

# Nancy Makri

## List of Publications by Citations

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104  
papers

5,651  
citations

40  
h-index

74  
g-index

109  
ext. papers

6,057  
ext. citations

4  
avg, IF

6.51  
L-index

#	Paper	IF	Citations
104	Tensor propagator for iterative quantum time evolution of reduced density matrices. I. Theory. <i>Journal of Chemical Physics</i> , <b>1995</b> , 102, 4600-4610	3.9	410
103	Tensor propagator for iterative quantum time evolution of reduced density matrices. II. Numerical methodology. <i>Journal of Chemical Physics</i> , <b>1995</b> , 102, 4611-4618	3.9	329
102	Numerical path integral techniques for long time dynamics of quantum dissipative systems. <i>Journal of Mathematical Physics</i> , <b>1995</b> , 36, 2430-2457	1.2	254
101	Quantum rates for a double well coupled to a dissipative bath: Accurate path integral results and comparison with approximate theories. <i>Journal of Chemical Physics</i> , <b>1994</b> , 101, 7500-7519	3.9	253
100	Path integrals for dissipative systems by tensor multiplication. Condensed phase quantum dynamics for arbitrarily long time. <i>Chemical Physics Letters</i> , <b>1994</b> , 221, 482-491	2.5	242
99	Time-dependent self-consistent field (TDSCF) approximation for a reaction coordinate coupled to a harmonic bath: Single and multiple configuration treatments. <i>Journal of Chemical Physics</i> , <b>1987</b> , 87, 5781-5787	2.9	232
98	Time-dependent quantum methods for large systems. <i>Annual Review of Physical Chemistry</i> , <b>1999</b> , 50, 167-91	15.7	199
97	A semiclassical tunneling model for use in classical trajectory simulations. <i>Journal of Chemical Physics</i> , <b>1989</b> , 91, 4026-4036	3.9	186
96	Semiclassical influence functionals for quantum systems in anharmonic environments <sup>1</sup> Presented at the American Physical Society Meeting in Los Angeles, California, USA, March 19, 1998.1. <i>Chemical Physics Letters</i> , <b>1998</b> , 291, 101-109	2.5	172
95	Influence functionals with semiclassical propagators in combined forwardBackward time. <i>Journal of Chemical Physics</i> , <b>1999</b> , 110, 1343-1353	3.9	158
94	The Linear Response Approximation and Its Lowest Order Corrections: An Influence Functional Approach. <i>Journal of Physical Chemistry B</i> , <b>1999</b> , 103, 2823-2829	3.4	157
93	Improved Feynman propagators on a grid and non-adiabatic corrections within the path integral framework. <i>Chemical Physics Letters</i> , <b>1992</b> , 193, 435-445	2.5	139
92	ForwardBackward Semiclassical Dynamics without Prefactors. <i>Journal of Physical Chemistry A</i> , <b>1999</b> , 103, 7753-7756	2.8	135
91	Quantum Dissipative Dynamics: A Numerically Exact Methodology. <i>Journal of Physical Chemistry A</i> , <b>1998</b> , 102, 4414-4427	2.8	129
90	Feynman path integration in quantum dynamics. <i>Computer Physics Communications</i> , <b>1991</b> , 63, 389-414	4.2	125
89	Monte Carlo path integration for the real time propagator. <i>Journal of Chemical Physics</i> , <b>1988</b> , 89, 2170-2177	3.7	116
88	Exponential power series expansion for the quantum time evolution operator. <i>Journal of Chemical Physics</i> , <b>1989</b> , 90, 904-911	3.9	110

