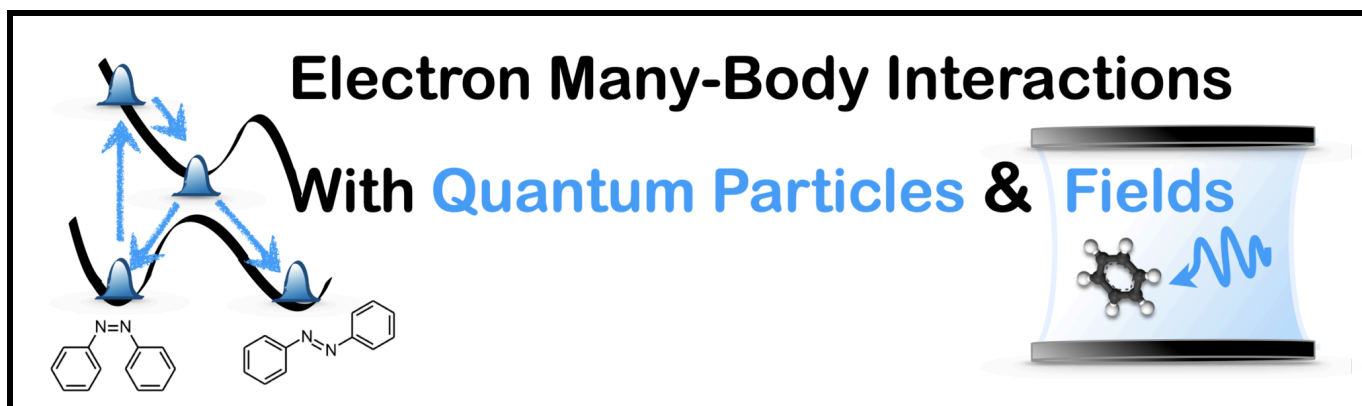


# Program and Book of Abstracts GDR N-Body Workshop



*Strasbourg, January 15th-17th, 2025*  
*Collège Doctorale Européen,*  
*46 Boulevard de la Victoire*

## PROGRAM OF THE DAYS

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### Wednesday, January 15<sup>th</sup>

Chair: J. Toulouse

13:50 – 14:00 Welcome words, **the organizers**.

14:00 – 14:50 **Scott M. Garner**, Princeton University, USA.  
“Dynamics with Nuclear-Electronic Orbital Density Functional and Wavefunction Theories”

14:50 – 15:30 **Aurélien de la Lande**, Paris-Saclay University, France.  
“Density Functional Theory Approaches for Ab Initio Modelling of Radiation Chemistry”

15:30 – 15:55 **Damian Contant**, Sorbonne Université, Paris, France.  
“Evaluating nuclear forces with the Optimized Effective Potential approach”

16:00 – 16:40 **Coffee break**

Chair: M. Vacher

16:40 – 17:20 **Jean-Christophe Tremblay**, Lorraine University, France.  
“Molecular Quantum Dynamics in Stochastic Dissipative Media”

17:20 – 17:45 **Emmanuel Giner**, LCT, Sorbonne Université & CNRS, Paris, France.  
“A Rigorous Density Functional Formulation for QM-MM Problems in the Canonical Statistical Ensemble”

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### Thursday, January 16<sup>th</sup>

Chair: E. Fromager

08:40 – 09:35 **Thomas Ebbesen**, ISIS, Strasbourg, France.  
“Manipulating Matter by Strong Coupling to the Vacuum Electromagnetic Field”

09:35 – 10:00 **Lucien Dupuy**, Strasbourg University, LCQS, France.  
“Exact Factorization-based Surface Hopping Without Velocity Adjustment: appeal of phase-space formulation for non-adiabatic dynamics”

10:00 – 10:40 **Coffee break**

10:40 – 11:30 **Federica Agostini**, Paris-Saclay University, France.  
“Theory and simulation of ultrafast processes in molecules”

11:30 – 11:55 **Benjamin Bacq-Labreuil**, IPCMS, Strasbourg, France.  
“Towards an Ab Initio Theory for High-Temperature Superconductors”

12:15 – 14:00 **Lunch at the University restaurant “Le 32”**

Chair: S. Yalouz

14:00 – 14:50 **Heiko Appel**, Max Planck Institute, Hamburg, Germany.  
“Light-matter interactions within the Ehrenfest-Maxwell-Pauli-Kohn-Sham framework: fundamentals, implementation, and applications”

14:50 – 15:30 **Rémi Avriller**, LOMA, Bordeaux, France.  
“Chirality and Dimensionality in the Ultrastrong Light-matter Coupling Regime: from the Foucault pendulum to the Spyrograph game”

