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Exact solutions to three-dimensional time-dependent Schrödinger equation

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Abstract. With a view to obtain exact analytic solutions to the time-dependent Schrödinger equation for a few potentials of physical interest in three dimensions, transformation-group method is used. Interestingly, the integrals of motion in the new coordinates turn out to be the desired invariants of the systems.

Keywords. Schrödinger equation; dynamical invariants.

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1. Introduction

The study of exactly solvable potentials has attracted much interest since the early development of quantum mechanics. The explicit expressions for the eigenvalues, eigenfunctions and the scattering matrix give a better insight into the detailed properties of a dynamical system. The exact solution of time-dependent Schrödinger equation (TDSE) is possible only for a few potentials such as Coulomb and harmonic oscillator potentials. The usual approach for solving TDSE has been time-dependent (TD) perturbation theories which is probably the primary computational method. However, much could be gained from the study of exactly solvable TD models as analytic results are much easier to use, interpret and to generalize.

Recently, considerable efforts have been made [1–8] to develop various techniques to get exact solution of TDSE with varying degree of success and domains of applicability. Lewis and Riesenfield [9,10] developed the theory of invariants and used it to investigate the quantum state of TD Hamiltonian systems. Thereafter, several authors [11,12] used invariants in the study of coherent states, transition probabilities and squeezed states. Therefore, the existence and subsequent construction of dynamical invariants for a TD system is of prime importance as far as understanding of the system is concerned.

The purpose of this paper is to extend Ray [13] approach, which is based on the transformation-group technique introduced by Burgan *et al* [1], in which a scale and phase transformation of dependent variable and a scale transformation of the independent space–time variables reduce TDSE in some complicated form and then imposing a condition of form invariance of TDSE on the transformed equation which in turn modifies the potential. A further phase transformation of the dependent variable converts this new TDSE into a time-indepedent (TID) SE in one of the standard forms whose exact solutions are usually known. Interestingly, the Hamiltonian analog of the transformed TIDSE is a constant of motion. Thus, there is direct connection between the solutions of TDSE of a system and its dynamical invariants which can be constructed by a variety of methods [14,15].

The plan of the paper is as follows: In §2, the method developed by Ray [13] is generalized to study three-dimensional systems and examples are considered in §3. The results are discussed in §4.

2. The method

The TDSE ($\hbar = \mu = 1$) for a system described by $V(x, y, z, t)$ is written as

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z, t)\right]\Psi(x, y, z, t) = i\frac{\partial \Psi}{\partial t}. \tag{2.1}$$

Truax [4] has classified potentials for the TDSE, eq. (2.1), according to their space–time or kinematical algebra in a search for exactly solvable TD models. Here we use Ray approach [13], essentially based on the generalization of the group-transformation method of Burgan *et al* [1], to solve SE for some TD potentials.

Carry out the following transformations on wave function, space and time [1]

$$\Psi(x, y, z, t) = B(t)\exp[i\phi(x, y, z, t)]\psi(x', y', z', t'), \tag{2.2}$$

$$\begin{aligned} x' &= \frac{x}{C_1(t)} + A_1(t); \quad y' = \frac{y}{C_2(t)} + A_2(t); \\ z' &= \frac{z}{C_3(t)} + A_3(t); \quad t' = D(t), \end{aligned} \tag{2.3}$$

where $B(t)$ is a TD normalization.

Therefore, eq. (2.1) can be written after using eqs. (2.2) and (2.3) as

$$\begin{aligned} &-\frac{B}{2}\left[\frac{1}{C_1^2}\psi_{x'x'} + \frac{1}{C_2^2}\psi_{y'y'} + \frac{1}{C_3^2}\psi_{z'z'} + 2i\left(\frac{1}{C_1}\phi_x\psi_{x'} + \frac{1}{C_2}\phi_y\psi_{y'}\right.\right. \\ &\left.\left.+\frac{1}{C_3}\phi_z\psi_{z'}\right) + i(\phi_{xx} + \phi_{yy} + \phi_{zz})\psi - (\phi_x^2 + \phi_y^2 + \phi_z^2)\psi\right] + VB\psi \\ &= i\dot{B}\psi - B\phi_t\psi + iB\dot{D}\psi_{t'} + iB\left[\left(\dot{A}_1 - x\frac{\dot{C}_1}{C_1^2}\right)\psi_{x'}\right. \\ &\left.+\left(\dot{A}_2 - y\frac{\dot{C}_2}{C_2^2}\right)\psi_{y'} + \left(\dot{A}_3 - z\frac{\dot{C}_3}{C_3^2}\right)\psi_{z'}\right]. \end{aligned} \tag{2.4}$$

Here the subscripts (x, x'), (t, t') etc. represent differentiation with respect to these variables and dot indicates time derivative.

