

Commun. Theor. Phys. **75** (2023) 125601 (4pp) https://doi.org/10.1088/1572-9494/ad0f15

A significantly enhanced magnetic moment due to an electric dipole moment

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Received 17 September 2023, revised 20 November 2023
Accepted for publication 23 November 2023
Published 20 December 2023

Abstract

We demonstrate via first-principle calculations based on the density functional theory that the magnetic moment of a helium atom under a given magnetic field has a positive correlation with the electric dipole moment when an external electric field is applied to the system. Our calculation shows that the enhancement of the magnetic moment is significant due to the reduction of the triplet-singlet splitting. We argue that this finding can be generalized to organic molecules, especially to macromolecules where the structure induced an electric dipole moment which may give rise to significantly enhanced responses to the external magnetic field. These results suggest that considerable magnetic responses prevail, particularly in bio-molecules without an inversion center.

Keywords: magnetic moment, helium atom, electric dipole moment

(Some figures may appear in colour only in the online journal)

Introduction

Magnetic interactions have long been recognized as fundamental interactions that exist and play a crucial role in materials science, astrophysics [1, 2], and life science [3], etc, ranging from macroscopic, to mesoscopic and molecular scales [4–10]. It is commonly believed that magnetic interactions are considerable only in magnetic materials. These materials usually contain magnetic elements such as Fe, Co, Ni and Mn [7, 8, 10]. Recently, magnetic materials without traditional magnetic elements have been discovered in a few systems including graphene with zigzag edges [11], nanographene with sublattice imbalance [12], materials with topological frustrations [13], and most notably in two-dimensional CaCl crystals on graphene oxide substrates [14]. In addition to magnetically ordered materials, materials with strong magnetic responses can also be useful in applications. Therefore, it is important to search for novel mechanisms that could enhance magnetic responses.

In this work, we take the helium atom as an example system to show that the magnetic response has a positive correlation with the electric dipole moment of the atom. The electric dipole moment of the helium atom is induced by applying an external electric field. With such an electric field, the energy levels of the ground and excited states are altered [15]. Meanwhile, the response of the helium atom to external magnetic fields is significantly enhanced. We argue that such a phenomenon, i.e., the significantly enhanced magnetic response due to the finite electric dipole moment is common in molecules and nanostructures which can be explained via simple physical mechanisms. Our finding here gives a simple and straightforward understanding of the relationship between electricity and magnetism, which has profound implications in the study of molecules and nanostructures with broken inversion symmetry, either induced by external electric fields or intrinsic structures, particularly in biological molecules.

DFT calculations

All the density functional theory (DFT) calculations in this work are performed using the Gaussian 09 quantum chemistry