87	ForwardBackward Semiclassical Dynamics with Linear Scaling. <i>Journal of Physical Chemistry A</i> , <b>1999</b> , 103, 9479-9486	2.8	92
86	ForwardBackward semiclassical dynamics for quantum fluids using pair propagators: Application to liquid para-hydrogen. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 8592-8605	3.9	90
85	Filtered propagator functional for iterative dynamics of quantum dissipative systems. <i>Computer Physics Communications</i> , <b>1997</b> , 99, 335-354	4.2	87
84	Basis set methods for describing the quantum mechanics of a System Interacting with a harmonic bath. <i>Journal of Chemical Physics</i> , <b>1987</b> , 86, 1451-1457	3.9	83
83	ForwardBackward semiclassical dynamics for condensed phase time correlation functions. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 1634-1642	3.9	65
82	Tensor propagator with weight-selected paths for quantum dissipative dynamics with long-memory kernels. <i>Chemical Physics Letters</i> , <b>1996</b> , 249, 224-230	2.5	59
81	System-specific discrete variable representations for path integral calculations with quasi-adiabatic propagators. <i>Chemical Physics Letters</i> , <b>1993</b> , 210, 448-457	2.5	59
80	Correct short time propagator for Feynman path integration by power series expansion in $\hbar$ . <i>Chemical Physics Letters</i> , <b>1988</b> , 151, 1-8	2.5	57
79	Simulation of dynamical properties of normal and superfluid helium. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2005</b> , 102, 4230-4	11.5	56
78	Quantum-classical path integral: A rigorous approach to condensed phase dynamics. <i>International Journal of Quantum Chemistry</i> , <b>2015</b> , 115, 1209-1214	2.1	54
77	Iterative path integral formulation of equilibrium correlation functions for quantum dissipative systems. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 507-514	3.9	53
76	Coherent state semiclassical initial value representation for the Boltzmann operator in thermal correlation functions. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 9207-9212	3.9	51
75	Control of dissipative tunneling dynamics by continuous wave electromagnetic fields: Localization and large-amplitude coherent motion. <i>Physical Review E</i> , <b>1995</b> , 52, 5863-5872	2.4	51
74	Stochastic resonance and nonlinear response in double-quantum-well structures. <i>Physical Review B</i> , <b>1995</b> , 52, R2257-R2260	3.3	51
73	Iterative evaluation of the path integral for a system coupled to an anharmonic bath. <i>Journal of Chemical Physics</i> , <b>1999</b> , 111, 6164-6167	3.9	50
72	Quantum-classical path integral. I. Classical memory and weak quantum nonlocality. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 22A552	3.9	48
71	Short-Range Coherence in the Energy Transfer of Photosynthetic Light-Harvesting Systems. <i>Journal of Physical Chemistry A</i> , <b>1999</b> , 103, 9417-9422	2.8	46
70	Quantum-classical path integral. II. Numerical methodology. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 22A553	3.9	45

69	Finite Temperature Correlation Functions via ForwardBackward Semiclassical Dynamics <i>Journal of Physical Chemistry A</i> , <b>2001</b> , 105, 2851-2857	2.8	43
68	Time-dependent discrete variable representations for quantum wave packet propagation. <i>Journal of Chemical Physics</i> , <b>1995</b> , 102, 5616-5625	3.9	42
67	Quantum-Classical Path Integral Simulation of Ferrocene-Ferrocenium Charge Transfer in Liquid Hexane. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 4959-65	6.4	41
66	Iterative path integral calculation of quantum correlation functions for dissipative systems. <i>Chemical Physics</i> , <b>2001</b> , 268, 1-10	2.3	41
65	Blip decomposition of the path integral: exponential acceleration of real-time calculations on quantum dissipative systems. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 134117	3.9	40
64	Phase Space Features and Statistical Aspects of ForwardBackward Semiclassical Dynamics. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 6816-6825	3.4	38
63	On smooth Feynman propagators for real time path integrals. <i>The Journal of Physical Chemistry</i> , <b>1993</b> , 97, 2417-2424		38
62	Stabilization of localized states in dissipative tunneling systems interacting with monochromatic fields. <i>Journal of Chemical Physics</i> , <b>1997</b> , 106, 2286-2297	3.9	37
61	Real time path integral methods for a system coupled to an anharmonic bath. <i>Journal of Chemical Physics</i> , <b>1994</b> , 101, 6708-6716	3.9	37
60	Memory propagator matrix for long-time dissipative charge transfer dynamics. <i>Molecular Physics</i> , <b>2012</b> , 110, 1967-1975	1.7	36
59	FORWARD-BACKWARD SEMICLASSICAL SIMULATION OF DYNAMICAL PROCESSES IN LIQUIDS. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2004</b> , 03, 391-417	1.8	35
58	Monte Carlo Evaluation of ForwardBackward Semiclassical Correlation Functions with a Quantized Coherent State Density. <i>Journal of Physical Chemistry B</i> , <b>2002</b> , 106, 8390-8398	3.4	35
57	Dissipative tunneling in a bath of two-level systems. <i>Physical Review B</i> , <b>1999</b> , 60, 972-978	3.3	34
56	Exploiting classical decoherence in dissipative quantum dynamics: Memory, phonon emission, and the blip sum. <i>Chemical Physics Letters</i> , <b>2014</b> , 593, 93-103	2.5	32
55	Bohmian versus semiclassical description of interference phenomena. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 60-67	3.9	32
54	Iterative quantum-classical path integral with dynamically consistent state hopping. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 044108	3.9	31
53	Iterative blip-summed path integral for quantum dynamics in strongly dissipative environments. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 134101	3.9	29
52	Small matrix disentanglement of the path integral: Overcoming the exponential tensor scaling with memory length. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 041104	3.9	29

