful. For example, suppose we are worried about there possibly being a mistake in some of these formulas. How could we detect it? One way is that if we succeed in drawing some kind of graphical representation of these formulas, we could then inspect the graphs and look whether they seem to have kind of symmetry that feels reasonable to expect. If something seemed to be out of place in the graphical representation, that would be a sign of a possible mistake in the formulas.

Since the quantity $c_n(x, y)$ is supposed to be used in a similar way as a matrix in a matrix multiplication, we can decide that the parameter y has something to do with an "input process", and the parameter x has something to do with an "output process". The parameter y does not appear in the quantity $c_n(x, y)$ in any other way except in the factor $e^{-\frac{i}{\hbar}k_2 y}$, and the parameter x does not appear in the quantity $c_n(x, y)$ in any other way except in the factor $e^{\frac{i}{\hbar}k_1 x}$. Therefore we can decide that k_2 has something to do with an "input process", and that k_1 has something to do with an "output process". Let's start drawing figures of the terms in these quantities by turning k_2 into an arrow that points into the picture, by turning k_1 into an arrow that points out of the picture, and by turning the other parameters $k_3, k_4, k_5, \ldots$ into dots that are somewhere between.

The expression that gets the most repeated in the formulas for $c_1, c_2, c_3, \ldots$ is

$$\frac{\int\limits_{-\infty}^{\infty} e^{\frac{i}{\hbar}(k_j - k_{j'})x'} b(x') dx'}{\sqrt{\mu + k_{j'}^2} + \sqrt{\mu + k_j^2}}.$$

Since this expression depends on two indices j and j', and we just decided how to draw these two indices into a picture, we could decide that every occurence of this expression becomes a solid straight line between the two objects symbolizing j and j'. In other words, this expression is either a solid line between two dots, or a solid line between an arrow and a dot, or a solid line between the two arrows. In this expression the order of the indices j and j' matters, so we should augment the solid line with some direction symbol.

Let's put a triangle on the line so that it is like an arrow that points from j to j'.

Also the expression

$$\frac{1}{\sqrt{\mu + k_{j'}^2} + \sqrt{\mu + k_j^2}}$$

appears in the formulas without the integral in the numerator. Since this expression also depends on two indices j and j', it would be reasonable to make every occurence of this expression into some kind of connection too. We cannot use a solid line for this anymore, so let's turn this expression into a dashed curve between the two objects symbolizing j and j'. This expression is symmetric with respect to j and j', so the dashed line should not indicate direction in any way.

If we draw the arrows, dots, solid lines with triangles, and dashed curves as just decided, we obtain a picture shown in Figure 1. The picture seems to have a kind of symmetry that feels reasonable to expect. Regrettably, it is not immediately obvious how the graph series in Figure 1 could be extrapolated.

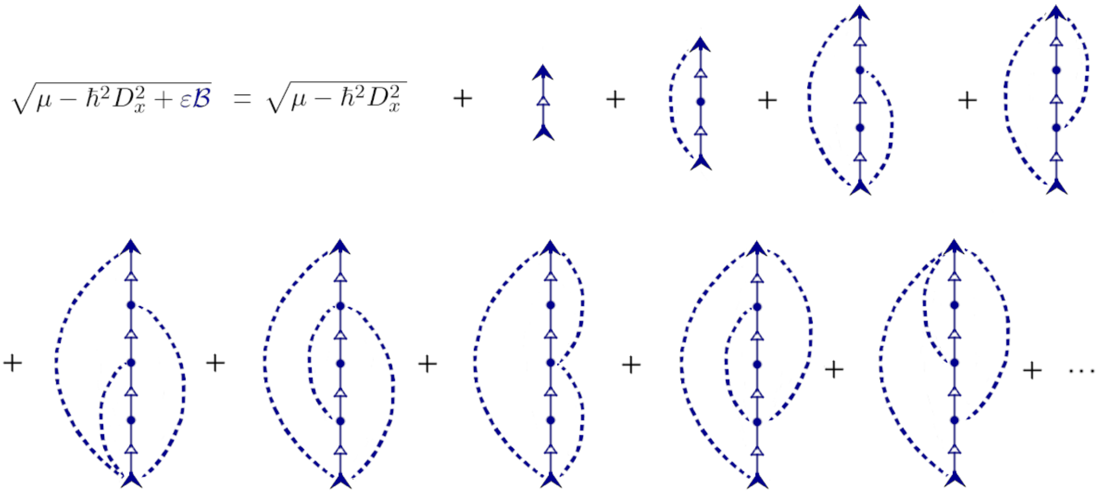

Figure 1: A graphical representation of the series approximation of the operator $\sqrt{\mu - \hbar^2 D_x^2 + \varepsilon \mathcal{B}}$. The way in which the arrows and dots are connected is based on the formulas for the quantities $c_1(x,y)$, $c_2(x,y)$, $c_3(x,y)$ and $c_4(x,y)$.

At this point it probably feels reasonable to consider a notation change, where we replace k_2 with k_{in}, k_1 with k_{out}, and carry out a translation of indices that turns the sequence $k_3, k_4, k_5, \ldots$ into a sequence $k_1, k_2, k_3, \ldots$. It would have required some skill to foresee this as a smart notation choice in the early stages of the calculation, but once the graphical representation has been drawn, this has become more obvious. I'll leave the already solved formulas for $c_1, c_2, c_3, \ldots$ the way they are, but let's do this notation change for the next step, where we move onto studying the operator $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla^2_{\mathbf{x}}}$.

Let's think about upgrading our series result into three dimensions. How could we accomplish this? We already know how Fourier transforms look in three dimensions, so we can make some obvious guesses based on this. We replace the one dimensional parameters $x', k_1, k_2, \ldots \in \mathbb{R}$ with three dimensional parameters $\mathbf{x}', \mathbf{k}_1, \mathbf{k}_2, \ldots \in \mathbb{R}^3$, the products $x'k_1$ with inner products $\mathbf{x}' \cdot \mathbf{k}_1$, and the squares k_1^2 with squares of the norms $\|\mathbf{k}_1\|^2$. We replace every occurence of the factor $2\pi\hbar$ with a factor $(2\pi\hbar)^3$. Here we should carefully notice that with an index j the relations $\mathbf{k}_j \notin \mathbb{R}$, $\mathbf{k}_j \in \mathbb{R}^3$, $(\mathbf{k}_j)_1 \in \mathbb{R}$, $(\mathbf{k}_j)_2 \in \mathbb{R}$ and $(\mathbf{k}_j)_3 \in \mathbb{R}$ are true.

