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Analytic solutions of the complex diffusion equation with aspects on quantum mechanics

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In this paper, we derive and compare the solutions of the real and complex diffusion equations obtained by the self-similar solution to each other. Additionally, possible quantum mechanical aspects are analyzed as well. In the second part of the study, a complex reaction–diffusion equation is investigated and compared to the quantum mechanical solutions of the corresponding Schrödinger equation with a power-law-type potential. We show that the same parameter ratio emerges in the quantum mechanical and the self-similar solutions as well, which is a remarkable property. For both investigated equations, the complex diffusion and complex reaction–diffusion equations, we found some solutions for which the absolute value squared has a convergent finite numerical integral. This is not a rigorous L^2 integrability condition but a good hint for that, which is a key property in quantum mechanics.

Keywords: Complex diffusion equation; self-similar solutions; Schrödinger equation.

1. Introduction

It is an evidence that diffusion (or heat conduction) is a fundamental physical process which attracted enormous intellectual interests from mathematicians, physicists and engineers in the last two centuries. The existing literature about diffusion (or again about heat conduction) is immense, therefore we just mention some basic textbooks.[1,2]

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We may perform a complex extension of the diffusion equation with an imaginary diffusion coefficient defining a complex field equation which is equivalent to the free Schrödinger equation. This is one of the cornerstones of nonrelativistic quantum mechanics. It is now clearly known[3] that quantum mechanics was born exactly hundred years ago in 1925 when Max Born first used the German phrase of "Über Quantenmechanik" in one of his papers.[4] The complete theory was worked out in the next year of 1925. This is the main motivation of our study. We would like to derive new results which lie between the Schrödinger equation and the classical diffusion process.

The achieved knowledge about the Schrödinger equation can also fill libraries. Some basic well-known textbooks are the following.[5,6a] The similarities and differences with ordinary diffusion can be studied in Refs. 7 or 8.

In our study, to derive analytic results, we apply the reduction mechanism which is a powerful tool to reduce nonlinear partial differential equations (PDE) or even nonlinear PDE systems to ordinary differential equations (ODEs) or ODE systems. Technically, we apply the self-similar Ansatz.

In our former studies, in a research paper[9] and in a book chapter,[10] we applied the self-similar Ansatz to the Madelung equation which is a fluid mechanical analogue of the Schrödinger equation. We derived that the fluid density is proportional to the square of the Bessel function with a quadratic argument. Therefore, the density function had countable infinite zeros which is a remarkable and less usual property in fluid mechanics and originated from quantum mechanics. Recently, Ván[11] analyzed and worked out the connection between quantum mechanics, superfluids and capillary fluids. Madelung fluids are capillary fluids. Thermodynamics is what links them together.

In a similar way, this paper presents specific solutions of the Schrödinger equation for infinite domain, using a self-similar transformation, which is different from the usual separation of time and space variables.

This study organically follows our former analysis in which we investigated the regular diffusion equation in depth.[12–14] The general basic mathematical and numerical aspects are covered in Refs. 15 and 16. Now, we extend our research to a diffusion equation which has a complex diffusion coefficient and therefore formally equivalent to the free Schrödinger equation. However, the Schrödinger equation is a complex field equation and a complex extension of the diffusion equation with an imaginary diffusion coefficient.

In the second part, we investigate one kind of a complex reaction–diffusion equation which is the form invariant to the Schrödinger equation with a power-law-type potential. We address the study to the one-dimensional Cartesian case only. After the exhaustive mathematical analysis of the solutions, we try to give a quantum mechanical interpretation of our results. Therefore, we investigate the parameter dependencies of the results and find a regime where the absolute value squared of the functions have a finite numerical integral which is a hint of L^2 integrability.

[a] We used the derivation given on pp. 64–65 for Eq. (5).

2. Theory and Results

Before we derive the generalized self-similar solutions for the Schrödinger equation, we briefly summarize our former results which were obtained for regular diffusion equation

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2}, \tag{1}$$

where $C(x,t)$ is the distribution of the particle concentration in space and time, and D is the diffusion coefficient and from physical reasons it is a positive real constant. From the mathematical point of view, the positivity of D assures the stability of the equation.

The function $C(x,t)$ fulfills the necessary smoothness conditions with existing continuous first and second derivatives. Numerous physics textbooks give us the derivation how the fundamental (the Gaussian) solutions can be obtained, e.g. the cross-diffusion case was discussed in Ref. 17. Solutions with concentration-dependent diffusion coefficients have also been evaluated.[18] In the well-known work of Bluman and Cole in 1969,[19] numerous analytic solutions were given for the diffusion equation, and they arrived to a certain level.

In our analysis, we apply the self-similar Ansatz in the form of $C(x,t) = t^{-\alpha} g(\frac{x}{t^\beta}) = t^{-\alpha} g(\eta)$, where α and β are the self-similar exponents being real numbers describing the temporal decay and spreading of the solution, $g(\eta)$ is called the shape function, and $\eta = \frac{x}{t^\beta}$ is the reduced variable defined from the original temporal and spatial variables. After some trivial algebraic step, the self-similar Ansatz leads us to the relations of $\alpha =$ arbitrary real number, $\beta = 1/2$, and to the clear-cut ODE of

$$-\alpha g - \frac{1}{2}\eta g' = D g''.$$

With the choice of $\alpha = 1/2$ and setting the first integration constant to zero ($c_1 = 0$), we get back the well-known Gaussian solution.

