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Variational Principle for a Schrödinger Equation with Non-Hermitian Hamiltonian and Position–Dependent Mass

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Abstract *A classical field theory for a Schrödinger equation with a non-Hermitian Hamiltonian describing a particle with position-dependent mass has been recently advanced by Nobre and Rego–Monteiro (NR) [Phys. Rev. A* **88** *(2013) 032105]. This field theory is based on a variational principle involving the wavefunction $\Psi(x,t)$ and an auxiliary field $\Phi(x,t)$. It is here shown that the relation between the dynamics of the auxiliary field $\Phi(x,t)$ and that of the original wavefunction $\Psi(x,t)$ is deeper than suggested by the NR approach. Indeed, we formulate a variational principle for the aforementioned Schrödinger equation which is based solely on the wavefunction $\Psi(x,t)$. A continuity equation for an appropriately defined probability density, and the concomitant preservation of the norm, follows from this variational principle via Noether's theorem. Moreover, the norm-conservation law obtained by NR is reinterpreted as the preservation of the inner product between pairs of solutions of the variable mass Schrödinger equation.*

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A Schrödinger equation for a particle with an effective, position-dependent mass has been recently introduced by Costa Filho, Almeida, Farias, and Andrade (CAFA).[1] This equation describes an interesting example of a quantum system with a dynamics governed by a non-Hermitian Hamiltonian, a subject that has attracted considerable attention recently (see for instance Refs. [2–4] and references therein). Another noticeable feature of the CAFA equation is that it is related to a deformed displacement operator, which has been found to be closely related to the Morse potential.[5] The CAFA proposal provides an intriguing alternative point of view on the dynamics of quantum particles with position dependent mass (see Refs. [6–9] and references therein for discussions on other approaches).

A field theory leading to the CAFA equation has been advanced by Rego–Monteiro and Nobre (RN).[10] This is a potentially important endeavor because it provides further support for the idea that it is possible to formulate a consistent quantum dynamics based on non-Hermitian Hamiltonians. In order to obtain the aforementioned field theory, and the concomitant variational principle, RN followed the procedure of introducing an auxiliary field besides the wave function Ψ appearing in the CAFA equation. This approach is well-known in mathematical physics for the formulation of variational principles leading to non-Hamiltonian evolution equations such as, for instance, the diffusion equation.[11] Motivated by their variational principle, RN also introduced a probability density, involving both the wave function and the auxiliary field, that satisfies a continuity equation.

The aim of our present contribution is to show that there is no need for an auxiliary field in order to formulate the variational principle for the CAFA equation. In fact, as we shall presently see, there is a variational principle for the CAFA equation involving solely the Ψ wave function and its complex conjugate, similarly to what occurs with the standard Schrödinger equation. An appropriate symmetry corresponding to this variational principle has an associated Noether's conserved current, leading to a probability density continuity equation.

The CAFA equation governs the behavior of the wave function Ψ corresponding to a quantum particle with a position dependent effective mass given by,

$$m_e = \frac{m}{(1+\gamma x)^2}\,, \tag{1}$$

where m is a constant with dimensions of mass and γ a constant with dimensions of inverse length. The CAFA equation reads,

$$\mathrm{i}\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\hat{D}_\gamma^2\Psi(x,t) + V(x)\Psi(x,t)\,, \tag{2}$$

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where $\hbar$ stands for the Planck constant and the operator $\hat{D}_\gamma$ is,

$$\hat{D}_\gamma = (1+\gamma x)\frac{\mathrm{d}}{\mathrm{d}x}\,. \tag{3}$$

The CAFA equation can be re-cast directly in terms of the effective mass m_e,

$$\mathrm{i}\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2}\Psi(x,t) - \frac{\hbar^2}{2}\Big[\frac{\mathrm{d}}{\mathrm{d}x}\Big(\frac{1}{2m_e}\Big)\Big] \times \frac{\partial\Psi(x,t)}{\partial x} + V(x)\Psi(x,t)\,. \tag{4}$$