15:30 – 15:55 **Benjamin Tirado**, Materials Physics Center, Donostia, Spain.  
“Design of quantum circuits to study dissipative processes in plasmonic systems”

16:00 – 18:00 **Poster session and aperitif**

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### Friday, January 17<sup>th</sup>

Chair: M. Vacher

08:45 – 09:35 **Enrico Ronca**, Perugia University, Italy.  
“Strong Light-Matter Coupling by Ab-Initio Methodologies”

09:35 – 10:00 **Jérémy Morere**, LPCT - CNRS and Université de Lorraine, Nancy, France.  
“Arbitrariness of the degree of complexity of nested commutators in equation-of-motion formalism”

10:00 – 10:40 **Coffee break**

Chair: L. Dupuy

10:40 – 11:20 **Scott M. Garner**, Princeton University, USA.  
“Nuclear-Electronic Orbital Approach for Electronic and Vibrational Polaritons”

11:20 – 12:00 **Johannes Schachenmayer**, CESQ, Strasbourg, France.  
“Dark chemistry in the large-N limit”

12:00 – 12:10 Concluding remarks, **the organizers**.

# **List of Abstracts**

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# **Talks**

# Manipulating Matter by Strong Coupling to the Vacuum Electromagnetic Field

**Thomas W. EBBESEN**

USIAS & ISIS, University of Strasbourg & CNRS, France

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Over the past decade, the possibility of manipulating material and chemical properties by using hybrid light-matter states has stimulated considerable interest [1,2]. Such hybrid light-matter states can be generated by strongly coupling the material to the spatially confined electromagnetic field of an optical resonator. Most importantly, this occurs even in the dark because the coupling involves the electromagnetic fluctuations of the resonator, the vacuum field. After introducing the fundamental concepts, examples of modified properties of strongly coupled systems, such as chemical reactivity, charge and energy transport, magnetism, will be given to illustrate the broad potential of light-matter states.

## **References:**

- [1] F.J. Garcia Vidal, C. Ciuti, T.W. Ebbesen, Science 373, eabd336 (2021)
- [2] K. Nagarajan, A. Thomas, T.W. Ebbesen, J. Am. Chem. Soc. 143, 16877 (2021)

# Strong Light-Matter Coupling by Ab-Initio Methodologies

**Enrico RONCA**

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Manipulation of matter properties using strong coupling to photons is becoming a hot research topic in physics and chemistry [1,2]. Recent experimental studies demonstrated that strong-light matter coupling in optical cavities can be used to inhibit, catalyze and increment the selectivity of chemical reactions [1]. In the past few years, a lot of progress has been made in the field, but a complete understanding of the possibilities offered by cavity QED in chemistry is still far from being achieved.

In this talk, I will present some recent studies we performed using new ab-initio theoretical techniques developed in the group [3,4]. The predictive potential offered by these techniques will be exploited. The effects induced by quantum fields on several chemical phenomena going from photochemistry to chemical reactivity will be analyzed and discussed [3-6]. In the last part of the talk I will also mention how the chirality and magnetic properties of molecules can be manipulated inside an optical cavity [7,8,9].

## **References:**

- [1]. T. W. Ebbesen, *Acc. Chem. Res.*, 49, 2403, 2016.
- [2]. M. Ruggenthaler, N. Tancogne-Dejean, J. Flick, H. Appel and A. Rubio, *Nature Rev. Chem.*, 2, 0118, 2018.
- [3]. T. S. Haugland, E. Ronca, E. F. Kjørstad, A. Rubio, H. Koch, *Phys. Rev. X*, 10, 41043, 2020.
- [4]. R. R. Riso, T. S. Haugland, E. Ronca, H. Koch, *Nature Commun.*, 13, 1368, 2022.
- [5]. C. Schäfer, J. Flick, E. Ronca, P. Narang, A. Rubio, *Nature Commun.*, 13, 7817, 2022.
- [6]. R. R. Riso, T. S. Haugland, E. Ronca, H. Koch, *J. Chem. Phys.*, 156, 234103, 2022.
- [7]. R. R. Riso, L. Grazioli, E. Ronca, T. Giovannini, H. Koch, *Phys. Rev. X*, 13, 031002, 2023.
- [8]. A. Barlini, A. Bianchi, E. Ronca, H.Koch, *ArXiv*, 2402.10599, 2024.
- [9]. G. Thiam, R. Rossi, H. Koch, L. Belpassi, E. Ronca, *ArXiv*, 2409.12757, 2024.