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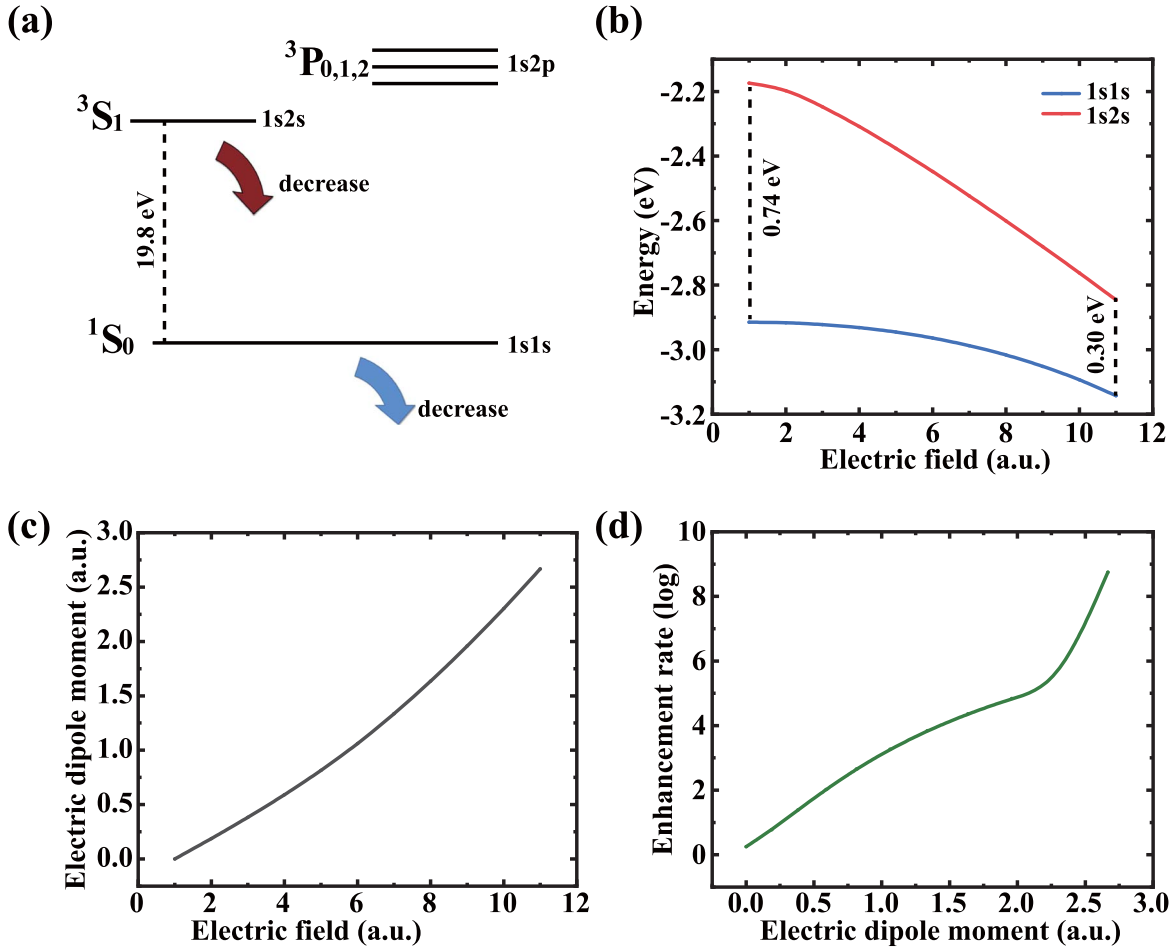

Figure 1. Calculated results of helium influenced by external electric fields. (a) Scheme of the lowest states and the energy gap. The big, curved arrows denote that the energy levels decreased due to the introduction of the external electric field. (b) Change of energy levels as the external electric field increases. (c) Change of the electric dipole moment as the external electric field increases. (d) Enhancement rate of the average magnetic moment as a function of the electric dipole moment. Here, a.u. denotes the atomic unit, where 1 a.u. = 2.542 Debye for the electric dipole moment, and 1a.u. = 51.423 V Angstrom^{-1} for the electric field.

package. The density function is chosen to be B3lyp, which is enough for the calculation of small atoms. To accurately describe the properties of the helium atom under the external electric field, AUG-c.c.-pVTZ basis set is applied for both single-point energy and electric dipole moment calculations. For the calculation of the excited states, time-dependent (TD) DFT is used considering the five lowest energy levels.

Results and discussion

The lowest energy levels of a helium atom are shown in figure 1(a). According to the Pauli exclusion principle, the two electrons are paired into a singlet state at the 1s state to form the ground state. In this state, both the spin and orbital angular momenta are zero, which corresponds to a vanishing magnetic moment. For the lowest excited state, one electron is in the 1s state while the other is in the 2s state. Their spins form the triplet state that can align with the external magnetic field. Therefore, the magnetic response of helium atom at finite temperature originates from the thermal population on the lowest excited state. The total magnetic moment of the lowest excited state is [16]:

$$M = Ng_J S\mu_B B_J\left(\frac{\mu_0 g_J S\mu_B B_J H}{k_B T}\right), \quad (1)$$

where N is the statistically average number of atoms occupying the excited state, g_J is the Lande factor, $S = 1$ describes the total spin angular momentum of the lowest excited state, $\mu_B = \frac{1}{2}$ a.u. $= 0.9274 * 10^{-23} A{\cdot}m^2$ is the Bohr magneton while a. u. denotes the atomic unit, B_J is the Brillouin function, and μ_0 is the permeability of vacuum. At temperatures that are not too high, the two electrons are mostly in their ground state, which is consistent with the common sense that helium is diamagnetic.