In order to obtain the CAFA equation from a variational principle, NR introduced the Lagrangian density,

$$\begin{aligned}\mathcal{L} =& \frac{\mathrm{i}\hbar}{2}\Phi(x,t)\partial_t\Psi(x,t) \\ &+ \frac{\hbar^2}{8}\Big[\frac{\mathrm{d}}{\mathrm{d}x}\Big(\frac{1}{m_e}\Big)\Big]\Phi(x,t)\partial_x\Psi(x,t) \\ &+ \frac{\hbar^2}{4m_e}\Phi(x,t)\partial_x^2\Psi(x,t) \\ &- \frac{1}{2}V(x)\Psi(x,t)\Phi(x,t) \\ &- \frac{\mathrm{i}\hbar}{2}\Phi^*(x,t)\partial_t\Psi^*(x,t) \\ &+ \frac{\hbar^2}{8}\Big[\frac{\mathrm{d}}{\mathrm{d}x}\Big(\frac{1}{m_e}\Big)\Big]\Phi^*(x,t)\partial_x\Psi^*(x,t) \\ &+ \frac{\hbar^2}{4m_e}\Phi^*(x,t)\partial_x^2\Psi^*(x,t) \\ &- \frac{1}{2}V(x)\Psi^*(x,t)\Phi^*(x,t)\,,\end{aligned} \tag{5}$$

involving the original wave function Ψ and an auxiliary field Φ. In the above equation ∂_x and ∂_t are shorthand notations for $\partial/\partial x$ and $\partial/\partial t$, respectively. In this paper we are going to use both notations, as well as the ∇-notation.

The action variational principle associated with the Lagrangian density (5) leads to the CAFA equation (2), together with a new differential equation governing the evolution of the auxiliary field Φ. This last equation is,

$$\begin{aligned}-\mathrm{i}\hbar\frac{\partial\Phi(x,t)}{\partial t} =& -\frac{\hbar^2}{2m_e}\frac{\partial^2\Phi(x,t)}{\partial x^2} \\ &- \frac{3\hbar^2\gamma(1+\gamma x)}{2m}\frac{\partial\Phi(x,t)}{\partial x} \\ &- \frac{\hbar^2\gamma^2}{2m}\Phi(x,t) + V(x)\Phi(x,t)\,.\end{aligned} \tag{6}$$

As already mentioned, this kind of scheme involving an auxiliary field provides a convenient way of formulating action variational principles for evolution equations that are not necessarily Hamiltonian or conservative (the auxiliary field is sometimes referred to as the "mirror-image" variable or field[11]). As paradigmatic examples of this approach we can mention, for instance, its application to the damped harmonic oscillator, and to the diffusion equation.[11] Variational principles obtained in this way are of considerable practical value in order to obtain, on the basis of an appropriate variational ansatz, approximate solutions to the evolution equation under study. From the fundamental point of view, however, these kind of variational principles are not as satisfactory as those based solely on the original field. The latter ones have the desirable features of providing highly "compressed" and economical descriptions of the system's dynamics and shedding light on the symmetries and conservation laws satisfied by the concomitant evolution equations. It is therefore of some interest to find out if the CAFA equation can be derived from a variational principle involving only the wave function Ψ and its complex conjugate Ψ^*. This is our purpose here. In order to answer the above question in a transparent way it will prove convenient to discuss an evolution equation slightly more general than the CAFA one. Let us consider the evolution equation (in N spatial dimensions),

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}g(\boldsymbol{x})\nabla[g(\boldsymbol{x})\nabla\Psi(\boldsymbol{x},t)] + V(\boldsymbol{x})\Psi(\boldsymbol{x},t)\,, \tag{7}$$

where $\boldsymbol{x}\in\mathcal{R}^N$, and $\nabla = (\partial/\partial x_1,\ldots,\partial/\partial x_N)$ is the N-dimensional ∇-operator. In the one-dimensional case with

$$g(x) = 1+\gamma x\,, \tag{8}$$

we recover the CAFA equation as a particular instance of Eq. (7). We now introduce the Lagrangian density,

$$\begin{aligned}\mathcal{L} =& \frac{\mathrm{i}\hbar}{g(\boldsymbol{x})}\Psi^*(\boldsymbol{x},t)\frac{\partial\Psi(\boldsymbol{x},t)}{\partial t} \\ &- \frac{\hbar^2}{2m}g(\boldsymbol{x})(\nabla\Psi^*(\boldsymbol{x},t))\cdot(\nabla\Psi(\boldsymbol{x},t)) \\ &- \frac{1}{g(\boldsymbol{x})}V(\boldsymbol{x})\Psi^*(\boldsymbol{x},t)\Psi(\boldsymbol{x},t)\,.\end{aligned} \tag{9}$$