In order to retain eq. (2.1) form invariant, equate the coefficients of $\psi_{x'}, \psi_{y'}$ and $\psi_{z'}$ on both sides of eq. (2.4). Thereby, one obtains a set of three first-order differential equations, which immediately give expressions for $\phi(x, y, z, t)$ as given below.

$$\phi = \frac{\dot{C}_1}{2C_1}x^2 - \dot{A}_1 C_1 x + \sigma_1(y, z, t),$$

$$\phi = \frac{\dot{C}_2}{2C_2}y^2 - \dot{A}_2 C_2 y + \sigma_2(x, z, t),$$

and

$$\phi = \frac{\dot{C}_3}{2C_3}z^2 - \dot{A}_3 C_3 z + \sigma_3(x, y, t),$$

where σ_1, σ_2 and σ_3 are integration constants, which can be adjusted in order to find a unique solution for ϕ, which is given as

$$\phi = \frac{1}{2}\left(\frac{\dot{C}_1}{C_1}x^2 + \frac{\dot{C}_2}{C_2}y^2 + \frac{\dot{C}_3}{C_3}z^2\right) - (\dot{A}_1 C_1 x + \dot{A}_2 C_2 y + \dot{A}_3 C_3 z). \qquad (2.5)$$

Now putting the value of ϕ from eq. (2.5) in eq. (2.4) and setting $C_1 = C_2 = C_3 = C$, we get

$$\begin{aligned} &-\frac{1}{2}(\psi_{x'x'} + \psi_{y'y'} + \psi_{z'z'}) + C^2 V\psi + \frac{1}{2}\ddot{C}C(x^2 + y^2 + z^2)\psi \\ &-C^2[(2\dot{A}_1\dot{C} + \ddot{A}_1 C)x + (2\dot{A}_2\dot{C} + \ddot{A}_2 C)y + (2\dot{A}_3\dot{C} + \ddot{A}_3 C)z]\psi \\ &+\frac{1}{2}C^4(\dot{A}_1^2 + \dot{A}_2^2 + \dot{A}_3^2)\psi - \frac{i}{2}C\left(3\dot{C} + 2C\frac{\dot{B}}{B}\right)\psi = iC^2\dot{D}\psi_{t'}. \end{aligned} \qquad (2.6)$$

To ensure that the above equation remains TDSE in new space and time coordinates, we should make the following choices:

$$C^2\dot{D} = 1,$$

which immediately reads as

$$t' = D(t) = \int \frac{\mathrm{d}t}{C^2}, \qquad (2.7)$$

and the term $-\frac{i}{2}C(3\dot{C} + 2C\frac{\dot{B}}{B})$ in eq. (2.6) must be zero to ensure a real potential, which gives the normalization term $B(t)$ in terms of $C(t)$ as

$$B(t) = \frac{1}{C\sqrt{C}}. \qquad (2.8)$$

Note that the expression for $B(t)$ is different when compared to one- [13] and two- [5] dimensional systems.