## Dark Chemistry in the Large-N Limit

**Johannes SCHACHENMAYER**

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Theoretically explaining experimental observations of cavity-modified physics and chemistry remains to be a major challenge, in particular for a large number of coupled molecules. Here I discuss our bottom-up approach with minimal many-body quantum optics models, which include electronic, photonic, and motional degrees of freedom in their simplest form. This talk will review how dark states acquire a "semilocalized" nature with unusual properties in terms of level statistics and other localization quantifiers. I then discuss how such states can play a crucial role for cavity-modified nuclear dynamics. As a main conclusion, I show that semilocalized states can produce exotic entangled quantum states of nuclear wave-packets. Surprisingly, those features can remain robust, also in a large-N limit.

# Theory and Simulation of Ultrafast Processes in Molecules

**Federica AGOSTINI**

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The interaction of light and matter is responsible for a variety of photophysical and photochemical phenomena occurring in nature, like photosynthesis, in the human body, like vision, and in technological devices, like photovoltaics. Theoretical modeling of these phenomena requires to be able to describe the complex interplay of electronic and nuclear motion beyond the Born-Oppenheimer approximation [1], i.e. including nonadiabatic effects, over ultrafast time scales ranging from femtoseconds to picoseconds.

The exact factorization of the electron-nuclear wavefunction is a formalism introduced in 2010 by Gross and coworkers to analyze and to simulate nonadiabatic processes [2,3]. Its original electron-nuclear formulation has been used to derive various flavors of trajectory-based algorithms [4,5] to simulate ultrafast relaxation processes initiated by photoexcitation, like photoisomerization [6] or photodissociation [7]. However, extensions of the original formalism to treat electron-only systems (exact electron factorization) [8,9] and photon-electron-nuclear systems (exact PEN factorization) [10, 11] have been proposed to study processes such as the dynamics of electrons in a strong laser field or photodynamics in the strong coupling regime.

In this talk, I will present an introduction to the theory of nonadiabatic ultrafast dynamics with the exact factorization and I will give an overview of its recent applications.

## **References:**

- [1] F. Agostini, B. F. E. Curchod, WIREs Comput. Mol. Sci. (2019).
- [2] A. Abedi, N. T. Maitra, E. K. U. Gross, Phys. Rev. Lett. (2010).
- [3] F. Agostini, E. K. U. Gross, Eur. Phys. J. B (2021).
- [4] S. K. Min, F. Agostini, E. K. U. Gross, Phys. Rev. Lett. (2015).
- [5] C. Pieroni, F. Agostini, J. Chem. Theory Comput. (2021).
- [6] C. Pieroni, E. Sangiogo Gil, L.-M. Ibele, M. Persico, G. Granucci, F. Agostini, J. Chem. Theory Comput. (2024).
- [7] A. Pollien, E. Villaseco Arribas, D. Lauvergnat, F. Agostini, Mol. Phys. (2024).
- [8]. A. Schild, E. K. U. Gross, Phys. Rev. Lett. (2017).
- [9] S. Giarrusso, F. Agostini, ChemPhysChem (2024).
- [10] L. Lacombe, N. M. Hoffmann, N. T. Maitra, Phys. Rev. Lett. (2019).
- [11] E. Sangiogo Gil, D. Lauvergnat, F. Agostini, J. Chem. Phys. (2024)

# Chirality and Dimensionality in the Ultrastrong Light-matter Coupling Regime: from the Foucault Pendulum to the Spyrograph Game

**Remi AVRILLER**

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We unveil the key-role of dimensionality in describing chiroptical properties of molecules embedded inside an optical Fabry-Pérot cavity.

For a 2D-layer configuration, we show that the interplay between molecular chirality and spatial dispersion of the cavity-modes, results in a gyrotropic coupling at the origin of a differential shift in polaritonic energy spectra. This differential shift is proportional to the gyrotropic coupling, while for 3D bulk-aggregate configurations it is shown to vanish.

We physically interpret the former 2D-chiral effect by analogy with the classical Newtonian motion of a fictitious particle in presence of 3D restoring force, and static magnetic field. The gyrotropic coupling is shown to directly perturbate the anholonomy angle of the classical trajectories, and the fictitious particle undergoes cyclotron gyrations upon entering the ultrastrong light-matter coupling regime.

