

Seminario de Química Física



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Salón de Actos de la Biblioteca

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Two-Hundred Years After Hamilton: Exploring New Formulations of Classical and Quantum Mechanics

This talk has three parts. The first part is an introduction to Hamilton's two monumental papers from 1834-1835, which introduced the Hamilton-Jacobi equation, Hamilton's equations of motion and the principle of least action [1]. These three formulations of classical mechanics became the three forerunners of quantum mechanics; but ironically none of them is what Hamilton was looking for -- he was looking for a "magical" function, the principal function $S(q_1, q_2, t)$, from which the entire trajectory history can be obtained just by differentiation (no integration) [2]. In the second part of the talk I argue that Hamilton's principal function is almost certainly more magical than even Hamilton realized. Astonishingly, all of the above formulations of classical mechanics can be derived just from assuming that $S(q_1, q_2, t)$ is additive, with no input of physics [3]. The third part of the talk will present a new formulation of quantum mechanics in which the Hamilton-Jacobi equation is extended to complex-valued trajectories [4], allowing the treatment of classically allowed processes, classically forbidden process and arbitrary time-dependent external fields within a single, coherent framework. The approach is illustrated for barrier tunneling, wavepacket revivals, nonadiabatic dynamics, optical excitation using shaped laser pulses and high harmonic generation with strong field attosecond pulses [5]

[1] W. R. Hamilton, On a General Method in Dynamics, Philosophical Transactions, Part 2, p. 247 (1834); *ibid.*, Second Essay on a General Method in Dynamics, Part 1, p. 95 (1835).

[2] M. Nakane and C. G. Fraser, The Early History of Hamilton-Jacobi Dynamics 1834-1837, *Centaurus* 44, 161 (2002); C. Lanczos, *The Variational Principles of Mechanics* (Oxford, 1949)

[3] D. J. Tannor, New derivation of Hamilton's three formulations of classical mechanics (preprint); *ibid.*, Duality of the Principle of Least Action: A New Formulation of Classical Mechanics, arXiv:2109.09094 (2021).

[4] Y. Goldfarb, I. Degani and D. J. Tannor, Bohmian mechanics with complex action: A new trajectory based formulation of quantum mechanics, *J. Chem. Phys.* 125, 231103 (2006); J. Schiff, Y. Goldfarb and D. J. Tannor, Path integral derivations of complex trajectory methods, *Phys. Rev. A* 83, 012104 (2011); N. Zamstein and D. J. Tannor, Overcoming the root search problem in complex quantum trajectory calculations, *J. Chem. Phys.* 140, 041105(2014).

[5] N. Zamstein and D. J. Tannor, Non-adiabatic molecular dynamics with complex quantum trajectories. I. The adiabatic representation, *J. Chem. Phys.* 137, 22A518 (2012); W. Koch and D. J. Tannor, Wavepacket revivals via complex trajectory propagation, *Chem. Phys. Lett.* 683, 306 (2017); W. Koch and D. J. Tannor, A three-step model of high harmonic generation using complex classical trajectories, *Annals of Physics*, 427, 168288 (2021).