One issue is that in the operator $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla^2_{\mathbf{x}}}$ the differential operator $\nabla^2_{\mathbf{x}}$ has been scaled differently than the differential operator D_x^2 in the operator $\sqrt{\mu - \hbar^2 D_x^2 + \varepsilon\mathcal{B}}$. We solve this issue by writing the operator of interest as

$$\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla^2_{\mathbf{x}}} \;=\; c\sqrt{m^2c^2 - \hbar^2\nabla^2_{\mathbf{x}} + \varepsilon\Big(2mM_U + \frac{\varepsilon}{c^2}M_U^2\Big)}.$$

Now we can use the previous series with substitutions $\mu = m^2c^2$ and $b = 2mU + \frac{\varepsilon}{c^2}U^2$. In attempt to compress our formulas as much as possible, let's use the notations

$$\hat{\psi}(\mathbf{k}_{\text{in}}) \;=\; \int\limits_{\mathbb{R}^3} e^{-\frac{i}{\hbar}\mathbf{k}_{\text{in}}\cdot\mathbf{y}}\psi(\mathbf{y})d^3y,$$

$$\hat{U}(\mathbf{k}) \;=\; \int\limits_{\mathbb{R}^3} e^{-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}'}U(\mathbf{x}')d^3x'$$

and

$$\widehat{U^2}(\mathbf{k}) \;=\; \int\limits_{\mathbb{R}^3} e^{-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}'}\big(U(\mathbf{x}')\big)^2 d^3x'.$$

The wide hat symbol is also above the number 2, so it means that the Fourier transform is calculated after the square operation. Let's also use the notation

$$E_{\mathbf{k}} \;=\; \sqrt{(mc^2)^2 + c^2\|\mathbf{k}\|^2}.$$

We are now ready to conclude that the effect of the operator $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla^2_{\mathbf{x}}}$ on a wave function $\psi(\mathbf{x})$ with small ε is approximately

$$\begin{aligned}
&\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla^2_{\mathbf{x}}}\psi(\mathbf{x}) \;=\; \sqrt{(mc^2)^2 - c^2\hbar^2\nabla^2_{\mathbf{x}}}\psi(\mathbf{x})\\
&+\; \frac{\varepsilon}{(2\pi\hbar)^6}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}2mc^2\hat{U}(\mathbf{k}_{\text{out}}-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})\\
&+\; \varepsilon^2\Big(\frac{1}{(2\pi\hbar)^6}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}\widehat{U^2}(\mathbf{k}_{\text{out}}-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})\\
&\quad-\; \frac{1}{(2\pi\hbar)^9}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\int\limits_{\mathbb{R}^3} d^3k_1\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_{\text{out}}-\mathbf{k}_1)}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_1}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})\Big)\\
&+\; \varepsilon^3\Big(-\frac{1}{(2\pi\hbar)^9}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\int\limits_{\mathbb{R}^3} d^3k_1\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_{\text{out}}-\mathbf{k}_1)}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_1}}\cdot\frac{\widehat{U^2}(\mathbf{k}_1-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})\\
&\quad-\; \frac{1}{(2\pi\hbar)^9}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\int\limits_{\mathbb{R}^3} d^3k_1\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}}}\cdot\frac{\widehat{U^2}(\mathbf{k}_{\text{out}}-\mathbf{k}_1)}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_1}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})\\
&\quad+\; \frac{1}{(2\pi\hbar)^{12}}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\int\limits_{\mathbb{R}^3} d^3k_1\int\limits_{\mathbb{R}^3} d^3k_2\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}})(E_{\mathbf{k}_2}+E_{\mathbf{k}_{\text{in}}})}\\
&\qquad\cdot\frac{2mc^2\hat{U}(\mathbf{k}_{\text{out}}-\mathbf{k}_2)}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_2}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})\\
&\quad+\; \frac{1}{(2\pi\hbar)^{12}}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\int\limits_{\mathbb{R}^3} d^3k_1\int\limits_{\mathbb{R}^3} d^3k_2\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}})(E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_1})}\\
&\qquad\cdot\frac{2mc^2\hat{U}(\mathbf{k}_{\text{out}}-\mathbf{k}_2)}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_2}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})\Big)\\
&+\; \varepsilon^4\Big(-\frac{1}{(2\pi\hbar)^9}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\int\limits_{\mathbb{R}^3} d^3k_1\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}}}\cdot\frac{\widehat{U^2}(\mathbf{k}_{\text{out}}-\mathbf{k}_1)}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_1}}\cdot\frac{\widehat{U^2}(\mathbf{k}_1-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})\\
&\quad+\; \frac{1}{(2\pi\hbar)^{12}}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\int\limits_{\mathbb{R}^3} d^3k_1\int\limits_{\mathbb{R}^3} d^3k_2\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}})(E_{\mathbf{k}_2}+E_{\mathbf{k}_{\text{in}}})}\\
&\qquad\cdot\frac{2mc^2\hat{U}(\mathbf{k}_{\text{out}}-\mathbf{k}_2)}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_2}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}}\cdot\frac{\widehat{U^2}(\mathbf{k}_1-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})\\
&\quad+\; \frac{1}{(2\pi\hbar)^{12}}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\int\limits_{\mathbb{R}^3} d^3k_1\int\limits_{\mathbb{R}^3} d^3k_2\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}})(E_{\mathbf{k}_2}+E_{\mathbf{k}_{\text{in}}})}\\
&\qquad\cdot\frac{2mc^2\hat{U}(\mathbf{k}_{\text{out}}-\mathbf{k}_2)}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_2}}\cdot\frac{\widehat{U^2}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})\\
&\quad+\; \frac{1}{(2\pi\hbar)^{12}}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\int\limits_{\mathbb{R}^3} d^3k_1\int\limits_{\mathbb{R}^3} d^3k_2\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}})(E_{\mathbf{k}_2}+E_{\mathbf{k}_{\text{in}}})}\\
&\qquad\cdot\frac{\widehat{U^2}(\mathbf{k}_{\text{out}}-\mathbf{k}_2)}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_2}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})\\
&\quad+\; \frac{1}{(2\pi\hbar)^{12}}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\int\limits_{\mathbb{R}^3} d^3k_1\int\limits_{\mathbb{R}^3} d^3k_2\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_{\text{in}}})(E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_1})}\\
&\qquad\cdot\frac{2mc^2\hat{U}(\mathbf{k}_{\text{out}}-\mathbf{k}_2)}{E_{\mathbf{k}_{\text{out}}}+E_{\mathbf{k}_2}}\cdot\frac{2mc^2\hat{U}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}}\cdot\frac{\widehat{U^2}(\mathbf{k}_1-\mathbf{k}_{\text{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}})
\end{aligned}$$

