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On a Complex Fundamental Solution of the Schrödinger Equation

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Abstract—A second-order Schrödinger differential operator of parabolic type is considered, for which an explicit form of a fundamental solution is derived. Such operators arise in many problems of physics, and the fundamental solution plays the role of the Feynman propagation function.

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In [1] (see also [2]), a fundamental solution of a parabolic equation with real coefficient (a Fokker–Planck–Kolmogorov equation) was obtained. In this paper, we use similar methods to investigate a parabolic equation with complex coefficients (the Schrödinger equation) and special initial conditions. For this equation, we obtain a complex fundamental solution, which is the Feynman propagation function.

1. STATEMENT OF THE PROBLEM AND THE RESULT

Let $x = (x_1, \dots, x_n) \in \mathbb{R}^n$ be a vector variable of dimension n, and let $t \in \mathbb{R}_+ = [0, +\infty)$ be a distinguished one-dimensional variable playing the role of time. We denote the class of complex-valued functions $u(t, x)$: $\mathbb{R}_+ \times \mathbb{R}^n \to \mathbb{C}$ having continuous partial derivatives ∂_t, ∂_{x_k}, and $\partial^2_{x_k x_l}$ $(k, l = 1, 2, \dots, n)$ on $\mathbb{R}_+ \times \mathbb{R}^n$ by $C^{1,2}(\mathbb{R}_+ \times \mathbb{R}^n; \mathbb{C})$.

We say that an operator $\mathcal{L}$ is a second-order complex operator if it has the form

$$\mathcal{L}[v] = \frac{(-i)^2}{2}\sum_{k,j=1}^n A_{kj}(t)\frac{\partial^2 v}{\partial x_k \partial x_j} + (-i)\sum_{k=1}^n\left(\sum_{j=1}^n \left(B_{kj}(t)x_j + c_k(t)\right)\right)\frac{\partial v}{\partial x_k} + \left(\sum_{k,j=1}^n F_{kj}(t)x_k x_j + \sum_{k=1}^n g_k(t)x_i + h(t)\right)v,$$

where the $A_{kj}(t)$, $B_{kj}(t)$, $c_k(t)$, $F_{kj}(t)$, and $g_k(t)$ with $k, j = 1, 2, \dots, n$, and $h(t)$ are real-valued functions depending only on time.

Accordingly, a second-order complex equation is an equation of the form

$$-i\hbar\dot{u} = \mathcal{L}[u]. \tag{1}$$

Remark 1. Note that Eq. (1) is an analogue of the multidimensional Schrödinger equation with Hamiltonian of the form

$$\mathcal{H} = \frac{1}{2}\sum_{k,j=1}^n A_{kj}(t)p_k p_j + \sum_{k=1}^n\left(\sum_{j=1}^n \left(B_{kj}(t)x_j + c_k(t)\right)\right)p_k + \left(\sum_{k,j=1}^n F_{kj}(t)x_k x_j + \sum_{k=1}^n g_k(t)x_i + h(t)\right)$$

on the right-hand side, where $p_k = -i\dfrac{\partial}{\partial x_k}$ is the momentum coordinate of a quantum particle (see, e.g., [4]).

Assumption A. The coefficients $A(t)$, $B(t)$, $F(t)$: $\mathbb{R}_+ \to \mathbf{M}_{n\times n}(\mathbb{R})$ of a second-order complex operator $\mathcal{L}$ are continuous functions on $\mathbb{R}_+$ having finite limits $A_0, B_0, F_0 \in \mathbf{M}_{n\times n}(\mathbb{R})$, respectively, as $t \to 0$. It is assumed that the matrix $A(t)$ is symmetric and the matrix A_0 is positive definite.

Suppose that a solution of the Cauchy problem

$$P' = -\frac{1}{\hbar}P\left(\frac{2}{\hbar}SA + B^{\mathrm{T}}\right) - \frac{1}{\hbar}\left(\frac{2}{\hbar}AS + B\right)P - \frac{2}{\hbar^2}A, \qquad P\big|_{t=0} = \mathbf{0} \in \mathbf{M}_{n\times n}(\mathbb{R}), \tag{2}$$

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where $S(t)$ is a symmetric solution of the problem

$$S' = \frac{2}{\hbar^2}SAS + \frac{1}{\hbar}(SB + B^{\mathrm{T}}S) + \frac{1}{2}(F + F^{\mathrm{T}}), \qquad S\big|_{t=0} = \mathbf{0} \in \mathbf{M}_{n\times n}(\mathbb{R}), \tag{3}$$

can be represented in a neighborhood of zero in the form

$$P(t) = -\frac{2t}{\hbar^2}A_0 + \frac{1}{\hbar^2}R(t), \tag{4}$$

where $R(t)$ is a matrix defined on the interval $[0, \varepsilon]$ for some constant $0 < \varepsilon \ll 1$.

