Hamilton-Jacobi approach to quantum mechanics via negative kinetic energies

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Negative kinetic energies can either be nonsense or convey a profound truth about the physical reality (e.g., antimatter in relativistic QED). In quantum mechanics, they are associated with some relevant manifestations (weak measurements, quantum backflow, Glauber quantum oscillator, etc.) and have been recently discovered in optics (optical backflow). Here, building on the analogy between optical waves and wave propagation of Hamilton-Jacobi (HJ) wave fronts, new effects caused by the Hamilton’s principal function $S_0$ that solves the HJ equation for negative kinetic energies are investigated. It turns out that the HJ wave function $\Psi^0_{HJ} = \exp(i S_0 / \hbar)$ reproduces correctly well-known Schrödinger’s wave functions of the vacuum state. The role of negative kinetic energies in establishing a no-contrast theorem regarding the quantum-classical correspondence is also emphasized in relation to the Hamilton’s principle of stationary action. Schrödinger and Heisenberg representations of quantum mechanics are thus demonstrated to be compatible with the HJ approach where negative kinetic energies are permitted. It is also shown how $\Psi^0_{HJ}$ shapes the wave functions at positive kinetic energies after the introduction of a quantum Babinet principle where the vacuum is regarded as the perfectly destructive interference of waves that manifest Aharonov-Berry superoscillatory behavior arising from phase singularities. Being these findings independent from the actual value of $\hbar$, the results obtained here are liberated from the classical limit ($\hbar \to 0$) that applies to the Hamilton’s principal function $S$ constrained to positive kinetic energies only. This work opens new avenues for further extension of the HJ theory at negative kinetic energies to the relativistic quantum arena.

Wave mechanics implies delocalization over the whole configuration space. Here, we apply this concept to the geometric interpretation of Hamilton-Jacobi (HJ) theory [1, 2]. It means that canonical momenta, calculated as the gradient of the Hamilton’s principal function $S$, are imaginary when referred to the so-called classically forbidden regions of the configuration space. However, based on the analogy between canonical momenta and index of refraction in optics [1, 2], whose imaginary component generates evanescent waves [3, 4], it is admissible that the Hamilton’s principal function $S$ (and the characteristic function $W = S + Et$) be complex-valued. Counting on this, we show that the wave front of $\Psi^0_{HJ} = \exp(i S / \hbar)$ satisfies basic quantum-mechanical laws independently from the value of the action unit $\hbar$.

A first consequence of delocalization and the presence of imaginary momenta is that negative kinetic energies are accessible. In quantum mechanics, they appear in some contexts (weak measurements [5, 6], quantum backflow [7, 8], Glauber quantum oscillator [9, 10]), but they are understood in optics as a manifestation of optical backflow [8], which has been recently observed [11]. Relying on the analogy between optics and the geometrical interpretation of the HJ approach to mechanics [1, 2], we expect some equally exotic physical effects caused by negative kinetic energies.

**Meaning of negative kinetic energies.** To make them appear, it suffices to consider the quantum-mechanical kinetic operator emerging from the identity between HJ equation and Schrödinger equation applied to $\Psi^0_{HJ}$ where $S$ is a complex-valued function (Supplementary Material S1)

$$\hat{T}_{QM} = \frac{1}{2m} p \otimes p - \frac{i \hbar}{2m} \nabla^2 W$$  \hfill (1)

In Eq. (1) the dyadic product $\otimes$ is introduced to take into account the possible complex values of $W$ (or $S$). Only when $\text{Im}(W) = 0$ (i.e., the classical case), the product $p \otimes p$ is the ordinary scalar product $p \cdot p = p^2$. Application of the operator to the state $\psi^0_{HJ} = \exp(i W_0 / \hbar)$ defined by negative kinetic HJ energies (i.e., $\text{Re}(W_0) = 0$) yields (Supplementary Material S1)

$$\hat{T}_{QM} \psi^0_{HJ} = \frac{1}{2m} (-[\nabla \text{Im}(W_0)]^2 - i \hbar \nabla^2 W_0) \psi^0_{HJ}$$  \hfill (2)

where only the spatial component $\psi^0_{HJ}$ of $\Psi^0_{HJ} = \exp(i S_0 / \hbar)$ is considered. Keeping this in mind, suppose now that $W$ is the solution to the reduced HJ equation of the simple harmonic oscillator at $E > 0$. Conditioning the
HJ wave function to represent the wave front implies that \( dS = pdq - Edt = 0 \) [1, 2]. In other terms, by virtue of the relationship between Hamilton’s principal function and Lagrangian \( dS/dt = L = T - V \), the kinetic and the potential energy must be equal in the classically allowed region, hence \( S = \) constant (i.e., Hamilton’s principle of stationary \( S \)) thanks to \( p = \pm im\omega q \). If so, outside of the classical region where \( E = 0 \), the condition becomes \( p = \pm im\omega q \) and, consequently, \( d^2W_0/dq^2 = im\omega \). This means that the term \(-i\hbar\nabla^2W_0/2m\) in Eq. (2) for the unidimensional oscillator has the precise meaning of the vacuum energy \( \hbar\omega/2 \) added to the more canonical kinetic energy. The elusive and fundamental lump of energy that is at the base of quantum mechanics [12] manifests itself in elementary wave interpretation of the HJ approach combined with Hamilton’s principle of stationary action! It can also be argued that the HJ state \( \psi_{HJ}^0 \) should have features related to the vacuum state and, indeed, this is demonstrated next. The dimensionless HJ equation for the normalized Hamilton’s characteristic function \( w = W/\hbar \) is (Supplemental Material S2)

