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A Note on the Relation between Potential Terms and Metric Matrices

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Abstract

The purpose of this paper is to introduce representation of kinetic fields in Schrödinger equations and to give the relation between potential terms and metric matrices via general structure of spaces rather than Euclidean spaces. We obtain two results from the point of view in Fourier analysis and pseudo-differential operators. One is the derivation of the potential terms in Schrödinger equations from the representation of kinetic fields by metric matrices in Schrödinger type equation, the other is the derivation the metric matrices in Schrödinger type equation from the potential terms in Schrödinger equation in the one-dimensional Euclidean space.

Keywords: *Schrödinger type equations, potential terms, metric matrices, Fourier transform, pseudo-differential operators*

1 Introduction

Let us consider the Cauchy problem for Schrödinger equations

$$i\hbar \frac{\partial}{\partial t}\psi(t,x) = H\psi(t,x) \tag{1}$$

and

$$\psi(0,x) = \psi_0(x), \tag{2}$$

where $\hbar$ denotes the Plank constant, H the Hamilton operator (Hamiltonian) and ψ_0 the initial data. A wavefunction in the Hilbert spaces is a complex-valued mapping

$$\psi : \mathbb{R} \times \mathbb{R}^n \to \mathbb{C} \tag{3}$$

satisfying the above Cauchy problem. When a quantum particle of mass $m > 0$ is in the potential $V(t, x)$, we can write

$$H = -\frac{\hbar^2}{2m}\Delta + V(t, x), \tag{4}$$

where Laplace operator (Laplacian) $\triangle$ is defined by

$$\triangle = \sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2}. \tag{5}$$

Our main results in this paper follow:

Theorem 1.1 *The Schrödinger type equation*

$$i\frac{\partial}{\partial t}\psi(t, x) = -\frac{1}{2}\nabla A(t, x)\nabla^T \psi(t, x) \tag{6}$$

is equivalent to the Schrödinger equation with potential terms

$$i\frac{\partial}{\partial t}\psi(t, x) = \left(-\frac{1}{2}\Delta + V(t, x)\right)\psi(t, x), \tag{7}$$

if

$$V(t, x) = \frac{1}{2}\nabla(E - A(t, x))\nabla^T, \tag{8}$$

where $A(t, x)$ is a metric matrix or coefficients of the second order differential operator.

Theorem 1.2 *Let $n = 1$. The Schrödinger equation with potential terms*

$$i\frac{\partial}{\partial t}\psi(t, x) = \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(t, x)\right)\psi(t, x) \tag{9}$$

is equivalent to the Schrödinger type equation

$$i\frac{\partial}{\partial t}\psi(t, x) = -\frac{1}{2}\frac{\partial}{\partial x}a(t, x)\frac{\partial}{\partial x}\psi(t, x), \tag{10}$$

if

$$a(t, x) = 1 - 2\left(\frac{\partial}{\partial x}\right)^{-1} V(t, x)\left(\frac{\partial}{\partial x}\right)^{-1}. \tag{11}$$

In should be remarked that we often use the natural unit system $\hbar = 1$ for simplicity.

2 Preliminary

2.1 Fourier Transform

Definition 2.1 *For an element $\psi = \psi(x)$ in Hilbert space $\mathbb{H}$, Fourier transform $\hat{\psi} = \hat{\psi}(\xi)$ is defined by*

$$\hat{\psi}(\xi) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} e^{-ix\cdot\xi}\psi(x)\ dx, \tag{12}$$

where $\xi \in \mathbb{R}^n$. We also write $\mathcal{F}\psi$ for $\hat{\psi}$.

Since x and ξ are canonically conjugate variables, $\hat{\psi}(\xi)$ is considered to be a wavefunction of ξ instead of x.

We have Plancherel formula [8]

$$\|\psi\| = \|\hat{\psi}\| \tag{13}$$

from the definition of Fourier transform.