This is the so-called fundamental solution and sometimes referred to as *source type* solution — by mathematicians — because for $t \to 0$ the $C(x,0) \to \delta(x)$. As far as we know, this is the simplest and shortest derivation to obtain the fundamental solution from the original PDE of Eq. (1). Therefore, this Ansatz is original among others and can help to find physically relevant disperse solutions to other physical systems like the Bénard convection problem[20] or a heated boundary layer flow.[21] By using the formula manipulating software package Maple 12 for general real α, the solutions read as

$$g(\eta) = \eta \cdot e^{-\frac{\eta^2}{4D}}\left(c_1 M\left[1-\alpha, \frac{3}{2}, \frac{\eta^2}{4D}\right] + c_2 U\left[1-\alpha, \frac{3}{2}, \frac{\eta^2}{4D}\right]\right), \tag{2}$$

where $M(\cdot,\cdot,\cdot)$ and $U(\cdot,\cdot,\cdot)$ are Kummer's M and Kummer's U functions. For more details, consult the NIST Handbook.[22]

In our former studies,[12–14] we analyzed the $\alpha \neq 1/2$ cases exhaustively, and found four different regimes:

- $1 - \alpha < 0$ the M function is a finite polynomial if α is an integer and larger than two,[13]
- $1 - \alpha = 0$ the M function is constant, the decay of solutions are determined by the Gaussian term,
- $0 < 1 - \alpha \leq 1$ the solutions have a local maxima and a decay to zero at large arguments,
- $1 < 1 - \alpha$ the solutions have oscillations proportional to the value of $(1 - \alpha)$ and have quicker decays to zero at larger $(1 - \alpha)$ values.

It is clear to see that most of the resulting functions have odd symmetry in terms of η, however it can be shown that for some α parameters, Kummer's U functions can have even symmetry[14] as well, which has far reaching consequences.

2.1. *Solutions of the complex diffusion equation*

Continue our analysis with the analogous problem, where the diffusion coefficient becomes complex. In other words, let's investigate the free Schrödinger equation — still in one Cartesian coordinate

$$\frac{\partial \Psi(x,t)}{\partial t} = i\hat{D}\frac{\partial^2 \Psi(x,t)}{\partial x^2}, \tag{3}$$

where $\hat{D} = \frac{\hbar}{2\,m} > 0$ is the real "diffusion coefficient" of the equation in the language of diffusion. (In the following, the solutions will be presented with the general diffusion coefficients $\hat{D}$, however in all the presented figures we apply $\hat{D} = 1/2$ which means atomic units $\hbar = m = 1$.) Just for completeness, we have to mention that Erwin Schrödinger investigated diffusion and heat conduction phenomena as well from the kinetic gas theoretical side.[23,24]

It is well known in quantum mechanics that the free Schrödinger equation has a disperse wave-packet solution which can be written in the form of

$$\Psi(x,t) = \frac{\sqrt[4]{2/\pi}}{\sqrt{1+2it}} \cdot e^{-\frac{x^2}{1+2it}},$$

when atomic units are used ($\hbar = m = 1$). The correctness of this formula can be proven with direct derivation and substitution to Eq. (3) considering $\hat{D} = 1/2$.

Exhaustive details and the properties of Gaussian wave-packets can be found in numerous text books like Refs. 6, 25 and 26.[b,c]

Before we derive and discuss our analytic solutions, we have to summarize other available results from the literature. We start with the work of Niederer[27] from 1972

[b] Formula of the wave packet on p. 58.
[c] A not so detailed derivation of the wave packet on pp. 57–59.

who used the maximal kinematic invariance group to solve the free Schrödinger equation. Shapovalov *et al.*[28] separated the variables of the stationary Schrödinger equation and presented numerous results. Numerous group theoretical studies were performed from various authors, we mention Beckers *et al.*[29] who investigated nonrelativistic quantum mechanical equations with the subgroups of the Euclidean group, where the Schrödinger or the Pauli equations were examined with different scalar and vector potentials.

On the other hand, for the time-independent Schrödinger equation, numerous exactly solvable potentials exist which have analytic solutions for the wave function and the energy eigenvalues. Some potentials can be exactly solved with the help of the supersymmetry and can be understood in terms of a few basic ideas which include supersymmetric partner potentials, shape invariance and operator transformations. Without completeness, we just give some works which contain additional references.[30–32] There are important recent solutions of the Schrödinger equation, which are related to heavy-light mesons,[33] diatomic molecules[34] or binding energies.[35] The multiplicity of solutions of the biharmonic nonlinear Schrödinger equation is discussed by Farkas and coworkers.[36] Finally, we mention that numerous additional quasi-exactly solvable models exist in quantum mechanics.[37]

It is crucial to emphasize that these studies do not mention our result in the form of Eq. (4). To derive the expression equation (2.1), the method of separation of variables was used, so the temporal "t" and the spatial "x" variable of the dynamics were handled separately, which is the crucial point.

The investigation of wave-packets dynamics is an interesting field in quantum mechanics which helps to visualize the possible wave-particle dualistic dynamics of the quantum particle. As an interesting point we may mention the nondispersive wave-packet solutions of Berry and Balázs which is based on Airy functions. Such solutions propagate freely without any envelope dispersion, maintaining its shape.[38] As an extra feature, it accelerates undisturbed in the absence of an external force field. Nevertheless, these properties do not violate Ehrenfest's theorem. Understanding quantum properties of matter via investigating the wave packed dynamics is a popular method; with an immense literature we just mention two reviews.[39,40]

The role and the source of time in quantum mechanics is an interesting and open-ended question and topics of scientific monographs and publications.[41,42]

As we learned earlier in the classical diffusion problem, one can find the fundamental solution applying self-similar Ansatz, where the time and the temporal variables are not separated (but remain connected) in the self-similar reduced variable $\eta = \frac{x}{t^\beta}$. In this sense, the classical diffusion process and the free Schrödinger equation "handles" space and time dynamical variables in a different way. However, to find the key results of this study, let's apply the same self-similar Ansatz as above $\Psi(x,t) = t^{-\alpha} f(\frac{x}{t^\beta}) = t^{-\alpha} f(\eta)$. The former physical meaning of α and β remains the same as was given above. To avoid later mixing, we mark with $f(\eta)$ the shape function. After the same trivial algebraic steps we get the same relations for the self-similar exponents: $\alpha =$ arbitrary real number, $\beta = 1/2$, and a very similar ODE as

Eq. (2) in the form of

$$-\alpha f - \frac{1}{2}\eta f' = i\hat{D} f''.$$

With the help of Maple 12, we can easily evaluate the general solution

$$f(\eta) = \tilde{c}_1 M\left[\alpha + \frac{1}{2}, \frac{3}{2}, \frac{i\eta^2}{4\hat{D}}\right]\eta + \tilde{c}_2 U\left[\alpha + \frac{1}{2}, \frac{3}{2}, \frac{i\eta^2}{4\hat{D}}\right]\eta, \tag{4}$$

where $\tilde{c}_1$ and $\tilde{c}_2$ are still usual real integration constants, and $M(\cdot,\cdot,\cdot)$ and $U(\cdot,\cdot,\cdot)$ are the Kummer's M and Kummer's U functions,[22] respectively. (Similarly to the real case, an alternative formulation is also available with the Hermite polynomials and the hypergeometric function properties of that formula is outside the scope of this study.) We concentrate and analyze the solutions which include the Kummer's functions.These two equations (Eqs. (2) and (4)) are the key results of our analysis.