\[
\left( \frac{\partial w}{\partial \xi} \right)^2 + \xi^2 = 2\epsilon \tag{3}
\]

where \( \xi = q/q_0 \) (with \( q_0 = \sqrt{\hbar/m\omega} \)) and \( \epsilon = E/\hbar\omega \). Taking \( \epsilon = 0 \) as before, the vacuum HJ solution is \( w_0 = \pm i\xi^2/2 \). This one leads to the regular (i.e., without divergence) HJ state

\[
\psi_{HJ}^0 = e^{-\xi^2/2} \tag{4}
\]

and we get straightforwardly the well-known Schrödinger’s vacuum state characterized by a Gaussian distribution. Note that, the spatial decay of Eq. (4) echoes the decaying amplitudes of evanescent optical waves occurring for imaginary indices of refraction. In this respect, the analogy between optics and HJ approach is again confirmed.

It is possible to extend the previous demonstration to other paradigmatic examples. For instance, extension to 2D problems can be summarized by the isotropic harmonic oscillator whose HJ wave function coincides exactly with Schrödinger’s (Supplemental Material S3). The hydrogen atom is instead an excellent example of a rather complicated 3D HJ problem that takes a new meaning if negative kinetic energies are allowed. The dimensionless HJ equation for the normalized radial component \( w_r = W_r/\hbar \) of the Hamilton’s characteristic function is (Supplemental Material S4)

\[
\left( \frac{\partial w_r}{\partial \rho} \right)^2 + \frac{j^2}{\rho^2} - \frac{2\rho}{\rho} = -\epsilon \tag{5}
\]

where \( \rho = r/r_0 \) (\( r_0 = \hbar^2/mk \) with \( k = e^2/4\pi\epsilon_0 \)), \( \lambda = \alpha/\hbar \), \( \eta \) is a parameter and \( \epsilon = 2\hbar^2\eta^2|E|/mk^2 \). Eq. (5) for purely rotational motion \( (\epsilon = 1 \) and \( \eta = \lambda \) has solution

\[
w_r^{rot} = \pm i\left( \rho - \frac{\lambda}{\rho} \right) \tag{6}
\]

and it is so easy to get the following regular radial HJ state

\[
R_{HJ}^{rot} = e^{i\omega_r^{rot} \rho} = \rho^\lambda e^{-\rho} \tag{7}
\]

where \( \lambda \) is an integer thanks to the conservation of the angular momentum \( \alpha_0 \) combined with the periodicity of the angular part of the HJ state (not shown). Eq. (7) brings out clearly the vacuum contribution \( \exp(-\rho) \) for \( \lambda = 0 \) (i.e., no rotation). Note also that again the imaginary momentum implied in Eq. (6) displays the exponential vacuum decay analogous to the decay of evanescent waves in optics. Another comment regards \( R_{HJ}^{rot} \) as the state expected for the classical circular Bohr orbits [13], which are of interest for advanced applications of Rydberg atoms [14]. At the same time, \( R_{HJ}^{rot} \) shows fundamental dependences of the more general Schrödinger’s wave function. Remarkably, these dependences have been obtained without any particular effort in comparison with the procedure employed to solve the Schrödinger’s radial equation. The use of Eq. (7) to solve the hydrogen atom is however available (Supplemental Material S5).

One question that is obvious at this point is the following: how is it possible to find imprints of genuinely quantum-mechanical manifestations in the classical HJ wave function? To underline the importance of such a question, it is worth mentioning that the classical limit \( \hbar \to 0 \) forbids \( \psi_{HJ} \) representing quantum-mechanical systems [15]. Dirac’s argument about the distinction between classical and quantum action is indeed commonplace in the community. But, the situation changes if negative kinetic energies are allowed. Thus, a first simple answer is that the classical limit has to be revised in light of negative kinetic energies which are by no means a purely classical manifestation. In pursuing this orientation, a more elaborated answer to the question is the following theorem.

\textit{No-contrast theorem.} For a particle of mass \( m \) subjected to a conservative potential \( V(q) \), the kinetic operator applied to the HJ wave function \( \psi_{HJ} = \Phi \exp(iS_{Re}/\hbar) \) is

\[
-\frac{\hbar^2}{2m} \nabla^2 \psi_{HJ} = -\frac{i\hbar}{2m} e^{iS_{Im}/\hbar} [\Phi \nabla^2 S_{Re} + 2V\Phi \cdot \nabla S_{Re} - (\hbar\nabla^2 \Phi)] + \frac{1}{2m} e^{iS_{Im}/\hbar} \Phi (\nabla S_{Re})^2 \tag{8}
\]