$$+ \frac{1}{(2\pi\hbar)^{12}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{out}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{in}} \int\limits_{\mathbb{R}^3} d^3k_1 \int\limits_{\mathbb{R}^3} d^3k_2 \frac{e^{\frac{i}{\hbar}\mathbf{k}_{\mathrm{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_{\mathrm{in}}})(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_1})}$$

$$\cdot \frac{2mc^2\hat{U}(\mathbf{k}_{\mathrm{out}}-\mathbf{k}_2)}{E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_2}} \cdot \frac{\widehat{U^2}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\mathrm{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\mathrm{in}}}} \hat{\psi}(\mathbf{k}_{\mathrm{in}})$$

$$+ \frac{1}{(2\pi\hbar)^{12}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{out}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{in}} \int\limits_{\mathbb{R}^3} d^3k_1 \int\limits_{\mathbb{R}^3} d^3k_2 \frac{e^{\frac{i}{\hbar}\mathbf{k}_{\mathrm{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_{\mathrm{in}}})(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_1})}$$

$$\cdot \frac{\widehat{U^2}(\mathbf{k}_{\mathrm{out}}-\mathbf{k}_2)}{E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_2}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\mathrm{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\mathrm{in}}}} \hat{\psi}(\mathbf{k}_{\mathrm{in}})$$

$$- \frac{1}{(2\pi\hbar)^{15}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{out}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{in}} \int\limits_{\mathbb{R}^3} d^3k_1 \int\limits_{\mathbb{R}^3} d^3k_2 \int\limits_{\mathbb{R}^3} d^3k_3 \frac{e^{\frac{i}{\hbar}\mathbf{k}_{\mathrm{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_{\mathrm{in}}})(E_{\mathbf{k}_3}+E_{\mathbf{k}_{\mathrm{in}}})(E_{\mathbf{k}_2}+E_{\mathbf{k}_{\mathrm{in}}})}$$

$$\cdot \frac{2mc^2\hat{U}(\mathbf{k}_{\mathrm{out}}-\mathbf{k}_3)}{E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_3}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_3-\mathbf{k}_2)}{E_{\mathbf{k}_3}+E_{\mathbf{k}_2}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\mathrm{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\mathrm{in}}}} \hat{\psi}(\mathbf{k}_{\mathrm{in}})$$

$$- \frac{1}{(2\pi\hbar)^{15}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{out}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{in}} \int\limits_{\mathbb{R}^3} d^3k_1 \int\limits_{\mathbb{R}^3} d^3k_2 \int\limits_{\mathbb{R}^3} d^3k_3 \frac{e^{\frac{i}{\hbar}\mathbf{k}_{\mathrm{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_{\mathrm{in}}})(E_{\mathbf{k}_3}+E_{\mathbf{k}_1})(E_{\mathbf{k}_3}+E_{\mathbf{k}_{\mathrm{in}}})}$$

$$\cdot \frac{2mc^2\hat{U}(\mathbf{k}_{\mathrm{out}}-\mathbf{k}_3)}{E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_3}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_3-\mathbf{k}_2)}{E_{\mathbf{k}_3}+E_{\mathbf{k}_2}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\mathrm{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\mathrm{in}}}} \hat{\psi}(\mathbf{k}_{\mathrm{in}})$$

$$- \frac{1}{(2\pi\hbar)^{15}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{out}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{in}} \int\limits_{\mathbb{R}^3} d^3k_1 \int\limits_{\mathbb{R}^3} d^3k_2 \int\limits_{\mathbb{R}^3} d^3k_3 \frac{e^{\frac{i}{\hbar}\mathbf{k}_{\mathrm{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_{\mathrm{in}}})(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_2})(E_{\mathbf{k}_2}+E_{\mathbf{k}_{\mathrm{in}}})}$$

$$\cdot \frac{2mc^2\hat{U}(\mathbf{k}_{\mathrm{out}}-\mathbf{k}_3)}{E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_3}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_3-\mathbf{k}_2)}{E_{\mathbf{k}_3}+E_{\mathbf{k}_2}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\mathrm{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\mathrm{in}}}} \hat{\psi}(\mathbf{k}_{\mathrm{in}})$$

$$- \frac{1}{(2\pi\hbar)^{15}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{out}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{in}} \int\limits_{\mathbb{R}^3} d^3k_1 \int\limits_{\mathbb{R}^3} d^3k_2 \int\limits_{\mathbb{R}^3} d^3k_3 \frac{e^{\frac{i}{\hbar}\mathbf{k}_{\mathrm{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_{\mathrm{in}}})(E_{\mathbf{k}_3}+E_{\mathbf{k}_1})(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_1})}$$

$$\cdot \frac{2mc^2\hat{U}(\mathbf{k}_{\mathrm{out}}-\mathbf{k}_3)}{E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_3}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_3-\mathbf{k}_2)}{E_{\mathbf{k}_3}+E_{\mathbf{k}_2}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\mathrm{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\mathrm{in}}}} \hat{\psi}(\mathbf{k}_{\mathrm{in}})$$

$$- \frac{1}{(2\pi\hbar)^{15}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{out}} \int\limits_{\mathbb{R}^3} d^3k_{\mathrm{in}} \int\limits_{\mathbb{R}^3} d^3k_1 \int\limits_{\mathbb{R}^3} d^3k_2 \int\limits_{\mathbb{R}^3} d^3k_3 \frac{e^{\frac{i}{\hbar}\mathbf{k}_{\mathrm{out}}\cdot\mathbf{x}}}{(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_{\mathrm{in}}})(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_1})(E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_2})}$$