## **References:**

[1] R. Avriller, and C. Genet, *Chirality and dimensionality in the ultrastrong light-matter coupling regime*, ArXiv:2408.01275 (2024)



# Density Functional Theory Approaches for Ab Initio Modelling of Radiation Chemistry

**Aurélien DE LA LANDE**

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The importance of understanding the responses of matter subjected to ionizing radiation is significant in various fields, including medicine, aerospace and nuclear industries, and fundamental sciences. The development of attosecond sources and technologies opens fascinating possibilities for discovering the physicochemical processes induced by irradiation at ultrashort timescales ( $< \text{ps}$ ), but it also presents major challenges for theory and modeling, which are essential for interpreting experimental data.

Our group at the Institute of Physical Chemistry (CNRS, University of Paris-Saclay) has been developing a coherent body of new methods dedicated to radiation chemistry for several years [1,2]. These methods, implemented in the deMon2k code, are based on density functional theory. The inclusion of electron-nucleus coupling is achieved within the Born-Oppenheimer framework or via the multicomponent DFT formalism [3]. This formalism is available for both stationary and dynamical situations. Special attention has been given to optimizing performance, thanks to the auxiliary DFT framework and GPU-based implementation [4].

In this presentation, I will provide an overview of the current functionalities of deMon2k, as well as some recent application examples, including experiments on picosecond pulse radiolysis and attosecond pump-probe experiments.

## **References:**

- [1] Omar, K. A.; Hasnaoui, K.; de la Lande, A. *Annu. Rev. Phys. Chem.* 2021, 72 (1), 445–465.
- [2] Omar, K. A.; Korsaye, F. A.; Tandiana, R.; Tolu, D.; Deviers, J.; Wu, X.; Parise, A.; Alvarez-Ibarra, A.; Moncada, F.; Pedroza-Montero, J. N.; Mejía-Rodríguez, D.; Van-Oanh, N.-T.; Cailliez, F.; Clavaguéra, C.; Hasnaoui, K.; de la Lande, A. *The Eur. J. Phys. Special Topics* 2023, 232 (13), 2167–2193.
- [3] Mejía-Rodríguez, D.; de la Lande, A. *J. Chem. Phys.* 2019, 150 (17), 174115.
- [4] Martínez, P. A.; Vock, T.; Kharchi, L. R.; Pedroza-Montero, J. N.; Wu, X.; Hasnaoui, K.; de la Lande, A. *Comput. Phys. Commun* 2024, 295, 108946.

# Light-matter interactions within the Ehrenfest-Maxwell-Pauli-Kohn-Sham framework: fundamentals, implementation, and applications

**Heiko APPEL**

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This presentation is introducing the theoretical foundations and the implementation details of a density-functional approach for coupled photons, electrons, and effective nuclei in non-relativistic quantum electrodynamics that we have developed over the past years in our group at the Max Planck Institute for the Structure and Dynamics of Matter in Hamburg (Advances in Physics, 2019 Vol. 68, No. 4, 225–333, arXiv: 2409.08959v2). Starting point of the formalism is a generalization of the Pauli–Fierz field theory for which we establish a one-to-one correspondence between external fields and internal variables. Based on this correspondence, we introduce a Kohn-Sham construction which provides a computationally feasible approach for ab-initio light-matter interactions. In the mean-field limit, the formalism reduces to coupled Ehrenfest–Maxwell–Pauli–Kohn–Sham equations. Within this formalism, we show how to couple the time-evolution of the electromagnetic fields self-consistently with the quantum time-evolution of the electrons and nuclei. We present an implementation of the approach in the real-space real-time code Octopus (<https://octopus-code.org>) using the Riemann–Silberstein formulation of classical electrodynamics to rewrite Maxwell’s equations in Schrödinger form. Furthermore, adapting established multi-trajectory methods that have been developed for electron-nuclear problems to coupled electron-photon systems, we show how to recover quantum effects such as spontaneous emission in real-time from ensembles of Maxwell-Kohn-Sham trajectories.

# Dynamics with Nuclear-Electronic Orbital Density Functional and Wavefunction Theories

**Scott M. GARNER**

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The nuclear-electronic orbital (NEO) method treats electrons and select nuclei quantum mechanically on the same level, inherently capturing nuclear quantum effects such as nuclear delocalization, zero-point energy, and tunneling as well as non-Born—Oppenheimer effects. Multicomponent density functional theory (NEO-DFT) and time-dependent DFT (NEO-TDDFT) methods, as well as a range of wavefunction methods, including coupled-cluster and configuration interaction theories, have been developed. Hydrogen tunneling is known to exhibit multireference character, and as such NEO has been implemented with multistate density functional theory (NEO-MSDFT) and time-dependent configuration interaction (NEO-TDCI) to study proton tunneling dynamics. In this talk, I will review the NEO theories and will highlight the additional insights gained when incorporating the NEO method into real-time dynamics simulations.