51	Modular path integral methodology for real-time quantum dynamics. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 214108	3.9	27
50	Communication: Modular path integral: Quantum dynamics via sequential necklace linking. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 101101	3.9	27
49	Quantum-classical path integral with self-consistent solvent-driven reference propagators. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 13357-66	3.4	25
48	Symmetries and detailed balance in forwardBackward semiclassical dynamics. <i>Chemical Physics</i> , <b>2006</b> , 322, 23-29	2.3	25
47	Small Matrix Path Integral for System-Bath Dynamics. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 4038-4049	6.4	23
46	Path integral renormalization for quantum dissipative dynamics with multiple timescales. <i>Molecular Physics</i> , <b>2012</b> , 110, 1001-1007	1.7	21
45	Forward-backward semiclassical and quantum trajectory methods for time correlation functions. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 14442-52	3.6	20
44	Dynamics of reduced density matrices: Classical memory versus quantum nonlocality. <i>Journal of Chemical Physics</i> , <b>1998</b> , 109, 2994-2998	3.9	20
43	Multitime response functions and nonlinear spectra for model quantum dissipative systems. <i>Journal of Chemical Physics</i> , <b>2010</b> , 132, 134506	3.9	19
42	Path integral study of hydrogen and deuterium diffusion in crystalline silicon. <i>Journal of Chemical Physics</i> , <b>1998</b> , 108, 6819-6828	3.9	19
41	Direct determination of discrete harmonic bath parameters from molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 110-115	3.5	18
40	Wigner phase space distribution via classical adiabatic switching. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 114114	3.9	17
39	Direct Computation of Influence Functional Coefficients from Numerical Correlation Functions. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 4169-77	6.4	16
38	Universal delocalization rate in driven dissipative two-level systems at high temperature. <i>Physical Review E</i> , <b>1997</b> , 55, 2475-2478	2.4	16
37	Forward--backward semiclassical dynamics with information-guided noise reduction for a molecule in solution. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 11320-7	2.8	16
36	Effects of periodic driving on asymmetric two-level systems coupled to dissipative environments. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , <b>1998</b> , 31, 209-226	1.3	16
35	Real-Time Path Integral Simulation of Exciton-Vibration Dynamics in Light-Harvesting Bacteriochlorophyll Aggregates. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 8783-8789	6.4	16
34	Information guided noise reduction for Monte Carlo integration of oscillatory functions. <i>Chemical Physics Letters</i> , <b>2004</b> , 400, 446-452	2.5	15