We introduce the following notation:

$$Q(t) = -\frac{1}{2t}R(t)A_0^{-1}, \tag{5}$$

$$\bar{Q}(t) = [E + Q(t)]^{-1} - E, \tag{6}$$

$$\tilde{Q}(t) = \bar{Q}(t) + (A(t) - A_0)A_0^{-1}[E + \bar{Q}], \tag{7}$$

$$\tilde{q}(t) = \frac{1}{n}\operatorname{tr}\tilde{Q}. \tag{8}$$

Assumption B. For $0 \le t < \varepsilon$, the following improper integral exists and is finite:

$$\int_0^t \frac{\tilde{q}(s)}{s}ds < +\infty.$$

Suppose given the systems of differential equations

$$\begin{aligned} S' &= \frac{2}{\hbar^2}SAS + \frac{1}{\hbar}(SB + B^{\mathrm{T}}S) + \frac{1}{2}(F + F^{\mathrm{T}}),\\ q' &= \frac{1}{\hbar^2}(2SA + \hbar B^{\mathrm{T}})q + \frac{2}{\hbar}Sc + g,\\ r' &= \frac{1}{2\hbar^2}q^{\mathrm{T}}Aq + \frac{1}{\hbar}q^{\mathrm{T}}c + h, \quad \psi' = -\frac{1}{\hbar}\operatorname{tr}(AS) \end{aligned} \tag{9}$$

and

$$\begin{aligned} P' &= -\frac{1}{\hbar}P\left(\frac{2}{\hbar}SA + B^{\mathrm{T}}\right) - \frac{1}{\hbar}\left(\frac{2}{\hbar}AS + B\right)P - \frac{2}{\hbar^2}A,\\ m' &= -\frac{1}{\hbar}\left(\frac{2}{\hbar}AS + B\right)m - \frac{1}{\hbar^2}Aq - \frac{1}{\hbar}c,\\ C' &= C\cdot\frac{1}{\hbar^2}(\operatorname{tr}(AP^{-1})). \end{aligned} \tag{10}$$

Consider the Cauchy problem for the operator $i\hbar\frac{\partial}{\partial t} + \mathcal{L}$ introduced above:

$$-i\hbar\frac{\partial u}{\partial t} = \mathcal{L}[u], \qquad u\big|_{t=0} = \delta_y(x), \tag{11}$$

where $\delta_y(x)$ is the delta-function with singularity at $y \in \mathbb{R}^n$.

Theorem 1. *If assumptions* A *and* B *hold, then a solution of the Cauchy problem* (11) *is the function* $u(t, x)$ *equal to*

$$\begin{aligned} &\exp\left\{-\frac{x^{\mathrm{T}}S(t)x + q^{\mathrm{T}}(t)x + r(t) + i\psi(t)}{i\hbar}\right\}(1+i)C(t)\\ &\times\exp\left\{-\frac{\langle P^{-1}(t)(x - m(t;\,y)), (x - m(t;\,y))\rangle}{i\hbar}\right\}, \end{aligned} \tag{12}$$

where $S(t)$, $q(t)$, $r(t)$, *and* $\psi(t)$ *are solutions of system* (9) *with initial conditions* $S_{kj}(0) = q_l(0) = r(0) = \psi(0) = 0$ *for any* $k, j, l \in 1, 2, \ldots, n$; $P(t)$ *and* $m(t; y)$ *are solutions of the first two equations of system* (10) *with initial conditions* $P_{kj}(0) = 0$ *for any* $k, j \in 1, 2, \ldots, n$; $m(0) = y$; *and* $C(t)$ *is a particular solution of the third equation of system* (10) *having the form*

$$C(t) = \frac{\sqrt{\hbar^n}}{\sqrt{2i(-2i)^n(\pi t)^n\det A_0}}\exp\left\{-\frac{n}{2}\int_0^t\frac{\tilde{q}(s)}{s}ds\right\}. \tag{13}$$

2. AUXILIARY ASSERTIONS

The following assertion (an analogue of Theorem 3.1 in [3]) holds.

Lemma 1. *A nonvanishing function* $\rho \in C^{1,2}(\mathbb{R}_+\times\mathbb{R}^n; \mathbb{C})$ *of the form*

$$\rho(t, x) = \exp\left\{\frac{i}{\hbar}(x^{\mathrm{T}}S(t)x + q^{\mathrm{T}}(t)x + \tilde{r}(t))\right\}, \tag{14}$$

where $S \in \mathbf{M}_{n\times n}(\mathbb{R})$, *is a solution of the second-order complex equation* (1) *if and only if its coefficients* $S(t)$, $q(t)$, *and* $\tilde{r}(t)$ *satisfy the Riccati-type system of equations*

$$\begin{aligned} S' &= \frac{1}{2\hbar^2}(S^{\mathrm{T}}AS + SAS^{\mathrm{T}} + 2SAS)\\ &\quad + \frac{1}{\hbar}(SB + B^{\mathrm{T}}S^{\mathrm{T}}) + \frac{1}{2}(F + F^{\mathrm{T}}),\\ q' &= \frac{1}{2\hbar^2}(2SA + 2S^{\mathrm{T}}A + 2\hbar B^{\mathrm{T}})q + \frac{1}{\hbar}(Sc + S^{\mathrm{T}}c) + g,\\ \tilde{r} &= \frac{1}{2\hbar^2} + \frac{1}{2}q^{\mathrm{T}}Aq + \frac{1}{\hbar}(q^{\mathrm{T}}c - i\operatorname{tr}(AS)) + h. \end{aligned} \tag{15}$$

The following two lemmas are similar to those given in [1].