## Nuclear-Electronic Orbital Approach for Electronic and Vibrational Polaritons

**Scott M. GARNER**

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Real-time nuclear-electronic orbital (NEO) simulations numerically integrate the time-dependent Schrödinger for both electrons and select quantized nuclei in order to calculate spectra and simulate ultrafast dynamics. Coupling these simulations to a photonic cavity mode provides a platform in which both electronic and vibrational strong coupling can be studied at the same level of theory. In this talk, I will present results displaying joint nuclear-electronic dynamics when coupled to a cavity mode, including excited state intramolecular proton transfer.

# Molecular Quantum Dynamics in Stochastic Dissipative Media

**Jean-Christophe TREMBLAY**

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In this contribution, I will present our recent advances in the development of the stochastic multiconfiguration time-dependent Hartree method (sMCTDH) for open systems, which allows studying molecular dissipative quantum dynamics within a system-bath approach in the Lindblad form. [1,2]. Model systems will be used to demonstrate how thermodynamical properties emerge from coherent dynamics simulations, both in the weak and strong coupling regimes. Further, I will illustrate how specific forms of system-bath separations allow investigating dissipative quantum dynamics in the non-Markovian regime [3].

## **References:**

- [1] Mandal, S., Gatti, F., Bindech, O., Marquardt, R., & Tremblay, J. C. Multidimensional stochastic dissipative quantum dynamics using a Lindblad operator. *J. Chem. Phys.*, 156 (2022).
- [2] Mandal, S., Gatti, F., Bindech, O., Marquardt, R., & Tremblay, J. C. Stochastic multi-configuration time-dependent Hartree for dissipative quantum dynamics with strong intramolecular coupling. *J. Chem. Phys.*, 157(2022).
- [3] Mandal, S., Bindech, O., Marquardt, R., Gatti, F., & Tremblay, J. C. Quantized Vibrational Relaxation from Stochastic Non-Markovian System-Bath Dynamics. *J. Phys. Chem. B*, under review (2025).

# Exact Factorization-based Surface Hopping Without Velocity Adjustment: appeal of phase-space formulation for non-adiabatic dynamics

**Lucien DUPUY**

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Exact factorization formalism provides a fertile alternative to Born-Huang expansion for rigorous description of the correlation between two quantum subsystems. It is of great appeal for building mixed-quantum classical descriptions of non-adiabatic dynamics [2] as it relies on unique, inherently dynamical potentials driving the subsystems' interaction. This unambiguous prescription carries on to the classical limit for the slow subsystem, becoming amenable to fruitful and incremental trajectory-based approximations capturing non-adiabatic effects missed by more ad hoc algorithms.

In this talk, I will present a recent methodological development eliminating both the need for velocity adjustment and ad hoc decoherence correction from surface hopping. This is achieved by combining nuclear evolution from the quantum-classical Liouville equation [3] and electronic equation from exact factorization [4]. The resulting approach outperforms parent SH methods addressing only one of the two problems, as will be illustrated through simulation of photo-relaxation of uracil cation [5].

## **References:**

- [1]. Abedi, Maitra, Gross, Phys. Rev. Lett. 105, 123002 (2010)
- [2]. Villaseco Arribas, Agostini, Maitra, Molecules 27, 4002 (2022)
- [3]. Martens, J. Phys. Chem. A 123, 5, 1110–1128 (2019)
- [4]. Ha, Lee, Min, J. Phys. Chem. Lett. 9, 5, 1097–1104 (2018)
- [5]. Dupuy, Rikus, Maitra, J. Phys. Chem. Lett. 15, 10, 2643–2649 (2024)

# A Rigorous Density Functional Formulation for QM-MM Problems in the Canonical Statistical Ensemble

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In this talk I will present a recent theoretical framework allowing to couple classical DFT and electronic structure calculations in order to obtain in principle exact statistical properties in QM-MM calculations. The latter can be seen as an extension of the Levy-Lieb formulation of electronic DFT to the field of QM-MM calculations.

# Evaluating Nuclear Forces with the Optimized Effective Potential Approach

**Damian CONTANT**

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Knowing the forces exerted on the nuclei is important for determining equilibrium geometries and calculating vibrational modes. Forces also enable a fully quantum description of the nuclei via, e.g., Path Integral Molecular Dynamics [1], which is important for light elements like hydrogen. The accuracy achieved will, however, crucially depend on the level of description of the electron-electron interaction because it directly determines the potential energy surface of the nuclei.