where \( S_{Re} \) is the real part of the Hamilton’s principal function whereas the imaginary part \( S_{Im} \) is contained in \( \Phi = \exp(-S_{Im}/\hbar) \) that takes into account the presence of negative kinetic energies. Since the real part of \( S \) is solution to the ordinary HJ equation \([\nabla S_{Re}]^2 = 2m(E - V) \) (with \( E > V \)), Eq. (8) reduces to
\[-\frac{\hbar^2}{2m} \nabla^2 \Psi_{\text{HJ}} = (E - V)\Psi_{\text{HJ}}\]
\[-\frac{i\hbar}{2m} e^{iS_{\text{Re}}/\hbar} \left[ \Phi \nabla^2 S_{\text{Re}} + 2 \nabla \Phi \cdot \nabla S_{\text{Re}} - i\hbar \nabla^2 \Phi \right] \tag{9}\]

This equation becomes the time-independent Schrödinger equation for \(\Psi_{\text{HJ}}\) if
\[\Phi \nabla^2 S_{\text{Re}} + 2 \nabla \Phi \cdot \nabla S_{\text{Re}} - i\hbar \nabla^2 \Phi = 0 \tag{10}\]

The condition is obeyed as long as \(\Phi\) is solution to
\[\nabla^2 \Phi + (\nabla S)^2 \Phi = 0 \tag{11}\]

with \(s = S_{\text{Re}}/\hbar\). Following the prescriptions of the HJ approach, the substitution of \(\nabla S_{\text{Re}}\) with the canonical momentum \(p\) gives a precise meaning to Eq. (11): that is, \(p^2 \Phi = -\hbar^2 \nabla^2 \Phi\). In other terms, the amplitude \(\Phi\) resulting from negative kinetic energies is also solution to the Schrödinger equation! Given this, there is no surprise in the connection shown at the beginning between HJ equation at negative kinetic energies and the vacuum state. The overall conclusion of this reasoning is the no-contrast theorem that can be stated as follows: the HJ wave function \(\Psi_{\text{HJ}}\) satisfies the Schrödinger equation if \(S\) is the Hamilton’s principal function whose real and imaginary parts are solutions to their respective HJ equations.

The no-contrast theorem can be viewed from the perspective that stands behind this whole work: that is, wave-front propagation of \(\Psi_{\text{HJ}}\) according to the most classical wave equation
\[\left(\nabla^2 - \frac{1}{v_{ph}^2} \frac{\partial^2}{\partial t^2}\right) \Psi_{\text{HJ}} = 0 \tag{12}\]

where the modulus squared of the phase velocity holds for the vector \(v_{ph} = dq/dt\). The wave front satisfies the Hamilton’s principle of stationary action. It means that the phase of \(\Psi_{\text{HJ}}\) obeys \(dS_{\text{Re}} = 0\), or \(\nabla S_{\text{Re}} \cdot dq = Edt = 0\). This amounts to saying that solving for the energy, we find \(E = p \cdot v_{ph}\) and, when \(p\) and \(v_{ph}\) are parallel (it happens very often), the wave front transforms the time derivative in Eq. (12) as follows
\[\frac{\partial^2 \Psi_{\text{HJ}}}{\partial t^2} = -\frac{\hbar^2}{2m} \Psi_{\text{HJ}} = -\frac{v_{ph}^2}{\hbar^2} p^2 \Psi_{\text{HJ}} \tag{13}\]

The combination of Eqs. (12) and (13) is \(p^2 \Psi_{\text{HJ}} = -\hbar^2 \nabla^2 \Psi_{\text{HJ}}\) which proves how the wave-front propagation of the HJ wave function \(\Psi_{\text{HJ}}\) gives rise to the time-independent Schrödinger equation once we make the usual substitution \(p^2 = 2m(E - V)\). Besides, the time-dependent Schrödinger equation follows from the harmonic structure of \(\Psi_{\text{HJ}}\). Very importantly, these findings are valid for any value of the action unit \(\hbar\). This conclusion overturns the common idea that the HJ approach is just the classical limit \(\hbar \to 0\) of deeper quantum-mechanical laws [1, 2, 15]. On the other hand, it helps recalling that wave-front propagation of \(\Psi_{\text{HJ}}\) is actually what is really meant by Schrödinger himself [16] and it is surprising that the simplicity of such an interpretation remains hidden to many [17].

**Matrix mechanics.** The Heisenberg representation and its equation of motion can also be understood on the basis of \(\Psi_{\text{HJ}}\) acted upon by the evolution operator \([18, 19]\) (Supplementary Material S6). Recalling the definition of \(\Psi_{\text{HJ}}\) and the general HJ equation \((\partial S/\partial t = -H)\), two distinct cases can be distinguished. When the Hamiltonian is time independent, the connection to the Heisenberg picture is established by the unitary operator \(U(t, t_0) = \exp[-iH(t - t_0)/\hbar]\) whose action on the HJ wave function \(\Psi_{\text{HJ}}(t_0)\) is \(\Psi_{\text{HJ}}(t) = U(t, t_0)\Psi_{\text{HJ}}(t_0)\) and, as such, there is no difference in comparison with the common use of the time-evolution operator. When the Hamiltonian is time dependent, then the time component of the Hamilton’s principal function stems from the formal integration of the HJ equation: \(S = W(q) - \int_{t_0}^{t} H dt\). In this case, the evolution operator becomes \(U(t, t_0) = \exp(-i\int_{t_0}^{t} H dt/\hbar)\) and again it coincides with the canonical expression \([18, 19]\). The Dyson series of \(U(t, t_0)\) could also be reproduced considering the different time windows where the mechanical system evolves under the same value of \(S\) (distributed Hamilton’s principle). This demonstration is postponed to a specific publication where connections to the Heisenberg picture of quantum mechanics are explored in detail beyond what is reported in the supplementary information (Supplementary Material S6).