The action variational principle associated with the Lagrangian (9) reads,

$$\delta\int_{t_1}^{t_2}\mathrm{d}t\Big[\int\mathcal{L}\,\mathrm{d}^N x\Big] = 0\,, \tag{10}$$

which leads to,

$$\begin{aligned}&\delta\int_{t_1}^{t_2}\mathrm{d}t\Big\{\int\delta\Psi^*\Big[\frac{\mathrm{i}\hbar}{g(\boldsymbol{x})}\frac{\partial\Psi}{\partial t} + \frac{\hbar^2}{2m}\nabla[g(\boldsymbol{x})\nabla\Psi] - \frac{1}{g(\boldsymbol{x})}V\Psi\Big] \\ &\quad + \delta\Psi\Big[-\frac{\mathrm{i}\hbar}{g(\boldsymbol{x})}\frac{\partial\Psi^*}{\partial t} + \frac{\hbar^2}{2m}\nabla\Big[g(\boldsymbol{x})\nabla\Psi^* - \frac{1}{g(\boldsymbol{x})}V\Psi^*\Big]\Big]\Big\}\mathrm{d}^N x \\ &= 0\,.\end{aligned} \tag{11}$$

Defining now,

$$C(\boldsymbol{x},t) = \frac{\mathrm{i}\hbar}{g(\boldsymbol{x})}\frac{\partial\Psi}{\partial t} + \frac{\hbar^2}{2m}\nabla[g(\boldsymbol{x})\nabla\Psi] - \frac{1}{g(\boldsymbol{x})}V\Psi, \tag{12}$$

we obtain,

$$\delta\int\mathrm{d}t\Big\{\int\delta\Psi^*(\boldsymbol{x},t)C(\boldsymbol{x},t) + \delta\Psi(\boldsymbol{x},t)C^*(\boldsymbol{x},t)\Big\}\mathrm{d}^N x = 0. \tag{13}$$

Writing Ψ and C explicitly in terms of their real and imaginary parts,

$$\Psi(\boldsymbol{x},t) = \Psi_r(\boldsymbol{x},t) + \mathrm{i}\Psi_i(\boldsymbol{x},t)\,, \tag{14}$$

$$C(\boldsymbol{x},t) = C_r(\boldsymbol{x},t) + \mathrm{i}C_i(\boldsymbol{x},t)\,, \tag{15}$$

we can re-cast the variational principle (13) in the form,

$$2\delta\int \mathrm{d}t\Big\{\int \delta\Psi_r(\boldsymbol{x},t)C_r(\boldsymbol{x},t) - \delta\Psi_i(\boldsymbol{x},t)C_i(\boldsymbol{x},t)\Big\}\mathrm{d}^N x = 0\,. \tag{16}$$

Now, taking into account that an arbitrary variation $\delta\Psi$ of the complex wave function Ψ is tantamount to arbitrary and independent variations of its real and imaginary parts, one obtains from Eq. (16) that

$$C_r(\boldsymbol{x},t) = C_i(\boldsymbol{x},t) = 0\,, \tag{17}$$

meaning that,

$$\frac{\mathrm{i}\hbar}{g(\boldsymbol{x})}\frac{\partial\Psi}{\partial t} + \frac{\hbar^2}{2m}\nabla[g(\boldsymbol{x})\nabla\Psi] - \frac{1}{g(\boldsymbol{x})}V\Psi = 0\,, \tag{18}$$

which (after multiplying both members of Eq. (18) by $g(\boldsymbol{x})$) yields precisely Eq. (7). The evolution equation (18) can of course be obtained also by the conventional procedure of regarding the wave function Ψ and its complex conjugate Ψ^* as independent fields when implementing the variational principle associated with the Lagrangian,

$$\mathcal{L}(\Psi,\partial_t\Psi,\partial_{x_1}\Psi,\ldots,\partial_{x_N}\Psi,\Psi^*,\partial_t\Psi^*,\partial_{x_1}\Psi^*,\ldots,\partial_{x_N}\Psi^*)\,, \tag{19}$$