$$\cdot \frac{2mc^2\hat{U}(\mathbf{k}_{\mathrm{out}}-\mathbf{k}_3)}{E_{\mathbf{k}_{\mathrm{out}}}+E_{\mathbf{k}_3}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_3-\mathbf{k}_2)}{E_{\mathbf{k}_3}+E_{\mathbf{k}_2}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_2-\mathbf{k}_1)}{E_{\mathbf{k}_2}+E_{\mathbf{k}_1}} \cdot \frac{2mc^2\hat{U}(\mathbf{k}_1-\mathbf{k}_{\mathrm{in}})}{E_{\mathbf{k}_1}+E_{\mathbf{k}_{\mathrm{in}}}} \hat{\psi}(\mathbf{k}_{\mathrm{in}})\Big)$$

$$+ \cdots$$

Is it possible to draw a graphical representation of the operator $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}$ similarly as of the operator $\sqrt{\mu - \hbar^2 D_x^2 + \varepsilon\mathcal{B}}$? We cannot draw the graphs exactly the same way, because with $\sqrt{\mu - \hbar^2 D_x^2 + \varepsilon\mathcal{B}}$ there was only one b function, and with $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}$ we have two "b functions". One is $b \propto U$, and the other one is $b \propto U^2$. We can solve this issue by using two different types of solid connecting lines. Let's decide that every occurence of the expression

$$\frac{2mc^2\hat{U}(\mathbf{k}_{j'}-\mathbf{k}_j)}{E_{\mathbf{k}_{j'}}+E_{\mathbf{k}_j}}$$

gets turned into an ordinary solid line between two connection points, and that every occurence of the expression

$$\frac{\widehat{U^2}(\mathbf{k}_{j'} - \mathbf{k}_j)}{E_{\mathbf{k}_{j'}} + E_{\mathbf{k}_j}}$$

gets turned into a double solid line between two connection points. Every occurence of

$$\frac{1}{E_{\mathbf{k}_{j'}} + E_{\mathbf{k}_j}}$$

without a Fourier transform in the numerator will be a dashed curve. If we draw the arrows, dots, solid lines with triangles, double solid lines with triangles, and dashed curves like this, we obtain a picture shown in Figure 2.

Let's attempt to approximate this operator in the almost non-relativistic case, and focus only on the first order term of the series. Does it look like a good idea to use the approximation

$$\begin{aligned}\frac{1}{\sqrt{(mc^2)^2 + c^2\|\mathbf{k}_{\text{out}}\|^2} + \sqrt{(mc^2)^2 + c^2\|\mathbf{k}_{\text{in}}\|^2}} &= \frac{1}{2mc^2} - \frac{\|\mathbf{k}_{\text{out}}\|^2 + \|\mathbf{k}_{\text{in}}\|^2}{8m^3c^4} \\ &+ \frac{\|\mathbf{k}_{\text{out}}\|^4 + \|\mathbf{k}_{\text{out}}\|^2\|\mathbf{k}_{\text{in}}\|^2 + \|\mathbf{k}_{\text{in}}\|^4}{16m^5c^6} \\ &- \frac{5(\|\mathbf{k}_{\text{out}}\|^6 + \|\mathbf{k}_{\text{out}}\|^4\|\mathbf{k}_{\text{in}}\|^2 + \|\mathbf{k}_{\text{out}}\|^2\|\mathbf{k}_{\text{in}}\|^4 + \|\mathbf{k}_{\text{in}}\|^6)}{128m^7c^8} + O\Big(\frac{1}{c^{10}}\Big)?\end{aligned}$$

To justify this Taylor series, it is not sufficient to assume that ψ is almost non-relativistic. We must also assume that U doesn't have significant extremely steep slopes in it. We can make these assumptions, so let's see where this approximation leads to. The first order term of the series of the operator can be approximated to be

$$\begin{aligned}&\frac{\varepsilon}{(2\pi\hbar)^6}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\,\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}2mc^2\hat{U}(\mathbf{k}_{\text{out}} - \mathbf{k}_{\text{in}})}{E_{\mathbf{k}_{\text{out}}} + E_{\mathbf{k}_{\text{in}}}}\hat{\psi}(\mathbf{k}_{\text{in}}) \\ &= \frac{\varepsilon}{(2\pi\hbar)^6}\int\limits_{\mathbb{R}^3} d^3k_{\text{out}}\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\int\limits_{\mathbb{R}^3} d^3x'\int\limits_{\mathbb{R}^3} d^3y\; e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot\mathbf{x}}e^{-\frac{i}{\hbar}(\mathbf{k}_{\text{out}} - \mathbf{k}_{\text{in}})\cdot\mathbf{x}'}U(\mathbf{x}')\psi(\mathbf{y}) \\ &\quad\Big(1 - \frac{\|\mathbf{k}_{\text{out}}\|^2 + \|\mathbf{k}_{\text{in}}\|^2}{4m^2c^2} + \frac{\|\mathbf{k}_{\text{out}}\|^4 + \|\mathbf{k}_{\text{out}}\|^2\|\mathbf{k}_{\text{in}}\|^2 + \|\mathbf{k}_{\text{in}}\|^4}{8m^4c^4} \\ &\quad - \frac{5(\|\mathbf{k}_{\text{out}}\|^6 + \|\mathbf{k}_{\text{out}}\|^4\|\mathbf{k}_{\text{in}}\|^2 + \|\mathbf{k}_{\text{out}}\|^2\|\mathbf{k}_{\text{in}}\|^4 + \|\mathbf{k}_{\text{in}}\|^6)}{64m^6c^6} \\ &\quad + O\Big(\frac{1}{c^8}\Big)\Big)e^{-\frac{i}{\hbar}\mathbf{k}_{\text{in}}\cdot\mathbf{y}}\end{aligned}$$