Hence the expression for $\phi(x,y,z,t)$ in eq. (2.5) reduces to a simpler form as

$$\phi = \frac{1}{2}\frac{\dot{C}}{C}(x^2+y^2+z^2) - C(\dot{A}_1 x + \dot{A}_2 y + \dot{A}_3 z). \tag{2.9}$$

Finally, eq. (2.6) becomes

$$-\frac{1}{2}(\psi_{x'x'} + \psi_{y'y'} + \psi_{z'z'}) + V'(x',y',z',t')\psi = i\psi_{t'}, \tag{2.10}$$

where the potential V' is given by

$$\begin{aligned} V' = {} & VC^2 + \frac{1}{2}\ddot{C}C(x^2+y^2+z^2) - C^2[(2\dot{A}_1\dot{C} + \ddot{A}_1 C)x \\ & + (2\dot{A}_2\dot{C} + \ddot{A}_2 C)y + (2\dot{A}_3\dot{C} + \ddot{A}_3 C)z] \\ & + \frac{1}{2}C^4(\dot{A}_1^2 + \dot{A}_2^2 + \dot{A}_3^2). \end{aligned} \tag{2.11}$$

In the next section we will apply the above results in order to solve the TDSE for some TD three-dimensional dynamical systems.

3. Examples

Case 1

Consider a three-dimensional shifted rotating harmonic oscillator system described by the potential

$$\begin{aligned} V(x,y,z,t) = {} & a_1(t)x^2 + b_1(t)y^2 + c_1(t)z^2 + a_2(t)x \\ & + b_2(t)y + c_2(t)z + d(t). \end{aligned} \tag{3.1}$$

After using eq. (3.1) and the inverse transformations from eq. (2.3) in eq. (2.11), we get

$$\begin{aligned} V' = {} & C^3\left[\left(a_1 C + \frac{\ddot{C}}{2}\right)x'^2 + \left(b_1 C + \frac{\ddot{C}}{2}\right)y'^2 + \left(c_1 C + \frac{\ddot{C}}{2}\right)z'^2\right] \\ & + C^3\left[(a_2 - C\ddot{A}_1 - 2\dot{C}\dot{A}_1) - 2A_1\left(a_1 C + \frac{\ddot{C}}{2}\right)\right]x' \\ & + C^3\left[(b_2 - C\ddot{A}_2 - 2\dot{C}\dot{A}_2) - 2A_2\left(b_1 C + \frac{\ddot{C}}{2}\right)\right]y' \\ & + C^3\left[(c_2 - C\ddot{A}_3 - 2\dot{C}\dot{A}_3) - 2A_3\left(c_1 C + \frac{\ddot{C}}{2}\right)\right]z' + F(t'), \end{aligned} \tag{3.2}$$

where the function $F(t')$ is given by

$$
\begin{aligned}
F(t') = {} & C^3 A_1 \left[A_1 \left(a_1 C + \frac{\ddot{C}}{2} \right) - (a_2 - C\ddot{A}_1 - 2\dot{C}\dot{A}_1) \right] \\
& + C^3 A_2 \left[A_2 \left(b_1 C + \frac{\ddot{C}}{2} \right) - (b_2 - C\ddot{A}_2 - 2\dot{C}\dot{A}_2) \right] \\
& + C^3 A_3 \left[A_3 \left(c_1 C + \frac{\ddot{C}}{2} \right) - (c_2 - C\ddot{A}_3 - 2\dot{C}\dot{A}_3) \right] \\
& + C^2 d + \frac{1}{2} C^4 (\dot{A}_1^2 + \dot{A}_2^2 + \dot{A}_3^2).
\end{aligned}
\tag{3.3}
$$

Now we set parameters $A_1(t), A_2(t), A_3(t)$ and $C(t)$ in order to find a solution of SE for the system of eq. (3.1).

Let us consider $C(t)$ satisfying the following differential equations:

$$
\ddot{C} + 2a_1 C = \frac{k_1}{C^3}; \quad \ddot{C} + 2b_1 C = \frac{k_2}{C^3}; \quad \ddot{C} + 2c_1 C = \frac{k_3}{C^3},
\tag{3.4}
$$

where k_1, k_2 and k_3 are arbitrary constants. The potential parameters a_1, b_1 and c_1 can be written in terms of constants k_i's $(i = 1, 2, 3)$ from eq. (3.4) as

$$
\begin{aligned}
& 2(a_1 - b_1)C^4 = k_1 - k_2; \quad 2(a_1 - c_1)C^4 = k_1 - k_3; \\
& 2(b_1 - c_1)C^4 = k_2 - k_3.
\end{aligned}
\tag{3.5}
$$

The above relations may be used to find function $C(t)$ in terms of the potential parameters $a_1(t), b_1(t), c_1(t)$ and constants k_1, k_2 and k_3.