**Guiding effect.** The solution \(\Psi_{\text{HJ}}(t) = U(t, t_0)\Psi_{\text{HJ}}(t_0)\) to the time-dependent HJ equation has further implications. We suppose that the time dependence of the unitary operator is incorporated in a parameter \(s\) that is somehow related to the energy. Under this hypothesis, parametric dependences appear and it is well known that they are responsible for a variety of effects due to the occurrence of geometric phases in addition to the dynamical phase \([20, 21]\). In the context of this work, the focus is on the parametric dependence related to the vacuum. This one can be visualized as the state due to perfect destructive interference among waves \(\Psi_{\text{HJ}}\) containing phase singularities in the parameter space. Physical intuition has it as a form of Babinet’s principle according to which the diffraction pattern disappears if complementary diffracted fields are added together \([3]\). It means that the vacuum field density \(\rho_0 = |\Psi_{\text{HJ}}(0)|^2\) can be described as the resultant density of the summation of all possible densities \(|\Psi_{\text{HJ}}|^2\) containing their phase singularities in the parameter space. This idea draws its inspiration from phase effects in the event of Aharonov-Berry superoscillations \([22, 23]\). Then,
the multi-component Babinet’s principle can be stated as a simple Taylor expansion over the dimensionless time-dependent parameter $s$ treated as a variable in its own right

$$\rho_0(q, s) = \sum_{n=0}^{\infty} \frac{1}{n!} A_n(s_0, q) (s - s_0)^n$$  (14)

In Eq. (14), the phase singularity at $s = s_0$ is made explicit in the partial densities of the summation having their zeros of progressive order $n$. Thus, the contribution $\delta_n$ to the vacuum field caused by $n$-th singularity is contained in the ratio between $A_n(s_0, q)$ and $\psi_{HJ}^0$

$$\delta_n = \frac{A_n}{\psi_{HJ}^0} = \frac{1}{\psi_{HJ}^0} \left( \frac{d^n \rho_0}{dx^n} \right)_{x=s_0} = \frac{1}{2 n! \psi_{HJ}^0} \int_{s=s_0}^\delta \frac{\rho_0(q,z)}{(z-s_0)^{n+1}} dz$$  (15)

where the Cauchy integral has been introduced on the right-hand side as an alternative to the derivative and to show the pole at the singularity. The conclusion drawn from Eqs. (14) and (15) is that the vacuum state $\psi_{HJ}^0$ can be built as a series of fields vanishing when $s = s_0$. Furthermore, the fields are just a direct consequence of the vacuum density $\rho_0$ modified by the singularity at $s_0$ (pole in the integrand). The singularity is also important because it signals divergent phase velocities whose role in Bell-type experiments might be worth studying for quantum-mechanical correlations.

The guiding effect of the vacuum can be delineated considering canonical examples. For instance, taking the HJ solution of the harmonic oscillator at negative energies, the substitution $\xi \rightarrow \xi - s$ in Eq. (4) gives

$$\rho_0(\xi, s) = e^{-(\xi-s)^2}$$  (16)

that represents the vacuum density when the parameter is zero ($s = s_0 = 0$). The substitution is legitimated by the fact that the oscillator’s coordinate is a relative quantity with respect the oscillator length at rest. The Taylor expansion at $s_0 = 0$ of Eq. (16) coincides with Eq. (14) if we take

$$A_n(s, \xi) = e^{-(\xi-s)^2} H_n(\xi - s)$$  (17)

whereas the field contribution to the vacuum near the singularity ($s \approx s_0 = 0$) is

$$\psi_{HJ} = \delta_n = e^{\xi^2/2} H_n(\xi)$$  (18)

as expected. Similarly, for the hydrogen atom, the density at negative energies is (see Eq. (7))

$$\rho_0(\rho, s) = (s \rho)^2 e^{-2s \rho}$$  (19)

that coincides with the vacuum density for $s = s_0 = 1$ and $\lambda = 0$. Note that the dependence on $s \rho$ is due to the definition of $\rho$ and $\epsilon$ in Eq. (5) and, as such, the parameter determines only a rescaling of $\rho$. The Taylor expansion of Eq. (14) is calculated after the expansion of the vacuum density $e^{-2s \rho}$ for positive values of $s$ (this condition implies Laguerre polynomials).

$$e^{-2s \rho} = s^{-\lambda} e^{-2s \rho} \sum_{m=0}^{\infty} \frac{L_m(2s)}{(s-1)^m}$$  (20)

and Eq. (14) is here reproduced if we take $A_m(1, \rho) = m! \rho^2 e^{-2s \rho} L_m(2s)$. This makes it possible to calculate the $m$-th contribution to the field at negative energies near the singularity at $s = 1$ (i.e., $\epsilon = 1$ corresponding to the usual Bohr orbits)

$$R_{HJ} = \delta_m = \rho^4 e^{-\rho} L_m(2\rho)$$  (21)

and if we replace the indices according to $\lambda = l$ and $m = n - l - 1$, the surviving Laguerre polynomials are $L_{n-l-1}(2\rho)$ with $l \leq n$. In the end, Eq. (21) is identical to the well-known result of the radial Schrödinger equation even though we did not solve it.