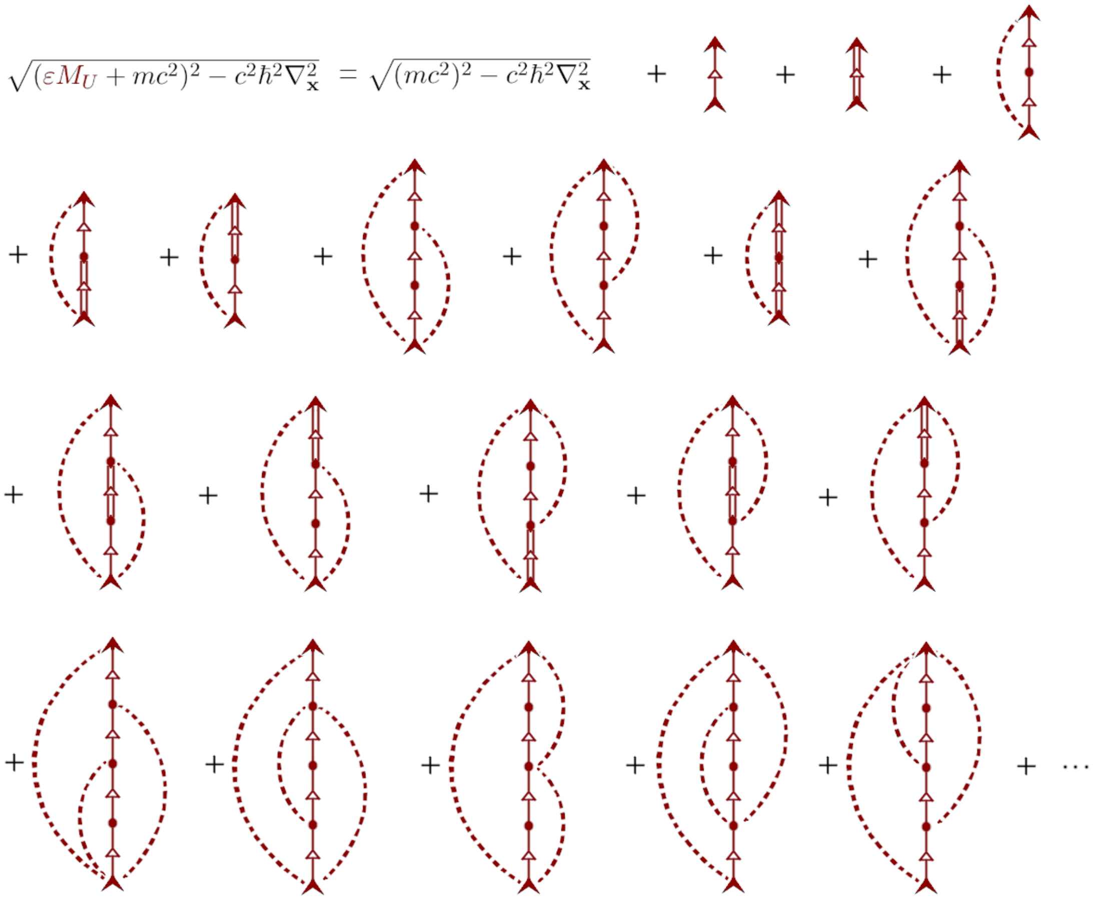

Figure 2: A graphical representation of the series approximation of the operator $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}$.

$$
\begin{aligned}
&= \frac{\varepsilon}{(2\pi\hbar)^6} \int\limits_{\mathbb{R}^3} d^3k_{\text{out}} \int\limits_{\mathbb{R}^3} d^3k_{\text{in}} \int\limits_{\mathbb{R}^3} d^3x' \int\limits_{\mathbb{R}^3} d^3y\; e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot(\mathbf{x}-\mathbf{x}')} e^{\frac{i}{\hbar}\mathbf{k}_{\text{in}}\cdot\mathbf{x}'} U(\mathbf{x}')\psi(\mathbf{y}) \\
&\quad \Big(1 - \frac{\|\mathbf{k}_{\text{out}}\|^2 - \hbar^2\nabla_{\mathbf{y}}^2}{4m^2c^2} + \frac{\|\mathbf{k}_{\text{out}}\|^4 - \hbar^2\|\mathbf{k}_{\text{out}}\|^2\nabla_{\mathbf{y}}^2 + \hbar^4(\nabla_{\mathbf{y}}^2)^2}{8m^4c^4} \\
&\quad - \frac{5(\|\mathbf{k}_{\text{out}}\|^6 - \hbar^2\|\mathbf{k}_{\text{out}}\|^4\nabla_{\mathbf{y}}^2 + \hbar^4\|\mathbf{k}_{\text{out}}\|^2(\nabla_{\mathbf{y}}^2)^2 - \hbar^6(\nabla_{\mathbf{y}}^2)^3)}{64m^6c^6} \\
&\quad + O\Big(\frac{1}{c^8}\Big)\Big) e^{-\frac{i}{\hbar}\mathbf{k}_{\text{in}}\cdot\mathbf{y}} \\
&= \frac{\varepsilon}{(2\pi\hbar)^6} \int\limits_{\mathbb{R}^3} d^3k_{\text{out}} \int\limits_{\mathbb{R}^3} d^3x' \int\limits_{\mathbb{R}^3} d^3y e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot(\mathbf{x}-\mathbf{x}')} \underbrace{\Big(\int\limits_{\mathbb{R}^3} d^3k_{\text{in}}\; e^{\frac{i}{\hbar}\mathbf{k}_{\text{in}}\cdot(\mathbf{x}'-\mathbf{y})}\Big)}_{=(2\pi\hbar)^3\delta(\mathbf{x}'-\mathbf{y})} U(\mathbf{x}') \\
&\quad \Big(1 - \frac{\|\mathbf{k}_{\text{out}}\|^2 - \hbar^2\nabla_{\mathbf{y}}^2}{4m^2c^2} + \frac{\|\mathbf{k}_{\text{out}}\|^4 - \hbar^2\|\mathbf{k}_{\text{out}}\|^2\nabla_{\mathbf{y}}^2 + \hbar^4(\nabla_{\mathbf{y}}^2)^2}{8m^4c^4} \\
&\quad - \frac{5(\|\mathbf{k}_{\text{out}}\|^6 - \hbar^2\|\mathbf{k}_{\text{out}}\|^4\nabla_{\mathbf{y}}^2 + \hbar^4\|\mathbf{k}_{\text{out}}\|^2(\nabla_{\mathbf{y}}^2)^2 - \hbar^6(\nabla_{\mathbf{y}}^2)^3)}{64m^6c^6} \\
&\quad + O\Big(\frac{1}{c^8}\Big)\Big)\psi(\mathbf{y})
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{\varepsilon}{(2\pi\hbar)^3} \int\limits_{\mathbb{R}^3} d^3k_{\text{out}} \int\limits_{\mathbb{R}^3} d^3y \; e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot(\mathbf{x}-\mathbf{y})} U(\mathbf{y}) \\
&\Big(1 \;-\; \frac{\|\mathbf{k}_{\text{out}}\|^2 - \hbar^2\nabla_{\mathbf{y}}^2}{4m^2c^2} \;+\; \frac{\|\mathbf{k}_{\text{out}}\|^4 - \hbar^2\|\mathbf{k}_{\text{out}}\|^2\nabla_{\mathbf{y}}^2 + \hbar^4(\nabla_{\mathbf{y}}^2)^2}{8m^4c^4} \\
&-\; \frac{5(\|\mathbf{k}_{\text{out}}\|^6 - \hbar^2\|\mathbf{k}_{\text{out}}\|^4\nabla_{\mathbf{y}}^2 + \hbar^4\|\mathbf{k}_{\text{out}}\|^2(\nabla_{\mathbf{y}}^2)^2 - \hbar^6(\nabla_{\mathbf{y}}^2)^3)}{64m^6c^6} \\
&+\; O\Big(\frac{1}{c^8}\Big)\Big)\psi(\mathbf{y}) \;=\; \cdots
\end{aligned}
$$

