New Phase Space Formulation of Quantum Mechanics for Nonadiabatic Systems

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We report recent progress on the phase space formulation of quantum mechanics with coordinate-momentum variables. The novel phase space mapping theory includes a unified framework for constructing the phase space mapping Hamiltonian, as well as a general phase space formulation of quantum mechanics for nonadiabatic systems where a finite number of discrete electronic states are mapped onto constraint space and nuclear degrees of freedom are mapped onto infinite space. It is shown that the conventional zero-point-energy parameter should be interpreted as a special case of a commutator matrix in the comprehensive phase space mapping Hamiltonian for nonadiabatic systems. Our applications range from gas phase to condensed phase systems, which include the spin-boson model for condensed phase dissipative two-state systems, the three-state photo-dissociation models, the seven-state Fenna-Matthews-Olson monomer that appears in photosynthesis in green sulfur bacteria, strongly coupled optical cavity-molecular matter systems used to control and manipulate chemical and physical processes, singlet-fission systems, and so forth.

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