Concluding remarks. Negative kinetic energies for imaginary canonical momenta resulting from the analogy between HJ theory and optics have been shown to manifest quantum features related to the fundamental role of the vacuum. Based on this, agreement with quantum-mechanical laws (origin of the vacuum energy, Schrödinger equation, Schrödinger wave functions, time-evolution operator for transition to Heisenberg representation and corresponding equation of motion) is found. Negative kinetic energies are also used to establish a theorem that reconciles quantum mechanics with geometric interpretation of HJ theory. In addition, the new concept of a quantum Babinet principle is introduced when the Hamiltonian is time dependent and phase effects are expected. Indeed, wave functions at positive energies are obtained as destructively interfering parametric fields generated by the interplay between vacuum and phase singularities. This approach leads to the novelty of an alternative to the calculation of wave functions without solving a wave equation, if not for the HJ equation at negative kinetic energy that provides the vacuum state. To conclude, solutions to the HJ equation at negative energies seem to suggest phase behavior that is reminiscent of the quantum potential of the de Broglie-Bohm formulation of quantum mechanics. It is worth noticing that, in this work, the actual value of $\hbar$ is unimportant and, for this reason, the reference to negative kinetic energies circumvents the classical limit ($\hbar \rightarrow 0$) according to which HJ equation has been disregarded in quantum physics. After this work, HJ approach is no longer at variance with quantum mechanics.

What is more, all of the above-mentioned ideas can be adjusted to relativistic contexts, which are the objective of an ongoing study.
Supplemental material

S1. Quantum-mechanical kinetic operator

The quantum-mechanical kinetic energy is calculated for the operator

$$\mathcal{T}_{QM} = -\frac{\hbar^2}{2m} \nabla^2$$

(S1.1)

When applied to $\Psi_{HJ} = \exp(iS/\hbar) = \exp(iW/\hbar)\exp(-iEt/\hbar)$, the Laplacian yields

$$\nabla^2 \Psi_{HJ} = \frac{1}{i\hbar^3} (i\hbar\nabla^2 W - \nabla W \otimes \nabla W) \Psi_{HJ}$$

(S1.2)

If the Hamilton’s characteristic function is a complex-valued function, its representation is $W = W_{Re} + iW_{Im}$ with $W_{Re} = Re(W)$ and $W_{Im} = Im(W)$. Based on this, the product $\nabla W \otimes \nabla W$ in Eq. (S1.2) is

$$p \otimes p = (\nabla W_{Re})^2 - (\nabla W_{Im})^2 + 2i\nabla W_{Re} \nabla W_{Im}$$

(S1.3)

and the operator in Eq. (S1.1) becomes

$$\mathcal{T}_{QM} = \frac{1}{2m} p \otimes p - \frac{i\hbar}{2m} \nabla^2 W$$

(S1.4)

When $W_{Re} = Re(W) = 0$, then the momentum is purely imaginary and the kinetic operator is

$$\mathcal{T}_{QM} = -\frac{1}{2m} (\nabla W_{Im})^2 - \frac{i\hbar}{2m} \nabla^2 W_{Im}$$

(S1.5)

S2. Hamilton-Jacobi (HJ) equation for the simple harmonic oscillator

The reduced HJ equation for the harmonic oscillator is [R1]

$$\frac{1}{2m} \left( \frac{\partial W}{\partial q} \right)^2 + \frac{1}{2} m\omega^2 q^2 = E$$

(S2.1)

where the momentum $p$ is the derivative of the Hamilton’s characteristic function $W$. Normalization to $\hbar$ is simply introduced by setting $W = \hbar W$ and, at the same time, the dimensionless coordinate $\xi = q/q_0$ is the new independent variable

$$\frac{\hbar^2}{2m q_0^2} \left( \frac{\partial W}{\partial \xi} \right)^2 + \frac{1}{2} m\omega^2 q_0^2 \xi^2 = E$$

(S2.2)

The definition of $q_0 = \sqrt{\hbar/m\omega}$ reduces Eq. S2.2 to

$$\left( \frac{\partial \xi}{\partial \rho} \right)^2 + \xi^2 = \frac{2E}{\hbar \omega}$$

(S2.3)

and normalization of the energy $\epsilon = E/\hbar \omega$ gives Eq. (3) of the main text.

