A new theoretical model to capture spin dynamics in Rydberg molecules

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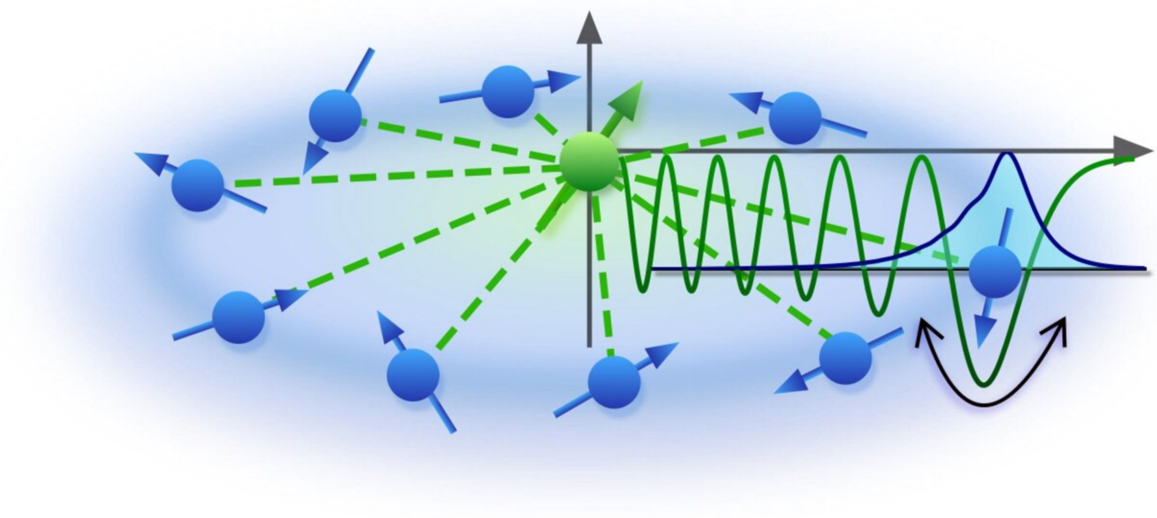

A schematic figure of the quantum Rydberg central spin model. Credit: Ashida et al.

Rydberg molecules are giant molecules made up of tens or hundreds of atoms bound to a Rydberg atom. These molecules have a permanent dipole (i.e., a pair of oppositely charged or magnetized poles), as one of their atoms is in a highly excited state.

Physicists have been studying Rydberg molecules both theoretically and experimentally for several years. Most studies investigating these molecules, however, have only focused on situations that do not involve quantum spins, as the many-body nature of Rydberg molecules makes analyzing their spin dynamics particularly challenging.

In a recent theoretical study, researchers at the University of Tokyo, the Chinese Academy of Sciences, Max Planck Institute and Harvard University were able to capture the interplay of the Rydberg-electron spin dynamics and the orbital motion of atoms using a new method that combines an impurity-decoupling transformation with a Gaussian ansatz. Their papers, published in *Physical Review Letters* and *Physical Review A*, introduce a new theoretical model that could also be applied to other quantum many-body problems.

"The analysis of spin dynamics in Rydberg molecules has remained a challenging problem due to their inherent many-body nature," Yuto Ashida, one of the researchers who carried out the study, told Phys.org. "The main aim of our research was to tackle this issue, advancing our understanding of out-of-equilibrium spin dynamics in spinful Rydberg gases."

The main challenge in investigating out-of-equilibrium spin dynamics in spinful Rydberg gases is that physicists must take into account the orbital motion of atoms and the impurity-environment entanglement mediated via the ultralong-range coupling simultaneously. This has so far made capturing the spin dynamics of Rydberg molecules very difficult.

"To the best of our knowledge, there is no theoretical approach applicable to this new type of quantum many-body problem," Ashida explained. "This is the reason why we developed a new variational approach applicable to solve a generic type of bosonic quantum impurity problem."

The new theoretical approach introduced by Ashida and his colleagues is based on an idea called "disentangling canonical transformation," which was introduced by the same research team in a previous paper, also published in *PRL*. The disentangling canonical transformation utilizes the parity symmetry to completely decouple the impurity and environment degrees of freedom, which ultimately allows the researchers to overcome the issues associated with capturing the spin dynamics in Rydberg gases in a very efficient way.

The variational method that Ashida and his colleagues used to capture the interplay of the Rydberg-electron spin dynamics and the orbital motion of atoms in Rydberg molecules combines the disentangling canonical transformation with a Gaussian ansatz for the bath of particles. This method allowed the researchers to unveil several features that are not present in traditional impurity problems.

One of these features is the interaction-induced renormalization of the absorption spectrum, which eludes simple explanations from molecular bound states. Using their variational method, the researchers were also able to observe long-lasting oscillations of the Rydberg-electron spin.

"The most interesting finding of our study was that the spin-precession dynamics have an unexpectedly long lifetime despite the nonintegrable nature of the present interacting many-body problem," Ashida said. "We interpret this feature as remnant of the integrability of the so-called central spin problem, which can be obtained if we take the infinite-mass limit in our model."

The observation that spin-precession dynamics in Rydberg molecules have a surprisingly long duration could have implications for several subfields of physics, including atomic, molecular and optical (AMO) physics. In fact, the presence of relaxation and thermalization in complex many-body systems is still an active research area in both AMO physics and statistical physics.

In the future, the variational model developed by the researchers and the analyses they conducted could also be applied to other systems in atomic physics and quantum chemistry. This is especially true for systems in which an electron excitation of a high orbital quantum number interacts with a spinful quantum bath.

"In our next studies, we would like to further extend our model to include nonzero angular momentum of the Rydberg electron," Ashida said. "Other open research questions include the generalization of our problem to fermionic bath, application of our general variational approach to other challenging quantum impurity problems. We hope that our studies will stimulate further research in these directions."

More information: Yuto Ashida et al. Quantum Rydberg Central Spin Model, *Physical Review Letters* (2019). DOI: 10.1103/PhysRevLett.123.183001

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