At this point we encounter some notational challenges. We would like to turn the occurences of $\|\mathbf{k}_{\text{out}}\|^2$ into $-\hbar^2\nabla_{\mathbf{x}}^2$, because only after this step can we integrate with respect to $\mathbf{k}_{\text{out}}$. However, we would also like to keep the factor $e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot(\mathbf{x}-\mathbf{y})}$ as a one factor, and we cannot move this factor on the right side of the occurences of $\|\mathbf{k}_{\text{out}}\|^2$ nicely, because it would interfere with the already present $\nabla_{\mathbf{y}}^2$ operations. Let's solve this issue by using a temporary special notation that the operator ${}_{\mathbf{x}}\nabla$ operates leftwards, meaning that for example a gradient of $f(\mathbf{x})$ could be written as $f(\mathbf{x})({}_{\mathbf{x}}\nabla)$. With this special notation we can calculate

$$
\begin{aligned}
\cdots \;&=\; \frac{\varepsilon}{(2\pi\hbar)^3} \int\limits_{\mathbb{R}^3} d^3k_{\text{out}} \int\limits_{\mathbb{R}^3} d^3y \; e^{\frac{i}{\hbar}\mathbf{k}_{\text{out}}\cdot(\mathbf{x}-\mathbf{y})} U(\mathbf{y}) \\
&\Big(1 \;+\; \frac{\hbar^2({}_{\mathbf{x}}\nabla^2 + \nabla_{\mathbf{y}}^2)}{4m^2c^2} \;+\; \frac{\hbar^4(({}_{\mathbf{x}}\nabla^2)^2 + {}_{\mathbf{x}}\nabla^2\nabla_{\mathbf{y}}^2 + (\nabla_{\mathbf{y}}^2)^2)}{8m^4c^4} \\
&+\; \frac{5\hbar^6(({}_{\mathbf{x}}\nabla^2)^3 + ({}_{\mathbf{x}}\nabla^2)^2\nabla_{\mathbf{y}}^2 + {}_{\mathbf{x}}\nabla^2(\nabla_{\mathbf{y}}^2)^2 + (\nabla_{\mathbf{y}}^2)^3))}{64m^6c^6} \;+\; O\Big(\frac{1}{c^8}\Big)\Big)\psi(\mathbf{y}) \\
&=\; \varepsilon \int\limits_{\mathbb{R}^3} d^3y \; \delta(\mathbf{x}-\mathbf{y})U(\mathbf{y}) \\
&\Big(1 \;+\; \frac{\hbar^2({}_{\mathbf{x}}\nabla^2 + \nabla_{\mathbf{y}}^2)}{4m^2c^2} \;+\; \frac{\hbar^4(({}_{\mathbf{x}}\nabla^2)^2 + {}_{\mathbf{x}}\nabla^2\nabla_{\mathbf{y}}^2 + (\nabla_{\mathbf{y}}^2)^2)}{8m^4c^4} \\
&+\; \frac{5\hbar^6(({}_{\mathbf{x}}\nabla^2)^3 + ({}_{\mathbf{x}}\nabla^2)^2\nabla_{\mathbf{y}}^2 + {}_{\mathbf{x}}\nabla^2(\nabla_{\mathbf{y}}^2)^2 + (\nabla_{\mathbf{y}}^2)^3)}{64m^6c^6} \;+\; O\Big(\frac{1}{c^8}\Big)\Big)\psi(\mathbf{y}) \\
&=\; \varepsilon\Big(U(\mathbf{x})\psi(\mathbf{x}) \;+\; \frac{\hbar^2}{4m^2c^2}\Big(\nabla_{\mathbf{x}}^2\big(U(\mathbf{x})\psi(\mathbf{x})\big) \;+\; U(\mathbf{x})\nabla_{\mathbf{x}}^2\psi(\mathbf{x})\Big) \\
&+\; \frac{\hbar^4}{8m^4c^4}\Big((\nabla_{\mathbf{x}}^2)^2\big(U(\mathbf{x})\psi(\mathbf{x})\big) \;+\; \nabla_{\mathbf{x}}^2\big(U(\mathbf{x})\nabla_{\mathbf{x}}^2\psi(\mathbf{x})\big) \;+\; U(\mathbf{x})(\nabla_{\mathbf{x}}^2)^2\psi(\mathbf{x})\Big) \\
&+\; \frac{5\hbar^6}{64m^6c^6}\Big((\nabla_{\mathbf{x}}^2)^3\big(U(\mathbf{x})\psi(\mathbf{x})\big) \;+\; (\nabla_{\mathbf{x}}^2)^2\big(U(\mathbf{x})\nabla_{\mathbf{x}}^2\psi(\mathbf{x})\big) \\
&\quad+\; \nabla_{\mathbf{x}}^2\big(U(\mathbf{x})(\nabla_{\mathbf{x}}^2)^2\psi(\mathbf{x})\big) \;+\; U(\mathbf{x})(\nabla_{\mathbf{x}}^2)^3\psi(\mathbf{x})\Big) \;+\; O\Big(\frac{1}{c^8}\Big)\Big).
\end{aligned}
$$

If a term in the series of the operator $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}$ is proportional to ε^2, then it is also proportional to $\frac{1}{c}$ or a higher order of this. If a term is proportional to ε^3, then it is also proportional to $\frac{1}{c^2}$ or a higher order of this. If a term is proportional to ε^4, then it is also proportional to $\frac{1}{c^3}$ or a higher order of this, and so on. We see from here that it is possible to derive the non-relativistic Schrödinger equation with the potential term U out of the relativistic Schrödinger equation as a non-relativistic approximation, which is nice to know.