By introducing the external electric field, the energy levels of the ground and excited states as well as their wavefunctions are modified, which could also be derived by solving the Schrodinger's equation with a few approximations, i.e., variational theorem, and perturbation theory. We notice that the energy gap between the ground state and the 1st excited state (1s2s) is reduced as the electric field increases, as shown in figure 1(b). The reduction of the energy gap due to the electric field also gives rise to the

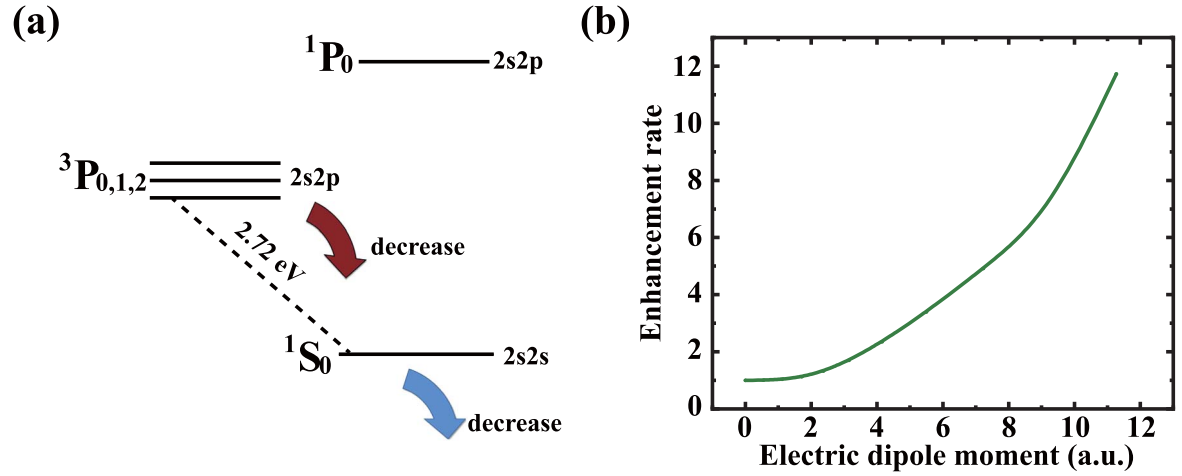

Figure 2. Calculated results of beryllium influenced by external electric fields. (a) Scheme of the lowest states and the energy gap. The big, curved arrows denote that the energy levels decreased with the introduction of external electric field. (b) Enhancement rate of the average magnetic moment as a function of the electric dipole moment. Here, a.u. denotes the atomic unit, where 1 a.u. = 2.542 Debye for the electric dipole moment, and 1a.u. = 51.423 V Angstrom^{-1} for the electric field.

reduction of the triplet-singlet splitting and thus an enhancement of the magnetic response. Meanwhile, the modified wavefunctions lead to a nonzero electric dipole moment of the atom under testing (figure 1(c)). We note that although the electric dipole moment does not directly induce the reduction of the energy gap, both of them are induced with the wavefunction shift by the external electric field, which means that the dipole moment should be a symbol of the energy gap shift together with the enhancement of magnetic response. We argue that the above features are quite general in molecules: Introducing an electric dipole (either by external electric fields or by breaking inversion symmetry) will accompany the reduction of the energy gap between the ground state and the lowest excited state, i.e., the triplet-singlet splitting, and therefore enhances the magnetic responses.