Definition 2.2 *For an element $\phi = \phi(\xi)$ in the Hilbert space $\mathcal{H}$, the inverse Fourier transform $\check{\phi} = \check{\phi}(x)$ is defined by*

$$\check{\phi}(x) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} e^{ix\cdot\xi}\phi(\xi)\ d\xi. \tag{14}$$

we also write $\mathcal{F}^{-1}\phi$ for $\check{\psi}$.

In our definition of the Fourier transform and the inverse Fourier transform, coefficients $(2\pi)^{-\frac{n}{2}}$ are used for the simple expression

$$\mathcal{F}^{-1}\mathcal{F}\psi = \psi, \quad \mathcal{F}\mathcal{F}^{-1}\phi = \phi \tag{15}$$

for any $\psi \in \mathcal{H}$ and any $\phi \in \mathcal{H}$.

2.2 Schrödinger Equations

A wavefunction ψ satisfies Schrödinger equations

$$i\frac{\partial}{\partial t}\psi(t,x) = H\psi(t,x), \tag{16}$$

where H denotes Hamiltonian. In quantum mechanics, we often use the form

$$H = -\frac{1}{2}\Delta + V(t,x), \tag{17}$$

where $V(t, x)$ is the potential in the quantum system depends on time t and space x, which represents interactions of electromagnetic forces for example.

Let us consider

$$i\frac{\partial}{\partial t}\psi(t, x) = \left(-\frac{1}{2}\Delta + V(t, x)\right)\psi(t, x) \tag{18}$$

for simplicity.

Schrödinger equation (18) is a partial differential equation (PDE) of evolution along time t. Therefore if initial data of $\psi(t, x)$ is given at $t = 0$, we can obtain the behavior of the wavefunction $\psi(t, x)$ for arbitrary time $t \in \mathbb{R}$. In fact, when $V(t, x)$ is imposed on appropriate conditions, if we give ψ_0 as initial data from the Hilbert space $\mathcal{H}$ to the equation, such as

$$\psi(0, x) = \psi_0(x), \tag{19}$$

there exists a unique solution to Schrödinger equation (18). It should be remarked that the estimate of energy

$$\|\psi(t, \bullet)\| \leq C\|\psi_0\| \tag{20}$$

holds with some $C > 0$ for any $t \in \mathbb{R}$. Moreover, we can take $C = 1$ and replace the inequality by the identity when $V = 0$.

Fourier transform plays an important role in solving Schrödinger equations. For an element ψ in Hilbelt spaces, integral by part yields

$$\begin{aligned}\mathcal{F}\left[\frac{\partial}{\partial x_j}\psi\right](t, \xi) &= (2\pi)^{-\frac{n}{2}}\int_{\mathbb{R}^n} e^{-ix\cdot\xi}\frac{\partial}{\partial x_j}\psi(x)\ dx \\ &= -(2\pi)^{-\frac{n}{2}}\int_{\mathbb{R}^n}\frac{\partial}{\partial x_j}(e^{-ix\cdot\xi})\psi(x)\ dx \\ &= i\xi_j(2\pi)^{-\frac{n}{2}}\int_{\mathbb{R}^n} e^{-ix\cdot\xi}\psi(x)\ dx \\ &= i\xi_j\hat{\psi}(\xi).\end{aligned} \tag{21}$$

In other words, the differential operator with respect to x is replaced by the multiplication of momentum. Moreover

$$-\triangle e^{ix\cdot\xi} = -\sum_{j=1}^{n}\frac{\partial^2}{\partial x_j^2}e^{ix\cdot\xi} = \sum_{j=1}^{n}\xi_j^2 e^{ix\cdot\xi} = |\xi|^2 e^{ix\cdot\xi} \tag{22}$$

indicates that the function $e^{ix\cdot\xi}$ is the eigenfunction of the operator $-\triangle$ corresponding to the eigenvalue of $|\xi|^2$. Hence, the inverse formula of Fourier transform