The essential differences between the solution of the real diffusion equation (2) and Eq. (4) are immediately visible. The first is the missing Gaussian multiplier function. The second no-less negligible difference is the complex argument of both Kummer's functions.

To perform an in-depth analysis, we have to systematically investigate the α dependencies of both Kummer's functions. To accelerate this process, it is useful to evaluate the first few Taylor expansion terms of these functions where we can clearly see the role of the α parameter.

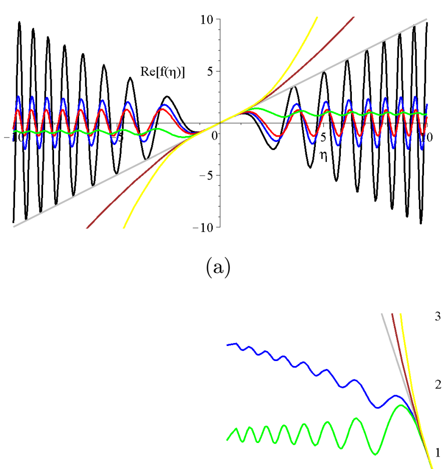
$$\begin{aligned} f(\eta) = \tilde{c}_1 &\left[\eta + \frac{i\cdot\left(\alpha+\frac{1}{2}\right)}{6\hat{D}}\eta^3 + \frac{\left(\alpha+\frac{1}{2}\right)\cdot\left(\alpha+\frac{3}{2}\right)}{120\hat{D}^2}\eta^5 \right.\\ &\left. + \frac{i\cdot\left(\alpha+\frac{1}{2}\right)\cdot\left(\alpha+\frac{3}{2}\right)\cdot\left(\alpha+\frac{5}{2}\right)}{5040\hat{D}^3}\eta^7 - \cdots\right]\\ &+ \tilde{c}_2\left[\frac{2\sqrt{\pi}}{\sqrt{\frac{i}{\hat{D}}}\Gamma\left(\alpha+\frac{1}{2}\right)} - \frac{2\sqrt{\pi}}{\Gamma(\alpha)}\eta \right.\\ &\left. + \frac{i\alpha\sqrt{\pi}}{\sqrt{i\cdot\hat{D}}\Gamma\left(\alpha+\frac{1}{2}\right)}\eta^2 - \frac{i\sqrt{\pi}\left(\alpha+\frac{1}{2}\right)}{3\hat{D}\Gamma(\alpha)}\eta^3 - \cdots\right]. \end{aligned} \tag{5}$$

Let us try to analyze the properties of this truncated finite series. The first term — Kummer's M function — is always an odd function and can be defined for arbitrary α. Furthermore, the odd members are real and the even members are purely complex. For negative half-integer α values we get finite polynomials. The second term — Kummer's U function — has a bit more tricky structure, — due to the analytic properties of the Gamma function[22] — for negative integer α values the function has even symmetry, and for negative half-integer α values (if $\alpha < -1/2$) the function has an odd symmetry. For all positive α values, the function has no even or odd symmetry. The exact α parameter dependence of the solution is a complicated problem. To solve this difficulty, we apply an empirical method and evaluate the shape functions $f(\eta)$s for various α values. Due to the complex argument of the solution, we present the real, the complex and the absolute value of the solution. First, Fig. 1 shows the results for Kummer's M function. Figures 1(a)–1(c) show the real, the imaginary and the absolute value of $M(\frac{1}{2}+\alpha, \frac{3}{2}, \frac{i\eta^2}{4\hat{D}}) \cdot \eta$ function for $\hat{D} = 1/2$. Having in mind Kummer's transformation formula[22] (Eq. (13.2.39))

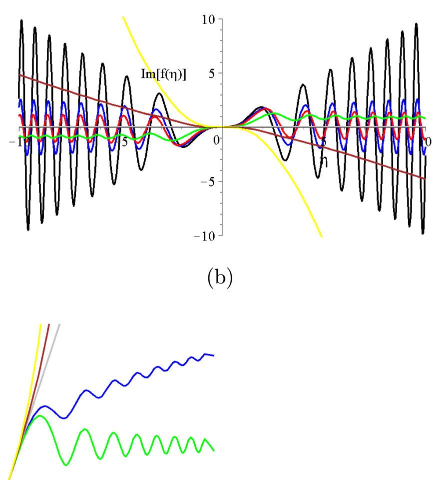
$$M(a,b,z) = e^z M(b-a,b,z), \tag{6}$$

we can find interesting unexpected identities during the analysis like $|M(0,\frac{3}{2},\frac{i\eta^2}{4\hat{D}})| = |M(\frac{3}{2},\frac{3}{2},\frac{i\eta^2}{4\hat{D}})|$, $|M(1,\frac{3}{2},\frac{i\eta^2}{4\hat{D}})| = |M(\frac{1}{2},\frac{3}{2},\frac{i\eta^2}{4\hat{D}})|$ or even $|M(\frac{4}{6},\frac{3}{2},\frac{i\eta^2}{4\hat{D}})| = |M(\frac{5}{6},\frac{3}{2},\frac{i\eta^2}{4\hat{D}})|$, for the Kummer's M functions only. This is the reason why only five curves are visible on Fig. 1(c). Some other curves coincide. A more detailed analysis showed that only for $0 < \alpha < 1/2$ we get oscillatory but decaying solutions, which could have physical interest later on.