Again choose the functions A_1, A_2 and A_3 in order to make the linear terms in V' of eq. (3.2) vanish. These choices are given by

$$
\begin{aligned}
& \ddot{A}_1 + 2\frac{\dot{A}_1 \dot{C}}{C} + \frac{A_1 k_1}{C^4} - \frac{a_2}{C} = 0, \\
& \ddot{A}_2 + 2\frac{\dot{A}_2 \dot{C}}{C} + \frac{A_2 k_2}{C^4} - \frac{b_2}{C} = 0, \\
& \ddot{A}_3 + 2\frac{\dot{A}_3 \dot{C}}{C} + \frac{A_3 k_3}{C^4} - \frac{c_2}{C} = 0.
\end{aligned}
\tag{3.6}
$$

Hence eqs (3.2) and (3.3) can be written, after using eqs (3.4) and (3.6), as

$$
V'(x', y', z', t') = \frac{1}{2}(k_1 x'^2 + k_2 y'^2 + k_3 z'^2) + F(t'),
\tag{3.7}
$$

and

$$
F(t') = -\frac{1}{2}(k_1 A_1^2 + k_2 A_2^2 + k_3 A_3^2) + \frac{1}{2}(\dot{A}_1^2 + \dot{A}_2^2 + \dot{A}_3^2) + \mathrm{d}C^2.
\tag{3.8}
$$

Therefore, the TDSE eq. (2.10) to be solved becomes

$$-\frac{1}{2}(\psi_{1x'x'}+\psi_{1y'y'}+\psi_{1z'z'})+\frac{1}{2}(k_1x'^2+k_2y'^2+k_3z'^2)\psi_1=i\psi_{1t'}, \tag{3.9}$$

after performing the phase change to ψ of the type

$$\psi(x',y',z',t')=\exp\left(-\int^{t'}F(\tau)\mathrm{d}\tau\right)\psi_1(x',y',z',t'). \tag{3.10}$$

Hence eq. (3.9) is identified as SE for three-dimensional TD harmonic oscillator for $k_1,k_2,k_3>0$ and reduces for a free particle system when $k_1=k_2=k_3=0$.

At this stage, if we define the operator

$$I'=-\frac{1}{2}\left(\frac{\partial^2}{\partial x'^2}+\frac{\partial^2}{\partial y'^2}+\frac{\partial^2}{\partial z'^2}\right)+\frac{1}{2}(k_1x'^2+k_2y'^2+k_3z'^2), \tag{3.11}$$

then one can write the general solution to eq. (3.9) as

$$\psi_1(x',y',z',t')=\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}C_{lmn}e^{-i(\lambda_l+\lambda_m+\lambda_n)t'}u_l(x')u_m(y')u_n(z'), \tag{3.12}$$

where C_{lmn} are constants which can be determined as

$$C_{lmn}=\langle u_l(x')u_m(y')u_n(z'),\psi_1(x',y',z',0)\rangle\,.$$

Here $u_l(x'),u_m(y'),u_n(z')$ are the orthonormal eigenfunctions of the operator I', and $\lambda_l,\lambda_m,\lambda_n$ are the constant eigenvalues of the Hermitian operator I'.

For the present case the eigenvalues are given by

$$\lambda_l=\left(l+\frac{1}{2}\right)\sqrt{k_1};\quad \lambda_m=\left(m+\frac{1}{2}\right)\sqrt{k_2};\quad \lambda_n=\left(n+\frac{1}{2}\right)\sqrt{k_3}. \tag{3.13}$$

Finally, the exact solution of eq. (2.1) for the potential, eq. (3.1), becomes

$$\begin{aligned}\Psi(x,y,z,t)=&\frac{1}{C\sqrt{C}}\exp\left(-\int^{t'}F(\tau)\mathrm{d}\tau\right)\\ &\times\exp\left[\frac{i}{2C}(\dot{C}(x^2+y^2+z^2)-2C^2(\dot{A}_1x+\dot{A}_2y+\dot{A}_3z))\right]\\ &\times\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}C_{lmn}\mathrm{e}^{-i(\lambda_l+\lambda_m+\lambda_n)\int(\mathrm{d}t/C^2)}\\ &\times u_l\left(\frac{x}{C}+A_1\right)u_m\left(\frac{y}{C}+A_2\right)u_n\left(\frac{z}{C}+A_3\right).\end{aligned} \tag{3.14}$$