Already on the simple (H<sub>2</sub>)<sub>2</sub> dimer, we find that most Density Functional Theory (DFT) methods give a poor description of the exchange and correlation (xc) effects [2]. Similar results are found on the solid molecular phases of hydrogen [3]. Only the more advanced methods, such as those based on the Random Phase Approximation (RPA), return results in good agreement with Quantum Monte Carlo, especially for the II-III phase transition of solid hydrogen in the megabar regime.

RPA methods can be formulated within the DFT framework, where the energies and density are obtained self-consistently under the action of a local Kohn-Sham potential. The xc part of this potential is obtained by solving the so-called Optimized Effective Potential (OEP) equation [4]. At self-consistency, forces can be determined through the Hellmann-Feynman theorem. However, we show that, whenever nonlocal pseudopotentials are used within the OEP formalism, extra force terms need to be calculated to account for exchange and correlation force contributions.

We have successfully implemented the OEP exchange term within the Quantum ESPRESSO plane-wave code [5], finding forces with excellent numerical accuracy on different molecular and solid systems [6]. This confirms the possibility of using computational methods based on the OEP formalism to predict force-related quantities.

## **References:**

- [1] T. Morresi et al., *Journal of Chemical Physics*, 154, 224108 (2021).
- [2] D. Contant, M. Casula, M. Hellgren, *Journal of Chemical Physics*, 161, 184107 (2024).
- [3] M. Hellgren, D. Contant, T. Pitts, M. Casula, *Physical Review Research*, 4, L042009 (2022).
- [4] S. Kümmel, L. Kronik, *Review of Modern Physics*, 80, 3 (2008).
- [5] P. Giannozzi et al., *Journal of Physics: Condensed Matter*, 29, 465901 (2017).
- [6] D. Contant, M. Hellgren, *Physical Review B*, 110, 125110 (2024).

# Towards an Ab Initio Theory for High-Temperature Superconductors

**Benjamin BACQ-LABREUIL**

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Significant progress towards a theory of high-temperature superconductivity in copper-oxide materials (cuprates) has been achieved via the study of effective one- and three-band Hubbard models. Nevertheless, material-specific predictions, while essential for constructing a comprehensive theory, remain challenging due to the complex relationship between real materials and the parameters of the effective models. By combining density functional theory and many-body methods to explicitly treat the electron-electron interactions, we show that the goal of material-specific predictions for high-temperature superconductors from first principles is within reach. We present a test case by applying our framework to two representative copper-oxide based families of materials usually called multilayer cuprates. They hold the record for highest superconducting temperature at ambient pressure. We explain material-specific properties such as the dependence of superconductivity on the number of consecutive copper-oxide planes, the larger propensity of mercury-based cuprates to superconduct, the link with magnetism, with the density of available electronic states, and other electronic properties. Our work establishes a framework for comprehensive studies of high-temperature superconducting cuprates, and unlocks opportunities for theoretical material design of high-temperature superconductors.



# Design of Quantum Circuits to Study Dissipative Processes in Plasmonic Systems

**Benjamin TIRADO**

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Plasmonic resonances in metallic nanoresonators, arising from collective oscillations of the free electrons in the metal, strongly enhance light-matter interactions. These resonances highly localize the electric field near the surface of the metal and, when coupled to quantum emitters such as molecules or quantum dots, profoundly modify the emission of light. The quantum emitter-metallic nanoresonator interaction has found applications in fields like molecular spectroscopy [1] and the manipulation of nonclassical photon states [2].

When a single quantum emitter that behaves as a two-level system (TLS) is considered, the Jaynes Cummings Hamiltonian [3] represents a simple and accurate approach to model the plasmon-emitter system. However, scaling to multiple emitters introduces high complexity in the classical computation, especially when including dissipative effects such as the losses of the plasmonic nanoresonator or the spontaneous decay of the emitter. The inclusion of many emitters is important for understanding collective phenomena and cooperative interactions that can be useful for multiqubit and long-range entanglement [4]. On the other hand, quantum computing is a promising approach that may be able to tackle these systems in an efficient manner.

This work leverages IBM quantum computers to simulate the dynamics of 1-dimensional emitter plasmonic nanoparticle networks. We assume weak coupling between the emitter and the nanoresonator so that the latter can be effectively removed through the Markovian approximation [5], which reduces the size of the Hilbert space and simplifies the overall quantum computations. We transform the dissipative time evolution into quantum circuits using ancillary qubits [6]. Trotterization of the resulting quantum circuit is performed to approximately represent the total time evolution and the simulation is launched on both noiseless and noisy backends. Finally, we compare the results obtained for the population dynamics with the exact solution of the master equation computed with classical software. The methodology developed in this work could pave the way for exploring larger, more complex networks of quantum emitters and plasmonic nanoresonators in an efficient way, suitable for noisy intermediate scale quantum computers (NISQ).