$$\psi(t, x) = (2\pi)^{-\frac{n}{2}}\int_{\mathbb{R}^n} e^{ix\cdot\xi}\hat{\psi}(t, \xi)\ d\xi \tag{23}$$

represents the expansion of the operator $-\triangle$ via eigenfunction $e^{ix\cdot\xi}$. If we take the Fourier transform both of the sides in the free Schrödinger equation with $V = 0$

$$i\frac{\partial}{\partial t}\psi(t,x) = -\frac{1}{2}\Delta\psi(t,x) \tag{24}$$

which describes the free field or the vacuum, then we obtain

$$i\frac{\partial}{\partial t}\hat{\psi}(t,\xi) = \frac{1}{2}|\xi|^2\hat{\psi}(t,\xi). \tag{25}$$

This equation is an ordinary differential equation with a variable t and a parameter ξ, so that we can solve

$$\hat{\psi}(t,\xi) = e^{-i\frac{|\xi|^2}{2}t}\hat{\psi}_0(\xi). \tag{26}$$

Since $\hat{\psi}$ is an expression of a wavefunction in momentum space $\mathbb{R}^n$, the inverse formula of Fourier transform implies the expression of the wavefunction in ordinary coordinate space

$$\psi(t,x) = (2\pi)^{-\frac{n}{2}}\int_{\mathbb{R}^n} e^{ix\cdot\xi}e^{-i\frac{|\xi|^2}{2}t}\hat{\psi}_0(\xi)\ d\xi. \tag{27}$$

From the relation (26) and Plancherel formula, we also have the energy estimate to the vacuum

$$\|\psi(t,\bullet)\| = \|\hat{\psi}(t,\bullet)\| = \|\hat{\psi}_0\| = \|\psi_0\|. \tag{28}$$

For instance, when we take Gaussian distribution

$$\psi_0(x) = e^{-\frac{1}{2}|x|^2} \tag{29}$$

as initial data in the vacuum, then we can calculate

$$\hat{\psi}_0(\xi) = e^{-\frac{1}{2}|\xi|^2} \tag{30}$$

by the definition of Fourier transform. Accordingly we have the wavefunction

$$\psi(t,x) = \{2\pi(1+it)\}^{-\frac{n}{2}}\, e^{-\frac{|x|^2}{2(1+it)}} \tag{31}$$

which satisfies the free Schrödinger equation (24). In this case, we have the decay rate of the survival probability

$$\overline{\psi(t,x)}\psi(t,x) = \left\{4\pi^2(1+t^2)\right\}^{-\frac{n}{2}}\, e^{-\frac{|x|^2}{1+t^2}} \leq (2\pi)^{-n}t^{-n}, \tag{32}$$

so that we obtain

$$|\psi(t,x)| \leq (2\pi)^{-n/2}t^{-n/2} \tag{33}$$

for any $t \in \mathbb{R}$ and $x \in \mathbb{R}^n$, as a pointwise estimate in the decay of the wavefunction.

This is a result of estimate for time decay in the free fields. We have already obtained the results [9] [6] for time decay property of wavefunctions or survival probabilities. Those results suggest that the decay rate is essentially based on the momentum distribution around the origin. We also know the example [2] for $n = 1$.

3 Representation of Kinetic Fields

The Schrödinger equation with potential terms

$$i\frac{\partial}{\partial t}\psi(t,x) = -\frac{1}{2}\triangle\psi(t,x) + V(t,x)\psi(t,x) \tag{34}$$

describes state of quantum partiles exist in the potential $V(t,x)$.

As generalization of Euclidean spaces $\mathbb{R}^n$ we introduce a metric g_{jk} $(j,k = 1,\dots,n)$ in order to define the coordinate system of a manifold. A metric g_{jk} may depend time and space variables $g_{jk} = g_{jk}(t,x)$.