For the construction of the dynamical invariant for the system eq. (3.1), one can follow the following prescription [15]: use the transformation equations (2.2) in equation of motion of the system and set the unknown coefficient functions of the transformed equation of motion in such a way that the equation of motion remains invariant under the transformation, which led an equation of motion for a TID system, from which constant of motion is obtained.

Therefore, the invariant for the system, eq. (3.1) is written as

$$I = \frac{1}{2}[(Cp_1 - \dot{C}x + \dot{A}C^2)^2 + (Cp_2 - \dot{C}y + \dot{A}C^2)^2 + (Cp_3 - \dot{C}z + \dot{A}C^2)^2] + \frac{k}{2}\left[\left(\frac{x}{C} + A\right)^2 + \left(\frac{y}{C} + A\right)^2 + \left(\frac{z}{C} + A\right)^2\right]. \tag{3.15}$$

The dynamical invariant I in eq. (3.15) can be obtained from I' in eq. (3.11) by carrying out inverse transformations of the type

$$I = \mathrm{e}^{i\phi} I' \mathrm{e}^{-i\phi}, \tag{3.16}$$

where ϕ is given by eq. (2.9) and C and A satisfy eqs (3.4) and (3.6) respectively. So there is a direct relationship between I and I' and the operator I' in eq. (3.11) has constant eigenvalues whereas the Hamiltonian of the system does not have constant eigenvalues.

Case 2

Consider the harmonic plus inverse harmonic oscillator potential

$$V(x,y,z,t) = a_1(t)x^2 + b_1(t)y^2 + c_1(t)z^2 + \frac{a_2}{x^2} + \frac{b_2}{y^2} + \frac{c_2}{z^2}. \tag{3.17}$$

Equation (2.11) for V', after using eq. (3.17) with inverse transformations from eq. (2.3), may be written as

$$\begin{aligned} V' = {} & C^3\left[\left(a_1C + \frac{\ddot{C}}{2}\right)x'^2 + \left(b_1C + \frac{\ddot{C}}{2}\right)y'^2 + \left(c_1C + \frac{\ddot{C}}{2}\right)z'^2\right] \\ & + a_2(x' - A_1)^{-2} + b_2(y' - A_2)^{-2} + c_2(z' - A_3)^{-2} \\ & - C^3\left[(\ddot{A}_1 + 2\dot{C}\dot{A}_1) + 2A_1\left(a_1C + \frac{\ddot{C}}{2}\right)\right]x' \\ & - C^3\left[(C\ddot{A}_2 + 2\dot{C}\dot{A}_2) + 2A_2\left(b_1C + \frac{\ddot{C}}{2}\right)\right]y' \\ & - C^3\left[(\ddot{A}_3 + 2\dot{C}\dot{A}_3) + 2A_3\left(c_1C + \frac{\ddot{C}}{2}\right)\right]z' + F(t'), \end{aligned} \tag{3.18}$$

where

$$F(t') = C^3 A_1\left[A_1\left(a_1C + \frac{\ddot{C}}{2}\right) + (\ddot{A}_1 + 2\dot{C}\dot{A}_1)\right]$$

$$+C^3 A_2 \left[A_2 \left(b_1 C + \frac{\ddot{C}}{2} \right) + (\ddot{A}_2 + 2\dot{C}\dot{A}_2) \right]$$
$$+C^3 A_3 \left[A_3 \left(c_1 C + \frac{\ddot{C}}{2} \right) + (\ddot{A}_3 + 2\dot{C}\dot{A}_3) \right]$$
$$+\frac{1}{2} C^4 (\dot{A}_1^2 + \dot{A}_2^2 + \dot{A}_3^2). \tag{3.19}$$