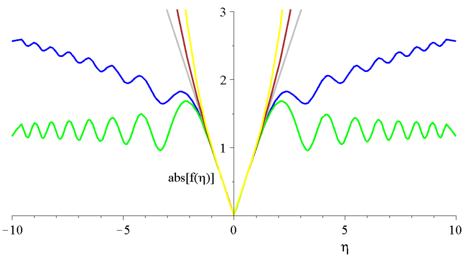
Figure 2 presents the real, imaginary and absolute values of the $U(\frac{1}{2}+\alpha,\frac{3}{2},\frac{i\eta^2}{4\hat{D}}) \cdot \eta$ function for the same α values. It is clear to see that, negative α values give divergent $f(\eta)$ shape functions which are from physical reasons out of our interest. Positive αs give decaying solutions at infinity with an additional cusp in the origin. (Cusp means



(a)



(b)



(c)

Fig. 1. (Color online) Panels (a)–(c) are the real, the complex and the absolute values of the $M(\frac{1}{2}+\alpha,\frac{3}{2},\frac{i\eta^2}{4\hat{D}}) \cdot \eta$ function in Eq. (4) for $\hat{D} = 1/2$. The black, blue, red, green, gray, brown and yellow lines are for $\alpha = 1, 2/3, 1/2, 0, -1/2, -2/3$ and -1, respectively.

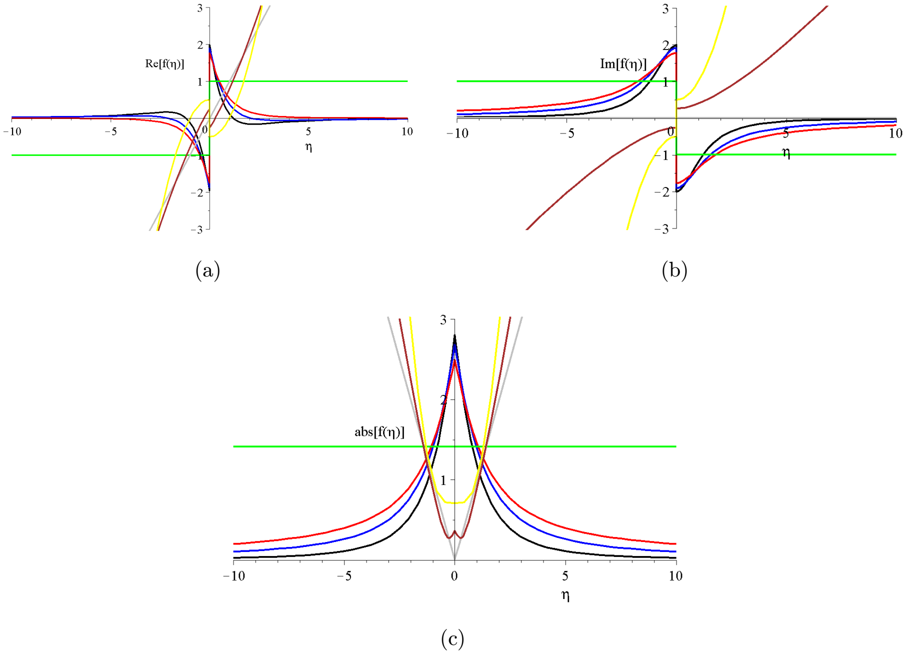


Fig. 2. (Color online) Panels (a)–(c) are the real, the complex and the absolute values of the $U(\frac{1}{2}+\alpha, \frac{3}{2}, \frac{i\eta^2}{4\hat{D}}) \cdot \eta$ function in for $\hat{D} = 1/2$. The black, blue, red, green, gray, brown and yellow lines are for $\alpha = -1, -2/3, -1/2, 0, 1/2, 2/3$ and 1, respectively.

now a point where the function has a finite numerical value but the derivative is indefinite.)

Figure 3 shows the absolute value squared of the wave function $|\Psi(x,t)|^2$ for Kummer's U and Kummer's M functions if $\alpha = 1/4$. We found that for $\alpha > 0$ all $|\Psi(x,t)|^2 = t^{-2\alpha}|U(\alpha+\frac{1}{2}, \frac{3}{2}, \frac{ix^2}{4\hat{D}t}) \frac{x}{t^{1/2}}|^2$ the function has a general temporal and spatial decay. For completeness we present the general absolute value squared of the wave function $|\tilde{c}_1 M(,,) + \tilde{c}_2 U(,,)|^2$ and we can see that the asymptotic decay remains the same.

As it is mentioned in the introduction, it is important to consider the physical relevancy of the solutions. In case of the Schrödinger equation, it is related to L^2 integrability, which means that the solution should belong to the Hilbert space in the sense described in Ref. 43. On more general grounds, the complex equation may have other solutions, with certain mathematical features. We performed a large number of numerical integration of $|t^{-2\alpha} \cdot U(\frac{1}{2}+\alpha, \frac{3}{2}, \frac{i\eta^2}{4\hat{D}}) \cdot \eta|^2$ to find out the convergence properties and we may say that for $\alpha \geq 1/2$ the convergence is easy to see with interval doubling. Table 1 shows the numerical values of the integral for a given parameter set. However, below 1/2 the convergence becomes very slow. We have no rigorous mathematical proof where lies the general convergence limit for α.