Lemma 2. *A function* $v \in C^{1,2}(\mathbb{R}_+\times\mathbb{R}^n; \mathbb{C})$ *of the form*

$$\begin{aligned} v(t, x) &= \frac{\widetilde{C}(t)}{\rho(t, x)}\\ &\times\exp\left\{\frac{i}{\hbar}\langle P^{-1}(t)(x - m(t)), (x - m(t))\rangle\right\}, \end{aligned} \tag{16}$$

where the coefficients $\widetilde{C}(t)$ *and* $m(t)$ *are defined by*

$$m = -\frac{1}{2}Pq \tag{17}$$

and

$$\widetilde{C} = \exp\left\{\frac{i}{\hbar}\left(\tilde{r} - \frac{1}{4}\langle Pq, q\rangle\right)\right\} \tag{18}$$

and the function $\rho(t, x)$ *satisfies* (14), *is a solution of the equation*

$$-i\hbar\frac{\partial v}{\partial t} = -\left\langle\frac{1}{2}A, \frac{\partial^2 v}{\partial x^2}\right\rangle - \frac{i}{\hbar}\left\langle\widehat{B}x + \hat{c}, \frac{\partial v}{\partial x}\right\rangle, \tag{19}$$

in which $\widehat{B} = 2AS + \hbar B$ *and* $\hat{c} = Aq + \hbar c$ *if and only if, after the change* $\widetilde{C}(t) = C(t)(1+i)$, *its coefficients satisfy system* (10).

Let $P(t)$ and $m(t; y)$ be solutions of the first two equations in system (10) with initial conditions $P_{ij}(0) = 0$ for $i, j \in 1, 2, \dots, n$ and $m(0) = y$, and let $C(t)$ be a particular solution of the third equation in system (10) of the form (13).

Consider the function $G(t, x; y)$: $\mathbb{R}_+ \times \mathbb{R}^n \times R^n \to \mathbb{C}$

$$G(t, x; y) = (1+i)C(t)$$
$$\times \exp\left\{\frac{i}{\hbar}\langle P^{-1}(t)(x - m(t; y)), (x - m(t; y))\rangle\right\}.$$

Lemma 3. *Let* $\phi(x)$: $\mathbb{R}^n \to \mathbb{R}$ *be a function of class* $C_0^\infty(\mathbb{R}^n)$. *Suppose that*

$$f(t, x) = \int_{\mathbb{R}^n}\phi(y)G(t, y; x)dy.$$

Then $f(t, x) \to \phi(x)$ *as* $t \to 0$.

3. PROOF OF THE MAIN STATEMENT

Proof of Theorem 1. Let us represent the solution of the Cauchy problem (11) as a product:

$$u(t, x) = \rho(t, x)v(t, x).$$

It is easy to see that the problem decomposes into the two subproblems

$$-i\hbar\frac{\partial\rho}{\partial t} = \mathcal{L}[\rho], \quad \rho|_{t=0} = 1 \tag{20}$$

and

$$-i\hbar\frac{\partial v}{\partial t} = \mathcal{F}[v], \quad v|_{t=0} = \delta_y(x), \tag{21}$$

where $\mathcal{L}$ is a second-order operator and $\mathcal{F}$ is the operator corresponding to the right-hand side of Eq. (19).

By virtue of Lemma 1, there exists a solution $\rho(t, x)$ of problem (20) which has the form (14), where $S(t)$, $q(t)$, $r(t)$, and $\psi(t)$ are solutions of system (9) with initial conditions $S_{ij}(0) = q_k(0) = r(0) = \psi(0) = 0$ for any $i, j, k \in 1, 2, \dots, n$.

Next, by virtue of Lemma 2, there exists a function $v(t, x)$ of the form (16), where $P(t)$, $m(t)$, and $C(t)$ are solutions of system (10). By virtue of Lemma 3, under the initial conditions $P_{ij}(0) = 0$ for any $i, j \in 1, 2, \dots, n$, $m(0) = y$ and

$$C(1) = \frac{\sqrt{\hbar^n}}{\sqrt{2i(-2i)^n\pi^n \det A_0}}\exp\left\{-\frac{n}{2}\int_0^1\frac{\tilde{q}(s)}{s}ds\right\}$$

we have $v(t, x) \to \delta_y(x)$ as $t \to 0$.

Obviously, under the initial conditions on $S(t)$, $q(t)$, $r(t)$, $\psi(t)$, $P(t)$, $m(t)$, and $C(t)$ specified above, the product $\rho(t, x)v(t, x)$ also tends to $\delta_y(x)$ as $t \to 0$.

This completes the proof of the theorem.

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