Considering a pile of helium atoms placed in a natural environment where the temperature is set as 300K, these atoms have a probability to be in the excited states due to thermal fluctuations. As the triplet-singlet splitting is reduced, the magnetic response can be substantially enhanced. This enhancement is related to the thermal population on the lowest excited state, which is described by the Boltzmann factor, considering the large gap between the ground state and the excited states [17]:

$$p = \exp\{-\Delta E/k_{\mathrm{B}}T\}, \tag{2}$$

where ΔE is the energy gap between the ground and the excited states, i.e., the triplet-singlet splitting, k_{B} is the Boltzmann constant, and T is the temperature. As shown in figure 1(b), the energy gap is notably reduced by the external electric field. In figure 1(d), we show the enhancement rate of the average magnetic moment at thermal equilibrium as a function of the electric dipole moment at room temperature. Here, the increase of the average magnetic moment reaches 10^8 as the electric dipole moment of the helium atom reaches 2.5 a.u.

We note that the initial occupation of the excited state is about 10^{-333} at room temperature since the initial energy gap between the ground state and the lowest excited state (1s2s) is as large as 19.8 eV. Therefore, the average magnetic moment of the helium atom due to only the external electric field is very difficult to observe since it requires a very large electric field which cannot be achieved in experiments. We emphasize that the above case study is only used to demonstrate the relationship between the electric dipole moment and the average magnetic moment, which can be applied to various systems beside helium atoms.

As an extension, we also calculate the energy shift of the ground state and the lowest excited state for beryllium. As the triplet-singlet gap decreases to 2.72 eV, the required electric field for an observable magnetic moment decreases considerably. For instance, the population of the lowest excited state ($1s^22s2p$) can be up to 10^{-9} with only an external electric field of 0.05 a.u., where the electric dipole moment is 11 a.u. Here, we consider only the lowest excited state of which the orbital momentum $L = 0$, whereas the other higher excited states are neglected due to their much smaller contributions. As a result, the average magnetic moment can reach to $1.4 * 10^{-9}$ a.u., which is much higher than that of a helium atom, while the external electric field is much lower. The scheme of the energy levels of a beryllium atom and the calculated enhancement rate of the average magnetic moment is shown in figures 2(a) and (b), respectively.

Finally, we point out that for realistic molecules and nanostructures, the situation becomes more complex, but the general principles demonstrated above can still hold. The couplings between atoms bring in more modulations to the wavefunction of the electrons, which can change the electric dipole moment of the molecule. Meanwhile, the energy gap between the adjacent states decreases even further with the increase of the atomic orbitals and the number of atoms in the system, which may lead to further enhancement of the reduction of the triplet-singlet splitting and hence the

magnetic response. These effects could be strong enough such that certain molecules are observed to be attracted to an external magnetic field at room temperature, even though they are often regarded as diamagnetic according to conventional ground state theories.

Conclusion

We have shown that the magnetic moment of atoms under an external magnetic field has a positive correlation with the electric dipole moment by considering a helium atom as an example, using DFT calculations. We note that the induced magnetic moment is still very small, $\sim 10^{-325}$ a.u. although it is enhanced by a factor of 10^8 due to an electric dipole moment of 2.5 a.u. which is induced by an external electric field. This value is too small to be observable which is due to the large triplet-singlet splitting. Moreover, only one excited state is considered in the calculation, where the orbital angular momentum of the excited state is zero. In realistic systems, especially in molecules containing multiple atoms, the triplet-singlet energy gap can be much smaller, while multiple excited states with a large magnetic moment may also exist. We believe that the principle revealed here can survive in some large molecules, although the calculation and considerations can be much more complex. In contrast, in helium atoms, the positive correlation between electricity and magnetism can be clearly demonstrated, and it can be expected that such positive correlation can be extended to complex molecule systems such as water. Therefore, magnetic responses of complex molecule systems with an intrinsic electric dipole moment may be strong enough to be directly observed in room temperature experiments as the recent experiment [18]. Furthermore, these discussions imply that magnetic interactions might be an essential ingredient in biological systems, as well as many other systems, since the electric dipole moments widely exist in various systems in this universe, and provide new insight to the understanding of the interactions that have not been fully understood.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (11974366), the Fundamental Research Funds for the Central Universities.

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