One question that should be recognized as interesting is that is the operator $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}$ local or non-local with respect to the potential U? This question means that if we fix some $\mathbf{x}$, is the behavior of $U(\mathbf{x})$ in an infinitesimal environment of $\mathbf{x}$ sufficient for the determination of the value $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}\psi(\mathbf{x})$, or could it be that this value is affected by $U(\mathbf{x}')$, where $\mathbf{x}'$ is far away from $\mathbf{x}$? The formula for $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}\psi(\mathbf{x})$ uses the Fourier transforms $\hat{U}$ and $\widehat{U^2}$ in a such way that it at least looks like that the effect from U could be non-local. People who know Fourier analysis of course know that the question cannot rigorously be answered based on this observation alone, because there could maybe be some cancellation phenomenon that eventually makes the effect local after all. Above we just learned that according to the almost non-relativistic approximation the effect of U is local. Some people might think that this result could be used to prove the locality in the fully relativistic situation too. The idea of the proof would be something like that the fully relativistic operator could be expressed as an infinite series of some simpler operations, and since the effects from the simpler operations are local, the local nature would be inherited by the fully relativistic operator. People who know rigorous calculus can see some problems with this proof attempt, because it would be using divergent series in the intermediate stages. Nonetheless, it wouldn't be an entirely nonsensical proof attempt. My understanding on this topic is that the correct answer is that the effect from U is actually non-local. When I was a university student, I asked a lot of physics questions from various places, and somebody from www.physicsforums.com showed me how to prove that the pseudo-differential operator $\sqrt{(mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}$ itself is non-local. I do not have a better source for this proof anymore, but anyway, the same proving technique can also be used to attempt to prove that $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}$ is non-local with respect to U. The proof of non-locality begins with these thoughts: Suppose $\mathbf{x} \mapsto f(\mathbf{x})$ is some function. If we write the Taylor series of the Fourier transform as

$$\begin{aligned}\hat{f}(\mathbf{k}) &= \int\limits_{\mathbb{R}^3} e^{-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x})d^3x = \int\limits_{\mathbb{R}^3} \Big(\sum_{n=0}^{\infty}\frac{1}{n!}\Big(-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big)^n\Big)f(\mathbf{x})d^3x \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\int\limits_{\mathbb{R}^3}\Big(-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big)^n f(\mathbf{x})d^3x,\end{aligned}$$

will this converge for all $\mathbf{k} \in \mathbb{R}^3$? Suppose there exists $R > 0$ with a property that $f(\mathbf{x}) = 0$ for all $\|\mathbf{x}\| > R$. Suppose that $\sup\limits_{\|\mathbf{x}\|\leq R} |f(\mathbf{x})| < \infty$. Then the inequality

$$\Big|\sum_{n=n_{\mathrm{A}}}^{n_{\mathrm{B}}} \frac{1}{n!}\int\limits_{\mathbb{R}^3} \Big(-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big)^n f(\mathbf{x})d^3x\Big| \;\leq\; \sum_{n=n_{\mathrm{A}}}^{n_{\mathrm{B}}} \frac{1}{n!}\int\limits_{\mathbb{R}^3} \Big|\frac{1}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big|^n |f(\mathbf{x})|d^3x$$

$$\leq \Big(\sup_{\|\mathbf{x}'\|\leq R} |f(\mathbf{x}')|\Big)\frac{4\pi R^3}{3}\sum_{n=n_{\mathrm{A}}}^{n_{\mathrm{B}}} \frac{1}{n!}\Big(\frac{\|\mathbf{k}\|R}{\hbar}\Big)^n$$

is true, and this is sufficient to imply that the Taylor series of $\hat{f}(\mathbf{k})$ converges for all $\mathbf{k}\in\mathbb{R}^3$. If there exists $R > 0$ with a property that $f(\mathbf{x}) = 0$ for all $\|\mathbf{x}\| > R$, we say that f has a bounded support.

Suppose we know that f has a bounded support and also that f is continuous in its domain $\mathbb{R}^3$. These two assumptions imply that $\max\limits_{\mathbf{x}\in\mathbb{R}^3} |f(\mathbf{x})|$ exists with a finite value. So we can also formulate the previous result by saying that if f has a bounded support and is continuous, then the Taylor series of $\hat{f}(\mathbf{k})$ converges for all $\mathbf{k}\in\mathbb{R}^3$. However, actually this only means that the Taylor series converges to something. Whether or not it converges to the right value $\hat{f}(\mathbf{k})$ is another matter. If we want to prove that the Taylor series converges to the right value, we should rigorously justify that

$$\int\limits_{\mathbb{R}^3}\Big(\sum_{n=0}^{\infty}\frac{1}{n!}\Big(-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big)^n\Big)f(\mathbf{x})d^3x \;=\; \sum_{n=0}^{\infty}\frac{1}{n!}\int\limits_{\mathbb{R}^3}\Big(-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big)^n f(\mathbf{x})d^3x$$

is true. The equation

$$\sum_{n=0}^{\infty}\frac{1}{n!}\int\limits_{\mathbb{R}^3}\Big(-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big)^n f(\mathbf{x})d^3x \;=\; \lim_{N\to\infty}\sum_{n=0}^{N}\frac{1}{n!}\int\limits_{\mathbb{R}^3}\Big(-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big)^n f(\mathbf{x})d^3x$$

$$= \lim_{N\to\infty}\int\limits_{\mathbb{R}^3}\sum_{n=0}^{N}\frac{1}{n!}\Big(-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big)^n f(\mathbf{x})d^3x$$

is true, since the order of an integral and a finite sum can always be changed. This means that the critical question is that how do we rigorously justify the equation

$$\lim_{N\to\infty}\int\limits_{\mathbb{R}^3}\sum_{n=0}^{N}\frac{1}{n!}\Big(-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big)^n f(\mathbf{x})d^3x \;=\; \int\limits_{\mathbb{R}^3}\lim_{N\to\infty}\sum_{n=0}^{N}\frac{1}{n!}\Big(-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big)^n f(\mathbf{x})d^3x?$$