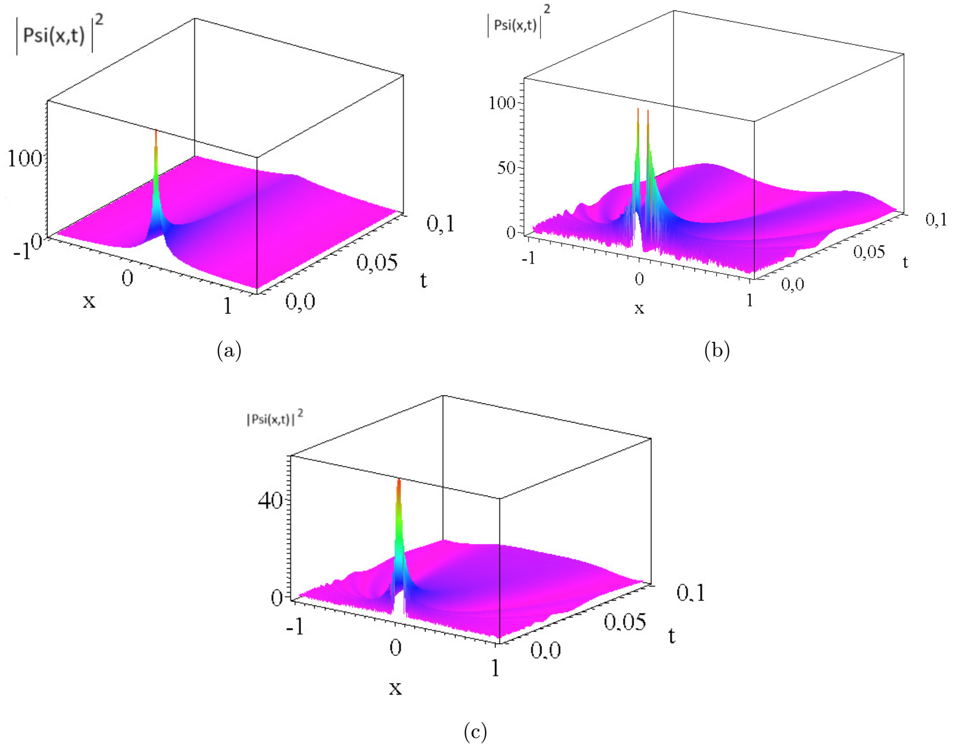


Fig. 3. The $|\Psi(x,t)|^2$ of Eq. (4) for $\alpha = 1/4$ and $\hat{D} = 1/2$. The subfigures (a) show Kummer's U function, (b) Kummer's M function and (c) is the linear combination of both with $\tilde{c}_1 = 0.5, \tilde{c}_2 = 1$, respectively.

Table 1. Convergence of the numerical integral of the function $|t^{-2\alpha} \cdot U(\frac{1}{2} + \alpha, \frac{3}{2}, \frac{ix^2}{4\hat{D}t}) \cdot \frac{x}{t^{1/2}}|^2$ in the interval of $[0 \ldots x_{\max}]$. The parameters are $t = 1$, $\hat{D} = 1/2, \alpha = 1/2$, considering 10 digits accuracy and default integration method in the Maple 12 software.

The upper limit of integration interval, $x_{\max}$	Numerical value of the integral
3.125	6.010
6.25	6.451
12.5	6.770
25	6.930
50	7.001
100	7.002

For the other function $|\Psi(x,t)|^2 = t^{-2\alpha}|M(\alpha + \frac{1}{2}, \frac{3}{2}, \frac{ix^2}{4\hat{D}t})\frac{x}{t^{1/2}}|^2$ the situation is a bit more different. For $\alpha = 1/4$, we get the lowest lying oscillating solution which has all local minimums equal to zero. All other solutions lie above this function. Having performed large number of numerical integration we can say with great certainty that no convergence can be achieved for any kind of α values.

3. The Role of an Additional Source Term

To complete our former equation with the additional and special source term, we arrive to the far analogous of the reaction–diffusion description:[44]

$$i\frac{\partial \Phi(x,t)}{\partial t} = -\hat{D}\frac{\partial^2 \Phi(x,t)}{\partial x^2} + V(x,t)\Phi(x,t), \tag{7}$$

where $\Phi(x,t)$ is the spacial- and temporal-dependent concentration, $V(x,t)\Phi(x,t)$ is the real source term, and $\hat{D}$ is still the diffusion coefficient. It is evidently form invariant to the time-dependent Schrödinger equation with an arbitrary potential $V(x,t)$.

Crucial for us in the following are the solutions of the $V(x) = ax^n$ interaction terms which are the space-dependent power-law type of potentials. (In quantum mechanics the greatest relevance has the harmonic oscillator potential where $a > 0 >$ and $n = 2$.) With different notations we still consider the self-similar Ansatz: $\Phi(x,t) = t^{-\alpha}h(x/t^{\beta}) = t^{-\alpha}h(\eta)$. Having done the derivation and having used that $x = \eta \cdot t^{\beta}$ after some algebraic step we get the following constraints:

$$\alpha + 1 = \alpha + 2\beta = \alpha - \beta n. \tag{8}$$

It is easy to see that $\beta = 1/2$, and α can be any real number therefore $n = -2$. This means that only for the

$$V(x) = -\frac{a}{x^2}, \tag{9}$$

time-independent potential, we arrive to an ODE of

$$-i\alpha h - i\frac{1}{2}\eta h' = -\hat{D}h'' - \frac{a}{\eta^2}h, \tag{10}$$

where prime means derivation with respect to η.

(From physical reasons, we consider the more relevant attractive interaction with the negative sign.) A remarkable feature of this potential is that being a homogeneous function of degree -2, which is the same as the modulus of the degree of the kinetic energy, is conformally invariant and thus the corresponding action functional is also invariant under the transformation of $q \to \lambda q$ and $t \to \lambda 2t$.[45]

The exact solution of Eq. (10) is given as

$$h(\eta) = c_1\frac{e^{\frac{i\eta^2}{8\hat{D}}}}{\sqrt{\eta}} \cdot \mathbf{M}_{\frac{1}{4}-\alpha,\frac{1}{4}\sqrt{1-\frac{4a}{\hat{D}}}}\left(\frac{i\eta^2}{4\hat{D}}\right) + c_2\frac{e^{\frac{i\eta^2}{8\hat{D}}}}{\sqrt{\eta}} \cdot \mathbf{W}_{\frac{1}{4}-\alpha,\frac{1}{4}\sqrt{1-\frac{4a}{\hat{D}}}}\left(\frac{i\eta^2}{4\hat{D}}\right), \tag{11}$$

now, however $\mathbf{M}()$ and $\mathbf{W}()$ are the Whittaker functions with possible complex arguments[22] which are the modified forms of the confluent hypergeometric equation and can be expressed with Kummer's M and Kummer's U functions.