S3. Hamilton-Jacobi (HJ) equation for the 2D isotropic harmonic oscillator

The reduced Hamilton-Jacobi equation for the 2D-IHO is available in Goldstein [R1] and, considering polar coordinates $r$ and $\theta$, it can be written for the Hamilton’s characteristic function $W$

$$\frac{1}{2m} \left( \frac{\partial W}{\partial r} \right)^2 + \frac{\alpha_\theta^2}{2mr^2} + \frac{1}{2} m\omega^2 r^2 = E$$

(S3.1)

with $\alpha_\theta$ indicating the constant angular momentum. Normalization to the action unit $\hbar$ helps in writing Eq. (S3.1) for the dimensionless characteristic function $w = W/\hbar$ whose derivative is taken with respect to the dimensionless radius $\rho = r/r_0$

$$\left( \frac{\partial w}{\partial \rho} \right)^2 + \frac{\lambda^2}{\rho^2} + \left( \frac{m\omega \rho^2}{\hbar} \right)^2 \rho^2 = \frac{2m\lambda^2}{\hbar^2} E$$

(S3.2)

where $\lambda = \alpha_\theta/\hbar$. The reference radius $r_0$ is arbitrary and a good choice is $r_0 = \sqrt{\hbar/m\omega}$ because it simplifies the coefficients of Eq. (S3.2). If we define the normalized energy $\epsilon = E/\sigma \omega$, the HJ equation becomes

$$\left( \frac{\partial \epsilon}{\partial \rho} \right)^2 + \frac{\lambda^2}{\rho^2} + \rho^2 = 2\epsilon$$

(S3.3)

The normalized characteristic function is separable in its radial and angular components: $w = w_r + \lambda \theta$. It means that the HJ equation can be specified to $w_r$ only, that is

$$\left( \frac{\partial w_r}{\partial \rho} \right)^2 + \frac{\lambda^2}{\rho^2} + \rho^2 = 2\epsilon$$

(S3.4)

Under the hypothesis of purely rotational motion, the normalized energy is $\epsilon = \lambda$ and Eq. (S3.4) takes an interesting form

$$\left( \frac{\partial w_r}{\partial \rho} \right)^2 = -\left( \rho - \frac{\lambda}{\rho} \right)^2$$

(S3.5)

It appears that the radial momentum is imaginary! On the other hand, the fact that the momentum could take imaginary values should not be surprising in view of the opto-mechanical analogy between linear momentum and index of refraction that can take imaginary values (i.e,
attenuation coefficient) [R2]. To avoid this apparent oddity, one might consider that the energy is \( E = m\omega^2 r^2 \) and, as such, the right-hand side of Eq. (S3.5) would be zero. Here, instead, the viewpoint of the wave interpretation of the HJ equation is assumed and the energy cannot be localized in space. This change of perspective has a fundamental impact on the solution of Eq. (S3.5)

\[
w_r = \pm i \left[ \frac{\rho^2}{2} - \lambda \ln(\rho) \right] \tag{S3.6}
\]

and, by virtue of Eq. S3.6, the spatial component of the HJ wave function is

\[
\psi_{\text{HJ}} = e^{iw_r/\hbar} = e^{i\omega_r + i\lambda \theta} = \rho^\lambda e^{-\rho^2/2} e^{i\lambda \theta} \tag{S3.7}
\]

Note that, when \( \lambda = 0 \) (implying no motion at all), the mere Gaussian wave function of the vacuum field appears. When \( \lambda \neq 0 \), then only integer values are allowed because of the periodicity of the wave function. The comparison of Eq. (S3.7) with the solutions found in the literature of the corresponding quantum-mechanical problem shows the perfect correspondence between HJ wave functions and Schrödinger’s of purely rotational motion [R3, R4].

**S4. Peculiarity of the Hamilton’s function of the hydrogen atom.**

The reduced Hamilton-Jacobi equation for the Kepler problem that emulates the hydrogen atom is available in Goldstein [R1]. It is summarized below considering spherical coordinates \( r, \theta \) and \( \varphi \)

\[
\frac{1}{2m} \left( \frac{\partial W_r}{\partial r} \right)^2 + \frac{a_\varphi^2}{2mr^2} - \frac{k}{r} = E \tag{S4.1}
\]

where \( W_r \) is the radial component of the separable Hamilton’s characteristic function \( W = W_r + W_\theta + W_\varphi \).

The potential energy is specified here for the hydrogen atom and, for this reason, \( k = e^2/4\pi\varepsilon_0 \). In addition,

\[
a_\varphi^2 = \left( \frac{\partial W_\varphi}{\partial \varphi} \right)^2 + \frac{a_\theta^2}{\sin^2(\theta)} \tag{S4.2}
\]

Since \( \varphi \) is an ignorable variable, \( a_\varphi \) is constant and determines the azimuthal component of \( W : W_\varphi = a_\varphi \varphi \).