## **References:**

- [1] Willets KA, Van Duyne RP. (2007). *Annu Rev Phys Chem.*; 58:267-97.
- [2] Hoang, T. B., Akselrod, G. M., & Mikkelsen, M. H. (2016). *Nano Letters*, 16(1).
- [3] Larson, J., & Mavrogordatos, T. (2021). *The Jaynes–Cummings Model and Its Descendants*.
- [4] Li, Y., & Argyropoulos, C. (2021). *Applied Physics Letters*, 119(21).
- [5] Breuer, H.-P., & Petruccione, F. (1985). *The Theory of Open Quantum Systems*.
- [6] del Re, L., Rost, B., Kemper, A. F., & Freericks, J. K. (2020). *Physical Review B*, 102(12).

# Arbitrariness of the Degree of Complexity of Nested Commutators in Equation-of-Motion Formalism

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When describing the reorganization of the electronic structure induced by the interaction between light and matter, one object is particularly crucial: the one-body reduced difference density matrix. The main motivation that led us to focus on this matrix is that it allows us to calculate the difference in the expectation value of the one-body operators between two electronic states without having to know these two states explicitly.

If we had access to the exact stationary eigenstates of the clamped-nuclei Hamiltonian of an N-electron molecular system, we could write an exact transition operator. In the equation-of-motion formalism (EOM), it is possible to prove that an arbitrary number of nested commutators involving this exact transition operator and second quantization operators allows us to write the exact expression of the density matrices of interest.

Since we don't generally have access to the exact transition operator, we need an approximate expression for these matrices. In the EOM formalism, the transition operator is usually substituted by one inspired by the operator that generates the central equation of the Random Phase Approximation (RPA) method. In the literature, the substitution operator is only involved within two nested commutators. Higher numbers of nested commutators aren't explored. Operators with four, six and eight nested commutators are small enough to be computed and it is returned that they do not fulfil the physical conditions to be an approximation of the one-body difference density matrix.

Without additional physical criterion to reject higher number of commutator operator, the molecular electronic transition representation is equivocal in the RPA-like approximation. We intend to show and justify that in that framework the choice of the number of nested commutators is not arbitrary, and that a minimum degree is required to express the elements of the density matrix. Under certain hypotheses, we will point out that there is a recursivity relation between different degrees of complexity, which allows to reject higher degrees.

**List of Abstracts**

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**Posters**

# State-Averaged Quantum Eigensolver for Polaritonic Chemistry: Circuit Design for Near-Term Quantum Computers

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The description of polaritonic systems at the ab initio level is computationally demanding, as it requires a high-level representation of the interaction between confined electromagnetic fields and the electronic structure of a molecule. In this work, we aim to address this challenge using a quantum algorithm, specifically the ensemble-VQE, which enables the calculation of both ground and excited states. Within this framework, we introduce a new type of quantum circuit ansatz designed to encode hybrid wavefunctions. This proposed extension is compact, making it particularly suitable for the NISQ (Noisy Intermediate-Scale Quantum) era, given the limitations of current noisy quantum devices. The extension is integrated into the algorithm to compute the three lowest-lying eigenstates of small systems within a cavity at the ab initio level, effectively capturing polaritonic effects such as the Rabi splitting.

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## Local Potential Functional Embedding Theory

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Accurate prediction of material behavior at the atomic and molecular level is essential in condensed matter physics and materials science. The many-body Schrödinger equation, while theoretically ideal, becomes computationally intractable as system size increases. Kohn-Sham Density Functional Theory (KS-DFT) offers a practical solution by approximating the system using a non-interacting framework. A big problem still needs to be solved, though: how to get close to the Hartree-exchange-correlation (Hxc) energy in order to understand complex electron-electron interactions, especially in systems with strong local electron correlations. In this work, we extend the Local Potential Functional Embedding Theory (LPFET), originally developed for the uniform Hubbard model, to provide a novel self-consistent approach for constructing the Hxc potential on a localized orbital basis. Our method bypasses traditional density functional approximations, instead employing orbital occupations in the spirit of the optimized effective potential method. This framework promises to enhance our ability to model strongly correlated systems, offering new insights into material behavior.