Here, we set $A_1 = A_2 = A_3 = 0$ in order to make V' TID and consider $C(t)$ which satisfy the following differential equations:

$$\ddot{C} + 2a_1 C = \frac{k_1}{C^3}; \quad \ddot{C} + 2b_1 C = \frac{k_2}{C^3}; \quad \ddot{C} + 2c_1 C = \frac{k_3}{C^3}, \tag{3.20}$$

where k_1, k_2 and k_3 are arbitrary constants as usual. Assuming a_2, b_2, c_2 as TID constants, then eq. (3.18) for V' reduces to

$$V' = k_1(t) x'^2 + k_2(t) y'^2 + k_3(t) z'^2 + \frac{a_2}{x'^2} + \frac{b_2}{y'^2} + \frac{c_2}{z'^2}, \tag{3.21}$$

and the TDSE eq. (2.1) turns to be TIDSE, i.e.

$$-\frac{1}{2}(\psi_{1x'x'} + \psi_{1y'y'} + \psi_{1z'z'})$$
$$+ \left(k_1 x'^2 + k_2 y'^2 + k_3 z'^2 + \frac{a_2}{x'^2} + \frac{b_2}{y'^2} + \frac{c_2}{z'^2} \right) \psi_1 = i\psi_{1t'}, \tag{3.22}$$

and Hermitian operator for the above equation becomes

$$I' = -\frac{1}{2} \left(\frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2} + \frac{\partial^2}{\partial z'^2} \right)$$
$$+ \left(k_1 x'^2 + k_2 y'^2 + k_3 z'^2 + \frac{a_2}{x'^2} + \frac{b_2}{y'^2} + \frac{c_2}{z'^2} \right). \tag{3.23}$$

Since in this case $F(t') = 0$, no phase transformation of the type of eq. (3.10) is required. Hence the exact solution of eq. (2.1) for harmonic plus inverse harmonic potential takes the form as

$$\Psi(x, y, z, t) = \frac{1}{C\sqrt{C}} \exp \left[\frac{i}{2C} (\dot{C}(x^2 + y^2 + z^2)) \right]$$
$$\times \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} C_{lmn} \mathrm{e}^{-i(\lambda_l + \lambda_m + \lambda_n) \int (\mathrm{d}t/C^2)} u_l$$
$$\times \left(\frac{x}{C} \right) u_m \left(\frac{y}{C} \right) u_n \left(\frac{z}{C} \right). \tag{3.24}$$

The invariant for the system described by eq. (3.17) can be obtained using Lie algebraic method [16], which is given as

$$I = \frac{1}{2}\left[k_1\left(\frac{\rho_1}{x}\right)^2 + k_2\left(\frac{\rho_2}{y}\right)^2 + k_3\left(\frac{\rho_3}{z}\right)^2 + a_2\left(\frac{x}{\rho_1}\right)^2 + b_2\left(\frac{y}{\rho_2}\right)^2 + c_2\left(\frac{z}{\rho_3}\right)^2 + (\rho_1 p_1 - p_1 x)^2 + (\rho_2 p_2 - p_2 y)^2 + (\rho_3 p_3 - p_3 z)^2\right], \tag{3.25}$$

where ρ_i, $i = 1, 2, 3$ are solutions of a set of three auxiliary equations of the form

$$\ddot{\rho}_i + 2\rho_i = \frac{k_i}{\rho_i^3}.$$

Once again one can obtain I from I' using eq. (3.16).

4. Summary and discussion

In the present work, we have derived the exact analytic solutions of TDSE of three-dimensional TD systems by applying the transformation-group method, which was previously demonstrated for one- [13] and two- [5] dimensional systems. We have extended the method in three dimensions and solved the TDSE for the shifted rotating harmonic oscillator and harmonic plus inverse harmonic potentials. Since the Hermitian operators I' (eqs (3.11) and (3.23)) and dynamical invariants I (eqs (3.15) and (3.25)) are related, if the invariant of a system is available, it can be used to get quantum states by solving TDSE analytically. As far as the applicability of this method is concerned, this works successfully for TD harmonic potentials, but may not produce analytic solutions for the systems having TD anharmonic potentials [15]. In such cases some TD terms may appear in V' which may not be eliminated even with further phase transformations of the type (eq. (3.10)).

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