Control of the Spin State of a Light Atom by Changing the Density of Surrounding Conduction Electrons

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Interests in spintronics are on the rise from both scientific and technological points of view. Since devices in spintronics involve active control and manipulation of spin degrees of freedom in solid-state systems, it is absolutely necessary to have a deeper understanding of fundamental interactions between electron spins and its solid-state environments. In view of this situation, we are interested in a composite system of an atom immersed into the otherwise homogeneous electron gas (EG).

In an isolated atom, the ground state obeys the Hund's multiplicity rule that requires the highest spin configuration compatible with the Pauli's exclusion principle. Physically this rule is interpreted as the consequence of an effectively larger nuclear charge in a higher spin configuration due essentially to the exchange effect.

Similarly in a uniform EG, the same effect favors spin polarization, bringing about the spontaneous spin-symmetry breaking or the spin-density-wave state which was proven to be the ground state at arbitrary electron densities within the Hartree-Fock (exchange only) approximation. The correlation effect, however, acts in the opposite direction and this effect is so strong in an EG as to lead eventually to the paramagnetic ground state for the majority of metals.

We have studied the ground state of the composite system (or pseudoatom) in the spin-density functional theory [1] and found several intriguing features such as (i) sharp transition from a spin-neutral state to a spin-polarized one with the decrease of the electron density of the EG, if the immersed atom is either B, C, N, or O; (ii) smooth evolution from the spin-polarized state of the pseudoatom to that of the negative ion of the corresponding isolated atom with the further decrease of the density; (iii) formation of the spherical combined spin density/charge density wave, which slowly decays with the distance from the immersed-atom site; and (iv) significant shrinkage of the size of the spin-polarized pseudoatom as compared with its spin-neutral counterpart.

In order to elaborate the first two points, we show the calculated total spin S of the ground-state pseudoatom as a function of r_s (the conventional parameter characterizing the electron density of the enveloping EG) in Fig. 1, which clearly indicates a spontaneous magnetization of the pseudoatom for r_s larger than some threshold value r_{sc}. The net electronic spin S depends on both r_s and the atomic number of the atom Z. This finds itself in contrast with the result for the net electronic charge around of the atom, which is uniquely determined by Z due to the full screening of a charge in the EG.

The steep fall in S near the critical point in Fig.1 is suggestive of a "phase transition" of the second order. In fact, S is found to exhibit a universal behavior in accordance with "the mean-field theory" or in proportion to $(r_s\text{-}r_{sc})^{0.5}$ for r_s near r_{sc}.

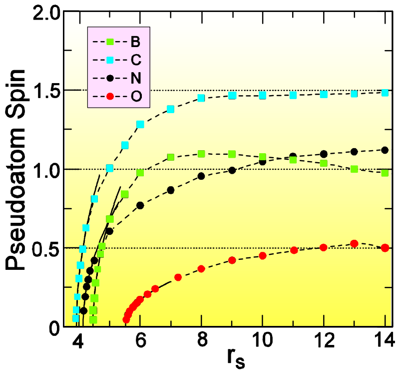

Fig. 1. Calculated total spin of the pseudoatom versus the EG density parameter r_s. Solid curves are the fittings of the data with the universal $(r_s\text{-}r_{sc})^{0.5}$ relation.

Generally, the obtained S is not a multiple of 1/2. This fundamental difference between an isolated atom and this pseudoatom is brought about by the contribution of an infinite number of delocalized electrons in the latter, implying a complicated many-body nature in this atom-EG composite system.

The trend in S at low densities (large r_s) has a clear qualitative interpretation: Because of the positive electron affinity (EA) of the B, C, and O isolated atoms (0.010, 0.046, and 0.054 a.u., respectively), each atom immersed into the EG in the limit of zero density should be reduced into a negative ion (NI) of the corresponding atom. According to the Hund's rule, the population of the 2p orbitals is with 2 electrons with spin up (^{3}P), 3 electrons with spin up (^{4}S), and 3 electrons with spin up and 2 electrons with spin down (^{2}P) for B^-, C^-, and O^- ions, respectively, corresponding to the total spin of 1, 3/2, and 1/2, respectively, which is clearly satisfied in Fig. 1 at large r_s. On the other hand, the NI of the N atom is unstable although long living (EA=−0.003 a.u.), and the slow growth of S of this pseudoatom between 1 and 3/2 at large r_s can be understood as the competition between the NI ^{3}P and atomic ^{4}S states.

Our model might be too primitive to discuss actual systems, but because of the sharpness of the transition in Fig. 1, we may suggest a novel method of spin manipulation by changing the carrier density in a system across the threshold. For example, we may think of an impurity atom in an appropriate semiconductor host, where the carrier density in the semiconductor will be altered by either applying the gate voltage in the FET (field-effect transistor) structure or optical pumping.

References

[1] V. U. Nazarov, C. S. Kim, and Y. Takada, *Phys. Rev. B* **72**, 233205:1-4 (2005).

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