According to Lebesgue's dominated convergence theorem this step is justified, if there exists a function $g:\mathbb{R}^3\to[0,\infty[$ with the properties

$$\int\limits_{\mathbb{R}^3} g(\mathbf{x})d^3x \;<\; \infty$$

and

$$\Big|\sum_{n=0}^{N}\frac{1}{n!}\Big(-\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}\Big)^n f(\mathbf{x})\Big| \;\leq\; g(\mathbf{x}) \qquad \forall\, N\in\{0,1,2,\ldots\}.$$

If we put

$$g(\mathbf{x}) \;=\; e^{\frac{\|\mathbf{k}\|R}{\hbar}}\Big(\sup_{\|\mathbf{x}'\|\leq R}|f(\mathbf{x}')|\Big)\chi_{\overline{B}(0,R)}(\mathbf{x}),$$

this works. Here $\chi_{\overline{B}(0,R)}(\mathbf{x})$ is an indicator function whose value is 1, if $\|\mathbf{x}\|\leq R$, and 0, if $\|\mathbf{x}\|>R$. We obtained a rigorous result that if $f(\mathbf{x})$ has a bounded support and is continuous, then the Fourier transform $\hat{f}(\mathbf{k})$ can be expressed as a Taylor series for all $\mathbf{k}$. This means that we can also use the conclusion that if the Taylor series of the Fourier transform $\hat{f}(\mathbf{k})$ diverges for some $\mathbf{k}$, then it must be so that $f(\mathbf{x})$ does not have a bounded support or that $f(\mathbf{x})$ is not continuous.

Next, let's define a function $f(\mathbf{x})$ with a formula

$$f(\mathbf{x}) \;=\; \frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^3} d^3k_{\textrm{out}}\int\limits_{\mathbb{R}^3} d^3k_{\textrm{in}}\;\frac{e^{\frac{i}{\hbar}\mathbf{k}_{\textrm{out}}\cdot\mathbf{x}}\hat{U}(\mathbf{k}_{\textrm{out}}-\mathbf{k}_{\textrm{in}})}{E_{\mathbf{k}_{\textrm{out}}}+E_{\mathbf{k}_{\textrm{in}}}}\hat{\psi}(\mathbf{k}_{\textrm{in}}).$$

We are going to need the claim that $\mathbf{x}\mapsto f(\mathbf{x})$ is continuous. What assumptions could we make to make this claim valid? If we assume that ψ and U belong to Schwartz space [4], we can then use Lebesgue's dominated convergence theorem to justify that $\lim\limits_{\mathbf{x}\to\mathbf{x}_0} f(\mathbf{x}) = f(\mathbf{x}_0)$. Let's impose these assumptions and continue under the knowledge that now $\mathbf{x}\mapsto f(\mathbf{x})$ is continuous.

Let's emphasize that we assume ψ to be fixed, and interpret the formula of f as a mapping $U\mapsto f$. We are interested in the question that is this mapping $U\mapsto f$ local or not. We define locality like this: We assume that there exists $R>0$ with a property that $U(\mathbf{x})=0$, if $\|\mathbf{x}\|>R$. Then, if $f(\mathbf{x})=0$ for all $\|\mathbf{x}\|>R$, we say that $U\mapsto f$ is local, and if $f(\mathbf{x})\neq 0$ for some $\|\mathbf{x}\|>R$, we say that $U\mapsto f$ is non-local. The definition of f can equivalently be stated as

$$\hat{f}(\mathbf{k}) \;=\; \int\limits_{\mathbb{R}^3} d^3k_{\textrm{in}}\;\frac{\hat{U}(\mathbf{k}-\mathbf{k}_{\textrm{in}})}{E_{\mathbf{k}}+E_{\mathbf{k}_{\textrm{in}}}}\hat{\psi}(\mathbf{k}_{\textrm{in}}).$$

We will attempt to prove that $U\mapsto f$ is non-local by proving that the Taylor series of $\hat{f}(\mathbf{k})$ diverges for some $\mathbf{k}$. If we extenend the mapping $\mathbb{R}^3\to\mathbb{R}$, $\mathbf{k}\mapsto E_{\mathbf{k}}$ into a complex mapping $\mathbb{C}^3\to\mathbb{C}$, the extended mapping is non-analytic at points $k_1^2+k_2^2+k_3^2=-m^2c^2$. The Taylor series of $\hat{U}(\mathbf{k}-\mathbf{k}_{\textrm{in}})$ converges for all $\mathbf{k}$, so this factor cannot have such points of non-analyticity that would cancel the points of non-analyticity of $E_{\mathbf{k}}$. This means that the Taylor series of the integrand $\frac{\hat{U}(\mathbf{k}-\mathbf{k}_{\textrm{in}})}{E_{\mathbf{k}}+E_{\mathbf{k}_{\textrm{in}}}}\hat{\psi}(\mathbf{k}_{\textrm{in}})$ with respect to $\mathbf{k}$ is diverging for some $\mathbf{k}$. Next, we would like to put forward a claim that since the Taylor series of the integrand is diverging, also the Taylor series of $\hat{f}(\mathbf{k})$ must be diverging for some $\mathbf{k}$. Is this correct? Regrettably, at the moment of writing this I don't know how to turn this argument into a fully rigorous form. If we remain open to all possibilities, it could maybe be so that the integral somehow makes the Taylor series converge after all. However, there is no obvious known mechanism that would make the integral work in a such way, so at this point it very much seems that the Taylor series of $\hat{f}(\mathbf{k})$ is diverging for some $\mathbf{k}$. Let's continue onto some final thoughts under the assumption that we now know the mapping $U \mapsto f$ to be non-local, even though a gap was left in the proof.

So it is so that the value $\sqrt{(\varepsilon M_U + mc^2)^2 - c^2\hbar^2\nabla_{\mathbf{x}}^2}\psi(\mathbf{x})$ is affected by $U(\mathbf{x}')$, where $\mathbf{x}'$ is far away from $\mathbf{x}$. A big question arises that what does this mean? Usually we want physics theories to have some reasonable locality properties. Could it be that this non-locality is a sign of all this being unphysical nonsense? I would advise people to keep in mind that we should already know the relativistic quantum theories to be overall difficult and paradoxical topic, and we should refrain from jumping to quick conclusions. We should recognize that the non-locality with respect to U is noteworthily strange, but it is still possible that eventually this turns out to be an ordinary physics paradox that can be solved somehow.

References

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