To solve Eq. S4.1, we proceed as shown for the 2D-IHO. Normalization to the action unit \( \hbar \) and reference to a 2 radius \( r_0 \) are introduced by setting \( w_r = W_r/\hbar \) and \( r = r_0 \rho \)

\[
\left( \frac{\partial w_r}{\partial \rho} \right)^2 + \frac{\lambda^2}{\rho^2} - \frac{2mr_0k}{\hbar^2 \rho} = \frac{2mr_0^2}{\hbar^2} E \tag{S4.3}
\]

with \( \lambda = a_\theta/\hbar \). The coefficients that depend on \( r_0 \) can be simplified by choosing the arbitrary value of \( r_0 \). With the benefit of hindsight, the choice is \( r_0 = \eta \hbar^2/mk \) where \( \eta \) is a parameter to be determined. Thus,

\[
\left( \frac{\partial w_r}{\partial \rho} \right)^2 + \frac{\lambda^2}{\rho^2} - \frac{2n}{\rho} = -\varepsilon \tag{S4.4}
\]

where, to take into account bound states, the minus sign has been extracted in the total energy normalized as follows

\[
\varepsilon = \frac{2n^2\hbar^2}{mk^2} |E| \tag{S4.5}
\]

For purely rotational motion to happen (i.e., circular motion), \( \varepsilon \) is equal to one and \( \eta \hbar \) has to be the angular momentum \( a_\theta \) implying \( \eta = \lambda \). This means that Eq. S4.4 becomes

\[
\left( \frac{\partial w_{\text{rot}}}{\partial \rho} \right)^2 = -\left( 1 - \frac{\lambda}{\rho} \right)^2 \tag{S4.6}
\]

whose solution is imaginary

\[
w_{\text{rot}} = \pm i \left( \rho - \frac{\lambda}{\rho} \right) \tag{S4.7}
\]

The double choice in the sign is removed by considering the corresponding HJ wave function that has to be finite under the limits \( \rho \to 0 \) and \( \rho \to \infty \)

\[
R_{\text{HJ}} = e^{i\omega_{\text{rot}}} = \rho^\lambda e^{-\rho} \tag{S4.8}
\]

and when \( \lambda = 0 \), the residual function shows the decay \( \exp(-\rho) \) that characterizes the vacuum.

**S5. Hamilton-Jacobi wave function for hydrogen atom**

The general HJ wave function for the hydrogen atom should incorporate radial motion besides rotational motion discussed in section S4. To fulfill the objective, the wave function is factorized according to

\[
\psi_{\text{HJ}} = e^{iW/\hbar} = R_{\text{HJ}} \Lambda \Theta e^{i\mu \varphi} \tag{S5.1}
\]

with \( \mu = a_\varphi/\hbar \). The function \( \Lambda \) is part of the radial component together with \( R_{\text{rot}}^{\text{HJ}} \). In other terms, the radial wave function is \( R = \exp(iW_r/\hbar) = R_{\text{rot}}^{\text{HJ}} \Lambda \). The remaining function \( \Theta \) is the polar part representing \( \exp(iW_\theta/\sigma) \) and, in addition, we have set \( \Phi = \exp(i\mu \varphi) \). Eq. S5.1 is now introduced in the wave-front condition \( \rho^2 \psi_{\text{HJ}} = -\hbar^2 \nabla^2 \psi_{\text{HJ}} \) resulting from the no-contrast theorem described in the main text (see discussion relative
to Eqs. (8)-(13) in the main text). In this way, calling Ω = Φ, we find
\[
\mathcal{V}^2 \psi_{\text{HJ}} = \frac{\psi_{\text{HJ}}}{r_0^2} \left[ \frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left( \rho^2 \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2 \sin(\theta)} \frac{\partial}{\partial \theta} \left[ \sin(\theta) \frac{\partial}{\partial \theta} \right] - \frac{\mu^2}{\rho^2 \sin^2(\theta)} \right]
\]
(S5.2)
and based on \( p^2 = \hbar^2 (2\eta / \rho - \epsilon) / r_0^2 \) (see Eq. S4.4), we conclude that
\[
- \left( \frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left( \rho^2 \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2 \sin(\theta)} \frac{\partial}{\partial \theta} \left[ \sin(\theta) \frac{\partial}{\partial \theta} \right] - \frac{\mu^2}{\rho^2 \sin^2(\theta)} \right) = \frac{2n}{\rho} - \epsilon
\]
(S5.3)
Comparison with the HJ equation in Eq. S4.4 shows clearly that the angular part of Eq. S5.3 is equal to
\[
\frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) \left[ \sin(\theta) \frac{\partial}{\partial \theta} \right] - \frac{\mu^2}{\rho^2 \sin^2(\theta)} = -\lambda^2
\]
(S5.4)
This equation has the well-known solution given by the associated Legendre function \( P_{l,l}^{\mu} (\cos \theta) \) for \( \lambda^2 = l(l + 1) \).