$$\begin{aligned} &\text{Whittaker } \mathbf{M}_{\lambda\mu}(z) = e^{-z/2}z^{\mu+1/2}M(\mu - \lambda + 1/2, 1 + 2\mu; z); \\ &\text{Whittaker } \mathbf{W}_{\lambda,\mu}(z) = e^{-z/2}z^{\mu+1/2}U(\mu - \lambda + 1/2, 1 + 2\mu; z). \end{aligned} \tag{12}$$

The Whittaker M and the Whittaker W are the irregular functions in the origin. Due to these relations, the Whittaker M function cannot be defined when its second parameter is a negative integer $\mu = -1, -2, -3, \ldots - N$ (NIST[22] Eq. (13.14.3)). Fortunately, this case never comes up in our system because the parameter $\sqrt{1 - 4a/\hat{D}}$ is either positive or complex. Note that due to the extra exponential function, the Whittaker functions cannot be represented to a finite polynomial at any parameters. (We have to make an important statement at this point. Our reduction mechanism makes it possible that any kind of time-dependent power-law-type potential in the form of $V_n(x,t) = \hat{a}x^n t^{-n-2}$ where $\hat{a}, n \in \mathbb{R}$ can be reduced to an ODE similar to Eq. (10). We found analytic solutions for the $n = -2, -1, 0, 1$ and 2 exponents only. We concentrate on the $n = -2$ case exclusively.)

In addition to the Coulomb and the harmonic oscillator problems, the $V(x) = -a/x^2$ potential has exotic properties and shows some anomalies in quantum mechanics. The problem has a remarkable wide literature, therefore without completeness we just mention some relevant studies.[45–54] (We also mention the literature for the spherical case as well, however the self-similar analysis of that case is the topic of our future study.) The potential has direct applications in classical celestial mechanics[55] or even in cosmology matter near horizon of a black hole.[56,57] This potential appears in such physical problems as the Efimov effect,[58] an electron near a bipolar molecule,[59–61] or an atom with magnetic moment in the magnetic field of a long solenoid[62] and a neutral atom in the electric field of a thin charged wire.[63,64]

Due to Essin and Grifith,[50] if the potential is restricted to positive coordinates ($x \geq 0$) and it is attractive, fulfilling the relation of $a > 1/8$ (in atomic units),[50] then it has finite negative bound states otherwise not. The wave functions are known for the negative energy bound states in the form of

$$\Phi(x) = N\sqrt{x}K_{ig}(\kappa x), \tag{13}$$

where $K_{ig}()$ stands for the modified Bessel functions[22] and for the positive energy scattering states as well. This is a linear combination of the two Hankel functions[22]

$$\Phi(x) = N\sqrt{x} \cdot [AH_{ig}^{(1)}(kx) + BH_{ig}^{(2)}(kx)], \tag{14}$$

where N, A, B are the normalization constants and $\kappa = \sqrt{-2E}$, $k = \sqrt{2E}$ and $g = 2a - 1/4$. The Hankel functions can be given with the help of the Bessel functions of the first and second kind in the form of

$$H_\nu^{(1)}(z) = J_\nu(z) + iY_\nu(z), \quad H_\nu^{(2)} = J_\nu(z) - iY_\nu(z), \tag{15}$$

where both the parameter ν and the argument z can be complex numbers. The total wave function has the well-known time-dependence of $\Phi(x,t) = \Phi(x)e^{-iEt}$ which is the common complex phase factor with the absolute value of unity. It is clear because the potential does not depend on time, therefore the Hamiltonian is conservative, and has the trivial time-dependence.

The real and complex parts are the usual cosine and sine functions, respectively.

Having in mind these information, let's analyze our solutions of Eq. (11). The shape function already has a complex phase factor of $\frac{i\eta^2}{2\hat{D}}$. The absolute value is unity, but the real and complex parts have a quadratic argument which means a linear chirp is a continuously enhancing frequency. The larger the diffusion coefficient $\hat{D}$ the slower the linear chirp. We saw earlier in the quantum relation that the $a = 1/8$ (in atomic units) shifts the potential to a regime where the system gets bounding eigenvalues. Note that such a point is reflected in the second parameter of the Whittaker functions as well. The nominator $\sqrt{\hat{D} - 4a}$ becomes complex in atomic units at $a = 1/8$. The main parameter — which defines the global overall properties of the solutions — is the first parameter of the Whittaker functions $1/4 - \alpha$. Figure 4 presents the real, imaginary and absolute values of the Whittaker M function of Eq. (11) for different α values. Figure 5 presents the real, imaginary and absolute value of the Whittaker W function of Eq. (11) for different α values. We consider $\hat{D} = 1/2$ and $a = 1/4$ which means the potential has bound states as well. Note that both functions have odd symmetry for the real and for the imaginary parts as well. Both functions are zero in the origin. For positive α values, the solutions show oscillations and for negative values exploding behavior, which meets our