With a metric of fields, we can write the Schrödinger equation such as

$$i\frac{\partial}{\partial t}\psi(t,x) = -\frac{1}{2}\sum_{j=1}^{n}\sum_{k=1}^{n}\frac{\partial}{\partial x_j}\left(g_{jk}(t,x)\frac{\partial}{\partial x_k}\psi(t,x)\right), \tag{35}$$

which is also called the Schrödinger type equation.

Although metric g_{jk} represents arbitrary structure of manifolds, we should impose some restrictions in the Cauchy problem for Schrödinger type equations.

First, g_{jk} is real, that is

$$g_{jk} : (t,x) \in \mathbb{R}\times\mathbb{R}^n \to \mathbb{R}. \tag{36}$$

for any j and k possible. Second, g_{jk} is symmetric, that is

$$g_{kj} = g_{jk} \tag{37}$$

for any j and k possible.

Third, g_{jk} is elliptic, that is there exists $C > 0$ such that

$$\sum_{j=1}^{n}\sum_{k=1}^{n} g_{jk}(t,x)\xi_j\xi_k \geq C|\xi|^2 \tag{38}$$

holds for any $\xi = (\xi_1,\dots,\xi_n) \in \mathbb{R}^n$.

3.1 Exsistence and Uniqueness of Wavefunctions

Let us consider the Schrödinger type equation

$$i\frac{\partial}{\partial t}\psi(t,x) = -\frac{1}{2}\sum_{j=1}^{n}\sum_{k=1}^{n}\frac{\partial}{\partial x_j}\left(g_{jk}(t,x)\frac{\partial}{\partial x_k}\psi(t,x)\right) \tag{39}$$

with initial data $\psi(0,x) = \psi_0(x)$.

In the following discussion, $\Re z$ and $\Im z$ stand respectively for the real and the imaginary part of a complex number $z \in \mathbb{C}$. In order to estimate the energy for a wavefunction $\psi(t,x)$, we have

$$\begin{aligned}
\frac{d}{dt}\|\psi(t,\bullet)\|^2 &= \frac{d}{dt}\left(\psi(t,\bullet),\psi(t,\bullet)\right)\\
&= \left(\frac{d}{dt}\psi(t,\bullet),\psi(t,\bullet)\right) + \left(\psi(t,\bullet),\frac{d}{dt}\psi(t,\bullet)\right)\\
&= \left(\frac{d}{dt}\psi(t,\bullet),\psi(t,\bullet)\right) + \overline{\left(\frac{d}{dt}\psi(t,\bullet),\psi(t,\bullet)\right)}\\
&= 2\Re\left(\frac{d}{dt}\psi(t,\bullet),\psi(t,\bullet)\right)\\
&= 2\Re\left(-\frac{1}{2i}\sum_{j=1}^{n}\sum_{k=1}^{n}\frac{\partial}{\partial x_j}\left(g_{jk}(t,x)\frac{\partial}{\partial x_k}\psi(t,\bullet)\right),\psi(t,\bullet)\right)\\
&= -\Im\left(\sum_{j=1}^{n}\sum_{k=1}^{n}\frac{\partial}{\partial x_j}\left(g_{jk}(t,x)\frac{\partial}{\partial x_k}\psi(t,\bullet)\right),\psi(t,\bullet)\right)\\
&= \Im\sum_{j=1}^{n}\sum_{k=1}^{n}\left(g_{jk}(t,x)\frac{\partial}{\partial x_k}\psi(t,\bullet),\frac{\partial}{\partial x_j}\psi(t,\bullet)\right)
\end{aligned} \tag{40}$$