The radial part of Eq. S5.3 is then
\[
\frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) \left[ \sin(\theta) \frac{\partial}{\partial \theta} \right] - \frac{\mu^2}{\rho^2 \sin^2(\theta)} = \frac{2n}{\rho} - \epsilon \quad R = 0
\]
(S5.5)
After simple algebra, Eq. S5.5 reduces to
\[
\frac{\partial^2 \Lambda}{\partial \rho^2} + \left( \frac{\lambda+1}{\rho} - 1 \right) \frac{\partial \Lambda}{\partial \rho} + \lambda - \frac{2(\lambda+1-\eta)}{\rho} + 1 - \epsilon \Lambda = 0
\]
(S5.6)
where \( \lambda^2 = l(l + 1) \) has been used. The solution to this equation contains generalized Laguerre polynomials
\[
\Lambda = \kappa_l e^{-\rho(1+\sqrt{\epsilon})} \rho^{1-\lambda} L_{s(l+1/2)}^{2+1} \left( 2\sqrt{\epsilon} \rho \right)
\]
(S5.7)
with \( \kappa_l \) a constant and \( s \) given by
\[
s = -1 - l + \frac{\eta}{\sqrt{\epsilon}}
\]
(S5.8)
and turning this parameter into more familiar terms, i.e., \( s = n - l - 1 \), we find that \( \epsilon = \eta^2 / n^2 \). Based on Eq. S4.5, the result corresponds to an energy of \( |E| = mk^2 / 2n^2 \hbar^2 \). This implies that \( \eta = n \) and Eq. S5.7 is
\[
\Lambda = \kappa_l \rho^{1-\lambda} L_{n-l-1}^{2l+1} (2\rho)
\]
(S5.9)
At last, we can collect all the factors taking part in the global solution and, apart from a multiplicative constant \( \kappa \), the HJ wave function gains a familiar look
\[
\psi_{\text{HJ}} = e^{iW/\hbar} = \kappa \rho^{l} e^{-\rho L_{n-l-1}^{2l+1} (2\rho)} P_{l}^{\mu} (\cos \theta) e^{i\mu \phi}
\]
(S5.10)
This is exactly the Schrödinger’s wave function. In particular, calling \( a_0 = \hbar^2 / mk \) and introducing a redefinition of the radial coordinate such that \( \rho = 2r / n a_0 \), we recover the customary radial dependences of the Schrödinger’s wave function
\[
\psi_{\text{HJ}} = \kappa \rho^l e^{-\rho L_{n-l-1}^{2l+1} (2\rho)} P_{l}^{\mu} (\theta, \varphi)
\]
(S5.11)
with \( P_{l}^{\mu} \) indicating the spherical harmonics.

### S6. Time-evolution operator and Heisenberg representation of quantum mechanics

The structure of the HJ wave function is such that the Heisenberg representation can be easily reproduced. One manner to fulfill the purpose is through the time-evolution operator. In general the HJ equation can be written for the Hamilton’s principal function
\[
H \left( q, \frac{\partial}{\partial q}, t \right) = -\frac{\partial}{\partial t}
\]
(S6.1)
Integration of Eq. S6.1 is
\[
S = W(q) - \int_{t_0}^{t} \mathcal{H} dq
\]
(S6.2)
where the Hamilton’s characteristic function \( W(q) \) takes the role of a “constant” of integration because contains functional dependences on the coordinates \( q \) that do not appear in the time integration.

The incorporation of \( S \) in the HJ wave function leads to
\[
\Psi_{\text{HJ}} (t) = U(t, t_0) \Psi_{\text{HJ}} (t_0)
\]
(S6.3)
with
\[
U(t, t_0) = e^{-iH \int_{t_0}^{t} dt'}
\]
and taking the time derivative of \( \Psi_{\text{HJ}} \), we get the so-called Schrödinger equation for the time-evolution operator \( \mathcal{H} \)
\[
i \hbar \frac{\partial}{\partial t} U(t, t_0) = \mathcal{H} U(t, t_0)
\]
(S6.5)
The transition to the Heisenberg picture is carried out after the usual transformation from the operator \( \mathcal{O} \) in Schrödinger representation to \( \mathcal{O}_H \) in Heisenberg representation
\[
\mathcal{O}_H (t) = U^*(t, t_0) \mathcal{O} U(t, t_0)
\]
(S6.6)
The Heisenberg equation of motion follows directly after differentiation of Eq. S6.6.
The commutation rule between conjugate observables can also be easily obtained from the spatial HJ wave function $\psi_{HJ}$ of Eq. S6.4. The commutator in Heisenberg representation of the two observables $q_H$ and $p_H$ is an operator that, when applied to $\psi_{HJ} = \exp(iW/\hbar)$, becomes
\[
[q_H, p_H]\psi_{HJ} = q_H p_H \psi_{HJ} - p_H q_H \psi_{HJ},
\]
or
\[
[q_H, p_H]\psi_{HJ} = U^+(t, 0)(q_S p_S - p_S q_S)\psi_{HJ} U(t, 0) \quad (S6.7)
\]
where $t_0 = 0$ for simplicity of notation. But we recall that in the HJ approach the canonical momentum is $p = \nabla S = \nabla W$ and thus
\[
p\psi_{HJ} = \nabla W \psi_{HJ} = -i\hbar \left( \frac{i}{\hbar} \nabla W \right) \psi_{HJ} = -i\hbar \nabla \psi_{HJ} \quad (S6.8)
\]
which implies the assumption of the Schrödinger operator for the momentum $p_S = -i \hbar \nabla$. This results in
\[
[q_H, p_H]\psi_{HJ} = i\hbar \psi_{HJ} \quad (S6.9)
\]
or $[q_H, p_H] = i\hbar$ which is the thesis we wanted to prove. Therefore, the use of the HJ wave function is compatible with the Heisenberg approach to quantum mechanics.

**References for Supplementary Material.**