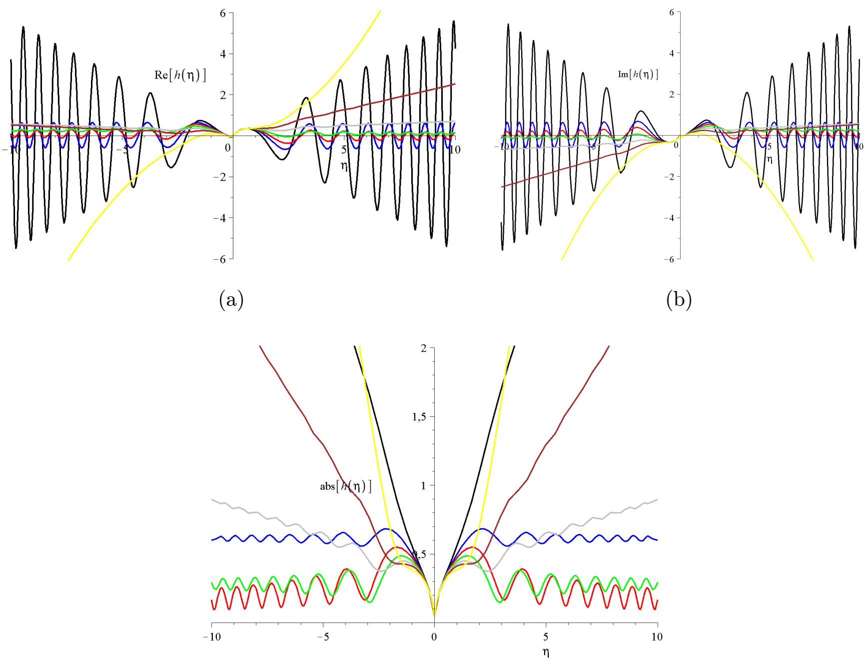
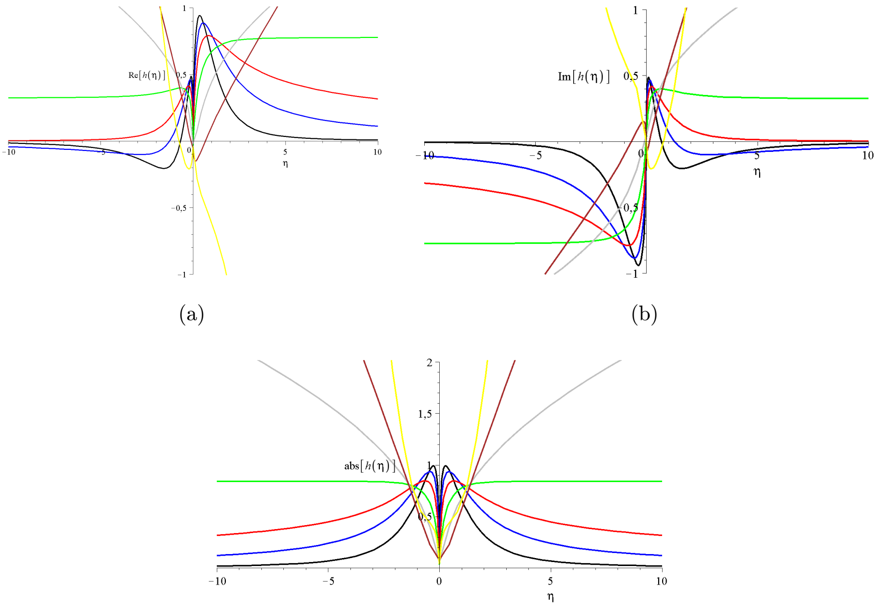


Fig. 4. (Color online) Panels (a)–(c)are the real, the complex and the absolute values of the $\frac{e^{\frac{i\eta^2}{8\hat{D}}}}{\sqrt{\eta}} \cdot \mathbf{M}_{\frac{1}{4}-\alpha,\frac{1}{4}\sqrt{1-\frac{4a}{\hat{D}}}}(\frac{i\eta^2}{4\hat{D}})$ function in for $\hat{D} = 1/2$ and $a = 1/4$. The black, blue, red, green, gray, brown and yellow lines are for $\alpha = 1, 1/2, 1/4, 0, -1/4, -1/2$ and -1, respectively.



(c)

Fig. 5. (Color Online) Panels (a)–(c) are the real, the complex and the absolute values of the $\frac{e^{\frac{i\eta^2}{8\hat{D}}}}{\sqrt{\eta}} \cdot \mathbf{W}_{\frac{1}{4}-\alpha,\frac{1}{4}\sqrt{1-\frac{4a}{\hat{D}}}}(\frac{i\eta^2}{4\hat{D}})$ function in for $\hat{D} = 1/2$ and $a = 1/4$. The black, blue, red, green, gray, brown and yellow lines are for $\alpha = 1, 1/2, 1/4, 0, -1/4, -1/2$ and -1, respectively.

experience. The Whittaker W functions decay for positive α values and explode for negative α values.

It is important to note that for some special parameters of the Whittaker functions, the derived solutions can be expressed with other elementary of special functions (see NIST[22] Eqs. (13.18.1)–(13.18.17)). The two most special cases are when all three parameters are fixed. The first leads to

$$M_{0,\frac{1}{2}}\left(\frac{i\eta^2}{4\hat{D}}\right) = 2\sinh\left(\frac{i\eta^2}{8\hat{D}}\right) \tag{16}$$

in the usual atomic units $\hat{D} = \frac{1}{2}, \alpha = -\frac{1}{4}$ and $a = -\frac{3}{8}$. The second one is

$$W_{0,\frac{1}{3}}\left(\frac{i\eta^2}{2\hat{D}}\right) = 2\sqrt{\pi} \cdot \left(\frac{3i\eta^2}{\hat{D}}\right)^{\frac{1}{6}} \cdot \mathrm{Ai}\left(\left[\frac{3i\eta^2}{\hat{D}}\right]^{\frac{2}{3}}\right), \tag{17}$$

where $\alpha = \frac{1}{4}$, $\hat{D} = \frac{1}{2}$ and $a = \frac{1}{8} - \frac{1}{9}$ and Ai() stand for the Airy function.[22] When only $\hat{D} = \frac{1}{2}$ is fixed, the following relation is valid:

$$M_{\kappa,\kappa-\frac{1}{2}}\left(\frac{i\eta^2}{4\hat{D}}\right) = W_{\kappa,\kappa-\frac{1}{2}}\left(\frac{i\eta^2}{4\hat{D}}\right) = M_{\kappa,-\kappa+\frac{1}{2}}\left(\frac{i\eta^2}{4\hat{D}}\right) = e^{-\left(\frac{i\eta^2}{4\hat{D}}\right)}\left(\frac{i\eta^2}{4\hat{D}}\right)^{\kappa}, \tag{18}$$

which can be fulfilled with arbitrary combinations of $(1+4\alpha)^2 = 1-8a$ (where $\kappa = 1/4-\alpha$ and $\kappa - 1/2 = \frac{1}{4}\sqrt{1-8a}$). A similar relation is true for

$$M_{\mu-\frac{1}{2},\mu}\left(\frac{i\eta^2}{4\hat{D}}\right) = 2\mu e^{\frac{z}{2}} z^{\frac{1}{2}-\mu} \cdot \gamma\left[2\mu, \left(\frac{i\eta^2}{4\hat{D}}\right)\right] \tag{19}$$