# A 1D Model for Hydrogen-Like Atoms: Towards Ab Initio QED

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In this work we are interested in an one-dimensional model of relativistic hydrogen-like atom using delta-potential interactions. It is motivated by the non-relativistic version of this model which leads to the same ground-state energy and radial wave function as the three-dimensional one. We are using an effective QED Hamiltonian which includes the effect of the vacuum polarization, and the creation of electron-positron pairs, but does not include the photons degree of freedom. In this model we are able to make accurate QED calculations which can be used to develop a more rigorous mathematical background for quantum calculations. This development could be a next step towards understanding QED effects and being able to do ab initio calculations based on a QED background.

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## **Range-Separated Density Functional Theory for Single-Photon Atomic Ionization**

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Advancements in attosecond physics increasingly demand theoretical models to explain measurement outcomes. This project aims at deriving and implementing the general linear-response Sternheimer equations for closed-shell atoms in order to investigate single-photon ionization. The present computational implementation covers the Hartree-Fock method, the local-density approximation, and their time-dependent counterparts, by means of a B-spline based code written in Fortran. As an introduction to range-separated density-functional theory, the locally range-separated hybrid version has been implemented as well. The results demonstrate accurate energy values and oscillator strengths for the Hartree-Fock method and the local-density approximation. Furthermore, the locally range-separated hybrid orbital energies align well with previous calculations. Finally, the time-dependent Hartree-Fock method offers huge improvements of the photoionization spectrum over the bare version. The time-dependent local-density approximation, offers a smaller improvement with respect to its bare version, however, at high energies, the correct behavior is recovered. Implementation of the linear-response Sternheimer equations for closed-shell atoms is currently ongoing.

# Modifying the Electronic Properties of the Topological Systems with Cavity

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Topological systems exhibit fascinating electronic applications due to their distinctive edge and zero-mode states. A central question is how these states interact with various environments, such as intense light. Similarly, hybrid quantum systems containing a few electrons, such as quantum dots, serve as valuable models for engineering topological electronic states. These systems have also garnered significant interest in cavity quantum electrodynamics (cavity QED) for their potential to achieve ultrastrong light-matter interactions. Their simplified architectures offer significant enhancements and optimizations in electron-photon coupling. In this study, we investigate modifications in electronic transport within single and double quantum dot arrays placed inside a cavity.

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## Polaritonic Chemistry Using the Density Matrix Renormalization Group Method

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The emerging field of polaritonic chemistry explores the behavior of molecules under strong coupling with cavity modes. Despite recent developments in ab initio polaritonic methods for simulating polaritonic chemistry under electronic strong coupling, their capabilities are limited, especially in cases where the molecule also features strong electronic correlation. To bridge this gap, we have developed a novel method for cavity QED calculations utilizing the Density Matrix Renormalization Group (DMRG) algorithm in conjunction with the Pauli–Fierz Hamiltonian. Our approach is applied to investigate the effect of the cavity on the S0–S1 transition of n-oligoacenes, with n ranging from 2 to 5, encompassing 22 fully correlated  $\pi$  orbitals in the largest pentacene molecule. Our findings indicate that the influence of the cavity intensifies with larger acenes. Additionally, we demonstrate that, unlike the full determinantal representation, DMRG efficiently optimizes and eliminates excess photonic degrees of freedom, resulting in an asymptotically constant computational cost as the photonic basis increases.

## Density Matrix Renormalization Group Approach Based on the Coupled-Cluster Downfolded Hamiltonians

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The Density Matrix Renormalization Group (DMRG) method has become a prominent tool for simulating strongly correlated electronic systems characterized by dominant static correlation effects. However, capturing the full scope of electronic interactions, especially for complex chemical processes, requires an accurate treatment of static and dynamic correlation effects, which remains a significant challenge in computational chemistry. This study presents a new approach integrating a Hermitian coupled-cluster-based downfolding technique, incorporating dynamic correlation into active-space Hamiltonians, with the DMRG method. By calculating the ground-state energies of these effective Hamiltonians via DMRG, we achieve a more comprehensive description of electronic structure. We demonstrate the accuracy and efficiency of this combined approach on selected mutireference systems.

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## QuantNBody: A Software Extension for Hybrid Fermion-Boson Systems

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Quantum many-body systems are ubiquitous in fields such as condensed matter physics, quantum information science and chemistry, to name a few. Studying these systems requires advanced numerical tools capable of addressing their inherent complexity. However, there are few tools available today that facilitate the easy numerical construction and study of fermionic and/or bosonic systems. To address these challenges, we introduce QuantNBody, a computational package that leverages the second quantization formalism to efficiently map the internal building blocks of quantum systems onto computable variables. In this work, we illustrate how QuantNBody provides a versatile and adaptable framework that can be easily applied to a variety of polaritonic systems with electron-boson interactions, all in a user-friendly manner.