and the property of g_{jk} implies

$$\begin{aligned}
&\overline{\sum_{j=1}^{n}\sum_{k=1}^{n}\left(g_{jk}(t,x)\frac{\partial}{\partial x_k}\psi(t,\bullet),\frac{\partial}{\partial x_j}\psi(t,\bullet)\right)}\\
&=\sum_{j=1}^{n}\sum_{k=1}^{n}\left(\frac{\partial}{\partial x_j}\psi(t,\bullet),g_{jk}(t,x)\frac{\partial}{\partial x_k}\psi(t,\bullet)\right)\\
&=\sum_{j=1}^{n}\sum_{k=1}^{n}\left(g_{jk}(t,x)\frac{\partial}{\partial x_j}\psi(t,\bullet),\frac{\partial}{\partial x_k}\psi(t,\bullet)\right)\\
&=\sum_{k=1}^{n}\sum_{j=1}^{n}\left(g_{kj}(t,x)\frac{\partial}{\partial x_k}\psi(t,\bullet),\frac{\partial}{\partial x_j}\psi(t,\bullet)\right)\\
&=\sum_{k=1}^{n}\sum_{j=1}^{n}\left(g_{jk}(t,x)\frac{\partial}{\partial x_k}\psi(t,\bullet),\frac{\partial}{\partial x_j}\psi(t,\bullet)\right).
\end{aligned} \tag{41}$$

Remember the identity $z - \bar{z} = 2\Im z$, we conclude

$$\frac{d}{dt}\|\psi(t,\bullet)\|^2 = 0 \tag{42}$$

which is equivalent to

$$\|\psi(t,\bullet)\| = \|\psi_0\|. \tag{43}$$

This energy estimate assures that there exists a unique wavefunction ψ in $\mathcal{H}$ for any time if we take initial data ψ_0 from Hilbert space $\mathcal{H}$. After all, we have the fact that the Cauchy problem for the above Schrödinger type equations is wellposed.

3.2 Matrix Representation in Schrödinger Equations

Definition 3.1 *We define the nabla operator*

$$\nabla = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \cdots, \frac{\partial}{\partial x_n}\right) \tag{44}$$

as a vector expression of differential operators.

Laplacian is expressed by $\triangle = \nabla \cdot \nabla$.

As matrix representation of the metric g_{jk}, we use

$$A(t,x) = \begin{pmatrix} g_{11}(t,x) & g_{12}(t,x) & \cdots & g_{1n}(t,x) \\ g_{21}(t,x) & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ g_{n1}(t,x) & \dots & \dots & g_{nn}(t,x) \end{pmatrix}. \tag{45}$$

Then, we obtain the simple form

$$i\frac{\partial}{\partial t}\psi(t,x) = -\frac{1}{2}\nabla A(t,x)\nabla^T\psi(t,x) \tag{46}$$

for Schrödinger type equations with matrix the $A(t,x)$, where ∇^T denotes the transpose vector of ∇. When $A(t,x) = E$, the operator in the right-hand side is equal to Laplacian $\triangle$, so that the identity matrix E in $\mathbb{R}^{n\times n}$ represents the structure of the free field without potential terms.

3.3 Potential Representation via Metric

It is neccesary that

$$-\frac{1}{2}\nabla A(t,x)\nabla^T\psi(t,x) = -\frac{1}{2}\triangle\psi(t,x) + V(t,x)\psi(t,x), \tag{47}$$

if Schrödinger type equations and Schrödinger equations with potential terms are equivalent. Paying attention to $\triangle = \nabla E \nabla^T$, we obtain

$$V(t,x) = \frac{1}{2}\nabla(E - A(t,x))\nabla^T. \tag{48}$$

The potential term $V(t,x)$ in the left-hand side is represented by the operators including metric. It is trivial that $V(t,x) = 0$ if $A(t,x) = E$.

3.4 Representation of Metric Matrices via Potential

Contrary to the previous section, we represent metric matrices via potential terms. Because the number of the elements of a metric matrix A is $n \times n$, representation form of the metric matrix via potential terms is not unique. Hence, we seek a natural form of the coefficients of the second differential operators in Schr̈dinger type equations in $n = 1$.