and

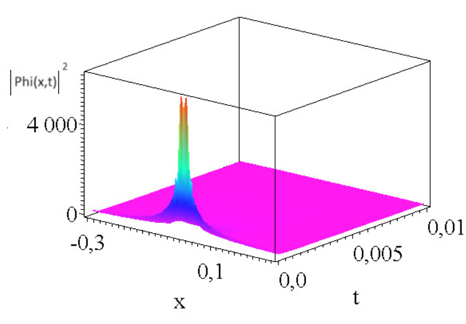
$$W_{\mu-\frac{1}{2},\mu}\left(\frac{i\eta^2}{4\hat{D}}\right) = e^{\frac{z}{2}} z^{\frac{1}{2}-\mu} \cdot \Gamma\left[2\mu, \left(\frac{i\eta^2}{4\hat{D}}\right)\right], \tag{20}$$

where $\gamma(a,z)$ and $\Gamma(a,z)$ are the incomplete lower and incomplete upper Gamma functions, for more information (NIST 8.2.1–8.2.2).[22] For $\hat{D} = \frac{1}{2}$, the relation between the two remaining parameters is $(3-4\alpha)^2 = 1-8a$.

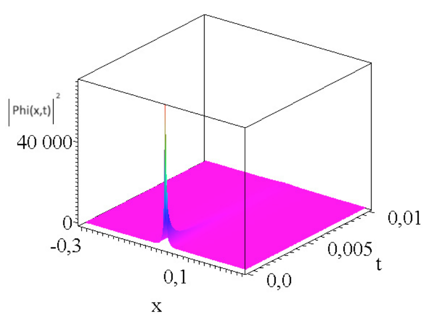
Another interesting case is when only the self-similar exponent is fixed $\alpha = -1/4$ it gives us the modified Bessel functions $I()$ and $K()$ with quadratic arguments

$$\begin{aligned} M_{0,\omega}\left(\frac{i\eta^2}{4\hat{D}}\right) &= 2^{2\omega+1/2} \cdot \Gamma(1+\omega) \cdot \sqrt{\frac{i\eta^2}{8\hat{D}}} \cdot I_\omega\left(\frac{i\eta^2}{8\hat{D}}\right), \\ W_{0,\omega}\left(\frac{i\eta^2}{4\hat{D}}\right) &= \sqrt{\frac{i\eta^2}{4\hat{D}\pi}} \cdot K_\omega\left(\frac{i\eta^2}{8\hat{D}}\right). \end{aligned} \tag{21}$$

For better transparency, we used the $\omega = \frac{1}{4}\sqrt{1-\frac{4a}{\hat{D}}}$ and $\Gamma()$ stands for the Gamma function again. There are additional relations available which reduce the Whittaker functions to parabolic cylinder functions (Eqs. (13.8.8)–(13.8.10)) or various orthogonal polynomials like Hermite (Eqs. (13.18.14)–(13.18.16))[22] or Laguerre polynomials (Eq. (13.18.17)).[22] With a far analogy — in general — we may say that the Whittaker M functions due to the inherent oscillations showing some similarities to some scattering quantum mechanical wave functions, however the Whittaker W functions look like wave function for some bound ground states. Figure 6 shows the absolute value squared of Eq. (11) $|\Phi(x,t)|^2$ for the parameter set of $\hat{D} = \alpha = 1/2$,



(a)



(b)

Fig. 6. The $|\Phi(x,t)|^2$ of Eq. (11) for $\alpha = 1/2$ and $\hat{D} = 1/2, a = 1/4$. The subfigures (a) show the Whittaker M and (b) Whittaker W function, respectively.

and $a = 1/4$. Both Whittaker functions have a very high and sharp peak in the origin and a very quick decay.

The crucial point is if we can find a parameter set for which the L^2 norm $|\Phi(x, t = t_0)|^2$ is finite. Our numerical experiences showed that for both the Whittaker W and Whittaker M functions, for the same parameter set $(\hat{D}, \alpha, a)$, convergence can be achieved. For the Whittaker W functions, the convergence is quite quick and valid even for $\alpha = 1$. For the oscillating Whittaker M function, the convergence is much weaker, we can only prove it with numerical integration using interval doubling. Usually we concentrate on the $a \leq 1/4$ values defining attractive potentials with bound states. For Whittaker M function, even for negative a values, the L^2 integral is convergent for $\alpha = 1/2$. Such solutions could have quantum mechanical relevance in the future.

4. Summary

In this study, we analyzed the complex diffusion and a special kind of reaction-diffusion equation with the self-similar Ansatz and presented numerous analytic solutions for various αs. For the complex diffusion equation, the solutions are proportional to the Kummer's M and Kummer's U functions with complex quadratic arguments. With exhaustive numerical calculations we showed that for $\alpha = 1/2$ the numerical integral of the $|t^{-2\alpha} \cdot U(\alpha + \frac{1}{2}, \frac{3}{2}, \frac{ix^2}{4\hat{D}t}) \cdot \frac{x}{t^{\frac{1}{2}}}|^2$ function has a finite numerical value.

In the second part of the study, a special form of the reaction–diffusion equation was investigated which is form invariant to the Schrödinger equation with a power-law type of space-dependent potential. We derived that for the $V(x) = -a/x^2, a > 0$ interaction the solutions can be expressed with the exponential and Whittaker M or Whittaker W functions with complex quadratic arguments. In quantum mechanics, this potential has unusual and remarkable properties with established literature discussing the properties of the analytic solutions. We found that the quantum mechanical solution and our self-similar solution have the same critical parameter. Finally, we found parameter sets where the numerical integral of the absolute value squared of our solutions is convergent. This is far from being a rigorous mathematical proof of L^2 integrability but a possible hint of such property. Future work is in progress to present a similar study to the spherically symmetric case where even the role of the angular momenta as parameter can be studied. It is evident that additional Fourier transformation, Wigner transformation or even the entropy of our solutions can be evaluated. We hope that our new solution will give new insight into the mathematical properties of the diffusion phenomena.

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