given by Eq. (9). In that case, Eq. (18) and its complex conjugate are equivalent, respectively, to the Euler–Lagrange equations derived from the Lagrangian (9),

$$\frac{\partial}{\partial t}\Big(\frac{\partial\mathcal{L}}{\partial(\partial_t\Psi^*)}\Big) + \Big[\sum_{i=1}^N\frac{\partial}{\partial x_i}\Big(\frac{\partial\mathcal{L}}{\partial(\partial_{x_i}\Psi^*)}\Big)\Big] - \frac{\partial\mathcal{L}}{\partial\Psi^*} = 0\,,\quad \frac{\partial}{\partial t}\Big(\frac{\partial\mathcal{L}}{\partial(\partial_t\Psi)}\Big) + \Big[\sum_{i=1}^N\frac{\partial}{\partial x_i}\Big(\frac{\partial\mathcal{L}}{\partial(\partial_{x_i}\Psi)}\Big)\Big] - \frac{\partial\mathcal{L}}{\partial\Psi} = 0\,. \tag{20}$$

Our previous procedure of explicitly considering independent variations of the real and the imaginary parts of Ψ was followed in order to emphasize that the complex conjugate wave function Ψ^* appearing in the Lagrangian (9) does not play the role of an independent "auxiliary field" (in the sense of NR).

The Lagrangian density (9) is invariant under the transformation

$$\Psi(\boldsymbol{x},t)\to\Lambda(\boldsymbol{x},t) = \mathrm{e}^{\mathrm{i}\theta}\Psi(\boldsymbol{x},t)\,,$$
$$\Psi^*(\boldsymbol{x},t)\to\Lambda^*(\boldsymbol{x},t) = \mathrm{e}^{-\mathrm{i}\theta}\Psi^*(\boldsymbol{x},t)\,, \tag{21}$$

characterized by the continuous, real parameter θ. Following a standard procedure[12–13] one can verify that this symmetry has an associated Noether conserved current leading to the continuity equation,

$$\frac{\partial}{\partial t}\Big[\frac{\partial\mathcal{L}}{\partial(\partial_t\Psi)}\Big(\frac{\partial\Lambda}{\partial\theta}\Big)_{\theta=0}\Big] + \sum_{i=1}^N\frac{\partial}{\partial x_i}\Big[\frac{\partial\mathcal{L}}{\partial(\partial_{x_i}\Psi)}\Big(\frac{\partial\Lambda}{\partial\theta}\Big)_{\theta=0}\Big] + \frac{\partial}{\partial t}\Big[\frac{\partial\mathcal{L}}{\partial(\partial_t\Psi^*)}\Big(\frac{\partial\Lambda^*}{\partial\theta}\Big)_{\theta=0}\Big] + \sum_{i=1}^N\frac{\partial}{\partial x_i}\Big[\frac{\partial\mathcal{L}}{\partial(\partial_{x_i}\Psi^*)}\Big(\frac{\partial\Lambda^*}{\partial\theta}\Big)_{\theta=0}\Big] = 0\,. \tag{22}$$

Defining now,

$$\rho = \frac{1}{g}\Psi\Psi^* = \frac{|\Psi|^2}{g}\,,\quad \boldsymbol{J} = \frac{\mathrm{i}\hbar}{2m}g[\Psi\nabla\Psi^* - \Psi^*\nabla\Psi]\,, \tag{23}$$

the continuity equation (22) can be re-written explicitly in terms of a density ρ and a density current $\boldsymbol{J}$, adopting the standard form,

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\boldsymbol{J} = 0\,. \tag{24}$$

As a consequence of Eq. (24) we obtain the preservation of the norm,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\rho\,\mathrm{d}^N x = \frac{\mathrm{d}}{\mathrm{d}t}\int\frac{1}{g(\boldsymbol{x})}\Psi(\boldsymbol{x},t)\Psi^*(\boldsymbol{x},t)\,\mathrm{d}^N x = 0\,. \tag{25}$$