The condition that Schr̈dinger type equations and Schr̈dinger equations with potential terms are equivalent is

$$-\frac{1}{2}\frac{\partial}{\partial x}\left(a(t,x)\frac{\partial}{\partial x}\psi(t,x)\right) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi(t,x) + V(t,x)\psi(t,x). \tag{49}$$

For some point $x_0 \in \mathbb{R}$, integrating around x implies

$$\begin{aligned} & a(t,x)\frac{\partial}{\partial x}\psi(t,x) - a(t,x_0)\frac{\partial}{\partial x}\psi(t,x_0) \\ & = \frac{\partial}{\partial x}\psi(t,x) - \frac{\partial}{\partial x}\psi(t,x_0) - 2\int_{x_0}^{x} V(t,y)\psi(t,y)\ dy. \end{aligned} \tag{50}$$

We know that $u(t,x_0) \to 0$ when $x_0 \to \infty$. Therefore,

$$a(t,x)\frac{\partial}{\partial x}\psi(t,x) = \frac{\partial}{\partial x}\psi(t,x) - 2\int_{\infty}^{x} V(t,y)\psi(t,y)\ dy. \tag{51}$$

Now, we put

$$Q(t,x) = \frac{1}{2}(E - A(t,x)) \tag{52}$$

using the matrix $Q(t,x) = [q(t,x)]$, the equation (49) becomes

$$\begin{aligned} \frac{\partial}{\partial x}q(t,x)\frac{\partial}{\partial x}\psi(t,x) &= V(t,x)\psi(t,x) \\ &= \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}\right)^{-1} V(t,x)\left(\frac{\partial}{\partial x}\right)^{-1}\frac{\partial}{\partial x}\psi(t,x). \end{aligned} \tag{53}$$

It is neccesary for the representation of metric matrices via potential terms that the relation

$$q(t,x) = \left(\frac{\partial}{\partial x}\right)^{-1} V(t,x)\left(\frac{\partial}{\partial x}\right)^{-1} \tag{54}$$

holds, where we assume the integral constant $q(t, x_0)$ is 0 in the choce of x_0. Hence, we have

$$A(t,x) = E - 2Q(t,x) = 1 - 2\left(\frac{\partial}{\partial x}\right)^{-1} V(t,x)\left(\frac{\partial}{\partial x}\right)^{-1} \tag{55}$$

for $n = 1$.

In the above discussion, for f satisfies

$$\xi^{-1}\hat{f}(\xi) \in \mathcal{H}, \tag{56}$$

we used

$$\left(\frac{\partial}{\partial x}\right)^{-1} f(x) = (2\pi)^{-\frac{n}{2}} \int_{-\infty}^{\infty} e^{ix\cdot\xi}\xi^{-1}\hat{f}(\xi)\, d\xi. \tag{57}$$

This defines the inverse of differential operators via Fourier transform.

In general, differential operators are expressed by

$$p(D)f(x) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} e^{ix\cdot\xi} p(\xi)\hat{f}(\xi)\, d\xi, \quad n = 1 \tag{58}$$

using a polynomial

$$p(\xi) = \sum_{j=0}^{N} c_j \xi^j = c_0 + c_1\xi + \cdots + c_N\xi^N. \tag{59}$$

Here f is N times differentiable and

$$D = -i\frac{\partial}{\partial x} \tag{60}$$

is the corresponding differential operator. It should be remarked from the expression via Fourier transform that f is N times differentiable if and only if $\xi^N\hat{f}$ belongs to $\mathcal{H}$. It is also clear that p may not a polynomial, and that p can be an arbitrary function for natural extension.

4 Concluding Remarks

We have proven the necessary and sufficient condition for the equivalence between Schrödinger type equation and Schrödinger equation with potential terms.

We can derive the potential terms in Schrödinger equation from the representation of fields in Schrödinger type equation, while we can derive the metric matrices in Schrödinger type equation from the potential terms in Schrödinger equation only in $n = 1$. The latter claim in $n \geq 2$ remains open.

It is possible to discuss the mathematical structure of wavefunctions in Schrödinger equation via Riemannian manifolds instead of potential terms.

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