33	Modular path integral for discrete systems with non-diagonal couplings. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 074110	3.9	14
32	All-Mode Quantum-Classical Path Integral Simulation of Bacteriochlorophyll Dimer Exciton-Vibration Dynamics. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 5028-5038	3.4	14
31	Quantum stochastic resonance in the strong-field limit. <i>Physical Review A</i> , <b>2004</b> , 70,	2.6	14
30	Blip-summed quantum-classical path integral with cumulative quantum memory. <i>Faraday Discussions</i> , <b>2016</b> , 195, 81-92	3.6	12
29	ForwardBackward semiclassical dynamics with single-bead coherent state density. <i>Molecular Physics</i> , <b>2008</b> , 106, 443-453	1.7	12
28	Wigner Distribution by Adiabatic Switching in Normal Mode or Cartesian Coordinates and Molecular Applications. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 5446-5458	6.4	12
27	On iterative path integral calculations for a system interacting with a shifted dissipative bath. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 074112	3.9	11
26	Modular path integral for finite-temperature dynamics of extended systems with intramolecular vibrations. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 044124	3.9	11
25	Small Matrix Path Integral with Extended Memory. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 1-6	6.4	10
24	Efficient matrix factorisation of the modular path integral for extended systems. <i>Molecular Physics</i> , <b>2021</b> , 119, e1797200	1.7	9
23	ExcitonVibration Dynamics in J-Aggregates of a Perylene Bisimide from Real-Time Path Integral Calculations. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 201-210	3.8	8
22	Non-equilibrium reactive flux: A unified framework for slow and fast reaction kinetics. <i>Journal of Chemical Physics</i> , <b>2017</b> , 147, 152723	3.9	7
21	Coherent State-Based Path Integral Methodology for Computing the Wigner Phase Space Distribution. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 4284-4294	2.8	7
20	Real-Time Path Integral Methods, Quantum Master Equations, and Classical vs Quantum Memory. <i>Journal of Physical Chemistry B</i> , <b>2019</b> , 123, 10470-10482	3.4	7
19	Quantum-classical path integral with a harmonic treatment of the back-reaction. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 184102	3.9	6
18	Low-temperature correlation functions via forwardBackward quantum dynamics. <i>Chemical Physics</i> , <b>2010</b> , 370, 15-19	2.3	5
17	Intramolecular Vibrations in Excitation Energy Transfer: Insights from Real-Time Path Integral Calculations.. <i>Annual Review of Physical Chemistry</i> , <b>2022</b> ,	15.7	5
16	Origin of vibrational features in the excitation energy transfer dynamics of perylene bisimide J-aggregates. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 114301	3.9	5

15	Small matrix modular path integral: iterative quantum dynamics in space and time. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 12537-12540	3.6	5
14	Time Evolution of Bath Properties in Spin-Boson Dynamics. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 8137-8151	3.4	4
13	Recovery of Purity in Dissipative Tunneling Dynamics. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 8592-8596	6.4	3
12	Electronic-vibrational density evolution in a perylene bisimide dimer: mechanistic insights into excitation energy transfer. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 15503-15514	3.6	3
11	Synthetic Control of Exciton Dynamics in Bioinspired Cofacial Porphyrin Dimers.. <i>Journal of the American Chemical Society</i> , <b>2022</b> ,	16.4	3
10	Small Matrix Path Integral for Driven Dissipative Dynamics. <i>Journal of Physical Chemistry A</i> , <b>2021</b> , 125, 10500-10506	2.8	2
9	Small Matrix Decomposition of Feynman Path Amplitudes. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 3825-3829	6.4	2
8	Quasiclassical Correlation Functions from the Wigner Density Using the Stability Matrix. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 2165-2174	6.1	1
7	Information-Guided Noise Reduction in Forward-Backward Semiclassical Dynamics. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 4-9	6.4	1
6	Quantum-Classical Path Integral Simulation of Excess Proton Dynamics in a Water Dimer Embedded in the Gramicidin Channel. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 627-638	6.4	1
5	Density matrix and purity evolution in dissipative two-level systems: II. Relaxation. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 5125-5133	3.6	1
4	Density matrix and purity evolution in dissipative two-level systems: I. Theory and path integral results for tunneling dynamics. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 5113-5124	3.6	0
3	Quantum-classical path integral evaluation of reaction rates with a near-equilibrium flux formulation. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, qua26618	2.1	0
2	Quantum quench and coherent-incoherent dynamics of Ising chains interacting with dissipative baths.. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 234705	3.9	0
1	Small Matrix Quantum-Classical Path Integral.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 3492-3498	6.4	0