Now, in order to clarify the meaning of the variational principle proposed by NR, let us consider the Lagrangian density,

$$\mathcal{L} = \frac{\mathrm{i}\hbar}{g(\boldsymbol{x})}\tilde{\Psi}^*(\boldsymbol{x},t)\frac{\partial\Psi(\boldsymbol{x},t)}{\partial t} - \frac{\hbar^2}{2m}g(\boldsymbol{x})(\nabla\tilde{\Psi}^*(\boldsymbol{x},t))\cdot(\nabla\Psi(\boldsymbol{x},t)) - \frac{1}{g(\boldsymbol{x})}V(\boldsymbol{x})\tilde{\Psi}^*(\boldsymbol{x},t)\Psi(\boldsymbol{x},t)\,, \tag{26}$$

which is obtained by replacing in Eq. (9) the complex conjugate Ψ^* of the wave function Ψ by the complex conjugate $\tilde{\Psi}^*$ of the new field $\tilde{\Psi}$, independent of Ψ. The Euler–Lagrange equations corresponding to the Lagrangian (26) lead again to the evolution equation (7) for Ψ, and to an evolution equation for $\tilde{\Psi}^*$ which, after complex conjugation, has exactly the form (7). That is, Ψ and $\tilde{\Psi}$ evolve according to the same Schrödinger equation. Now, the Lagrangian (26) is invariant under the transformation,

$$\Psi(\boldsymbol{x},t)\to\mathrm{e}^{\mathrm{i}\theta}\Psi(\boldsymbol{x},t)\,,\quad \tilde{\Psi}(\boldsymbol{x},t)\to\mathrm{e}^{\mathrm{i}\theta}\tilde{\Psi}(\boldsymbol{x},t)\,. \tag{27}$$

The conserved Noether current associated with the above symmetry leads to the continuity-like equation,

$$\frac{\partial P}{\partial t} + \nabla\cdot\boldsymbol{K} = 0\,. \tag{28}$$

where

$$P = (1/g(\boldsymbol{x}))\Psi\tilde{\Psi}^*,\quad \boldsymbol{K} = \frac{\mathrm{i}\hbar}{2m}g(\boldsymbol{x})[\Psi\nabla\tilde{\Psi}^* - \tilde{\Psi}^*\nabla\Psi]\,. \tag{29}$$

Equation (28), in turn, yields,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\frac{1}{g(\boldsymbol{x})}\tilde{\Psi}^*(\boldsymbol{x},t)\Psi(\boldsymbol{x},t)\,\mathrm{d}^N x = 0\,. \tag{30}$$

That is, the quantity

$$\int \frac{1}{g(\boldsymbol{x})} \tilde{\Psi}^*(\boldsymbol{x},t)\Psi(\boldsymbol{x},t)\,\mathrm{d}^N x\,, \tag{31}$$

which can be interpreted as an inner product between two time-dependent solutions of Eq. (7), is conserved under the concomitant dynamics.

After the identification,

$$\tilde{\Psi}^* \to g(x)\Phi\,, \tag{32}$$

it is plain that, in the particular case of one spatial dimension and g given by Eq. (8), the variational principle associated with the Lagrangian (26) is equivalent to the one proposed by NR, which is derived from the Lagrangian (5). In terms of the identification (32), the conserved norm found by NR is,

$$\frac{1}{2}\int \frac{1}{g(x)} (\tilde{\Psi}^*(x,t)\Psi(x,t) + \tilde{\Psi}(x,t)\Psi^*(x,t))\,\mathrm{d}x\,, \tag{33}$$

which turns out to be the real part of the (conserved) inner product between two different solutions of the CAFA equation. In the limit $\gamma \to 0$ we have $g \to 1$, the CAFA equation reduces to the standard (constant mass) Schrödinger equation, and the conserved norm found by NR reduces to the real part of the inner product between two time-dependent solutions of the usual Schrödinger equation.

Summing up, we have shown that the CAFA Schrödinger equation for a particle with an effective position-dependent mass can be derived from a variational principle involving only the wave function Ψ and its complex conjugate Ψ^*, with no need of introducing an auxiliary field. This variational principle leads, via Noether's theorem, to a conserved Noether current, and to the concomitant conservation of an appropriately defined norm. The auxiliary field appearing in the variational principle proposed by NR is itself, via the identification (32), closely related to a time-dependent solution of the CAFA equation. Consequently, the NR variational principle can be re-cast in terms of two independent solutions of the same equation: the CAFA one. Moreover, the conserved norm found by NR turns out to be the real part of the (also conserved) inner product between two solutions of the CAFA equation.

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