



## Entanglement of mixed quantum states for qubits and qudit in double photoionization of atoms



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### ABSTRACT

Quantum entanglement and its paradoxical properties are genuine physical resources for various quantum information tasks like quantum teleportation, quantum cryptography, and quantum computer technology. The physical characteristic of the entanglement of quantum-mechanical states, both for pure and mixed, has been recognized as a central resource in various aspects of quantum information processing. In this article, we study the bipartite entanglement of one electronic qubit along with the ionic qudit and also entanglement between two electronic qubits. The tripartite entanglement properties also have been investigated between two electronic qubits and an ionic qudit. All these studies have been done for the single-step double photoionization from an atom following the absorption of a single photon without observing spin orbit interaction. The dimension of the Hilbert space of the qudit depends upon the electronic state of the residual photoion  $A^{2+}$ . In absence of SOI, when Russell–Saunders coupling (L–S coupling) is applicable, dimension of the qudit is equal to the spin multiplicity of  $A^{2+}$ . For estimations of entanglement and mixedness, we consider the Peres–Horodecki condition, concurrence, entanglement of formation, negativity, linear and von Neumann entropies. In case of L–S coupling, all the properties of a qubit–qudit system can be predicted merely with the knowledge of the spins of the target atom and the residual photoion.

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### 1. Introduction

Quantum entanglement is a key prediction of quantum mechanics and one of the resources needed in quantum information (QI) processing [1,2]. In analogy to the classical information, QI also needs bits, called qubits. But, a bit in QI is a quantum system which has, at least, one observable requiring two-, or higher-, dimensional space for its characterization. A two-dimensional quantum system (e.g., a spin-1/2 particle) is called in QI as a quantum bit or qubit [3,4]. In general, a  $d$ -dimensional quantum system (with  $d > 2$ ) is called a qudit [5].

Availability of two or more qubits with entanglement is an essential ingredient for any quantum information related studies. Quantum entanglement is a nonlocal property that allows a set of qubit to express higher correlation that is not possible in classical systems.

Research into quantum entanglement was started in 1935 by Einstein, Podolsky and Rosen describing the EPR paradox [6]. The

flaw in EPR arguments was discovered by Bell [7], who proved that the principle of locality used in EPR paradox, was not consistent with the hidden variables interpretation of quantum theory. Bell's theorem conversely provides one of the possible methods to test whether two or more particles form an entangled state. The strong correlations among entangled particles can be used as resources of quantum cryptography [8], quantum teleportation [9] and quantum computation [10].

It is known that quantum correlation in qudit or multipartite system is stronger than in the bipartite system. The investigations performed hitherto have already shown that entanglement among more than two particles is not merely an extension of its bipartite counterpart but has instead several new and different properties which are more advantageous, as example, in super dense coding, quantum cloning, teleportation [11]. Koike et al. [12] have already demonstrated experimentally “1 → 2 quantum telecloning” for optical coherent states. To study QI at more fundamental levels, the multipartite entangled states, in addition, are also needed. It has been suggested [13] that the use of qudit can reduce the number of qubits by a function of  $\log_2 d$ . Qudit system is also useful in developing quantum communication protocols which provides greater security in quantum communication complexity [14].

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The bipartite states of photons which are entangled in higher than two dimension space have been generated in [15]. Being an excellent carrier of information, photon is not suitable for long term storage as it is immediately destroyed as soon as one tries to detect it. Some theories have been developed for studying the bipartite states of an electronic qubit and ionic qudit produced by photoionization [14]. One of the simplest processes for producing entangled particles with non-zero rest mass is double photoionization (DPI) in which simultaneously two electrons are ejected following absorption of a single photon in an atom or molecule [16,17]. Here we discuss DPI of an atom for generating bipartite entanglement for tripartite states of two electronic qubits (say  $e_1$  and  $e_2$ ) and an ionic qudit (say  $A^{2+}$ ) and also tripartite entanglement of the same system. These particles are entangled with respect to their spin-angular momenta in absence of spin orbit interaction (SOI). Furthermore, the electrons in DPI are emitted with all possible kinetic energies (subject to the conservation of the total energy) in all possible directions. Their spins can be quantized in any directions as well. The residual doubly charged positive ion (i.e., dication) of the target molecule may be left in any of its energetically accessible spin-angular states. Hence, the two photoelectrons and the dication are in a mixed state after DPI.

A pure separable (i.e., unentangled) state of two particles always satisfies Bell's inequalities [7]. A mixed state can be nonseparable (i.e., entangled) even without violating Bell's inequalities. Peres [18] and Horodecki [19] developed a condition which is equally applicable to both pure and mixed states. According to Peres and Horodecki condition, the density matrix for unentangled mixed states remains positive when subjected to partial transposition. A fundamental fact is that this condition is the necessary and sufficient condition for separability of  $2 \otimes 2$  and  $2 \otimes 3$  cases. Here, we explore theoretically the domain between pure highly entangled states and highly mixed weakly entangled states [20]. As a measure of entanglement, we consider Peres–Horodecki condition, entanglement of formation (EOF) [20], concurrence, negativity [21]. As a measure of mixedness and partial entanglement we consider linear and von Neumann entropies [22]. However in references [16] and [17] only free entanglement of bipartite system of two electronic qubits have been studied and the entanglement is quantified by Peres–Horodecki's NPT condition. The density matrices calculated in Refs. [16,17] have considered both, the real and imaginary parts of the outgoing wave function and the calculated density matrices can be used to some specific geometry. In order to calculate the density matrix of two electronic qubits we have considered only the real part of the outgoing wave function and the density matrix in this case can be applied to any geometrical configuration of the physical system. In case of tripartite system, both, free and bound entanglements have been studied considering negativity and Horodecki's inequality condition [4,13], respectively.

In Section 2, we briefly describe the density operator (DO) and states for DPI of an atom. This operator corresponds to the case when the ionizing electromagnetic radiation is in a pure state of polarization and the target atom is in its ground state before DPI. This DO is used to derive an expression for the density matrix (DM) needed to study the quantum entanglement properties of the spin states of the photoelectrons and photoion in Russell–Saunders coupling when SOI is not taken into account. In Section 3, we study the entanglement in DPI for qubits and qudit system. A quantitative application of entangled properties in DPI of Neon is presented in Section 4. Finally Section 5 contains the conclusion part.

## 2. Density operators

Let us consider the DPI process of simultaneous emission of two electrons ( $e_1, e_2$ ) from an atom A due to absorption of a single

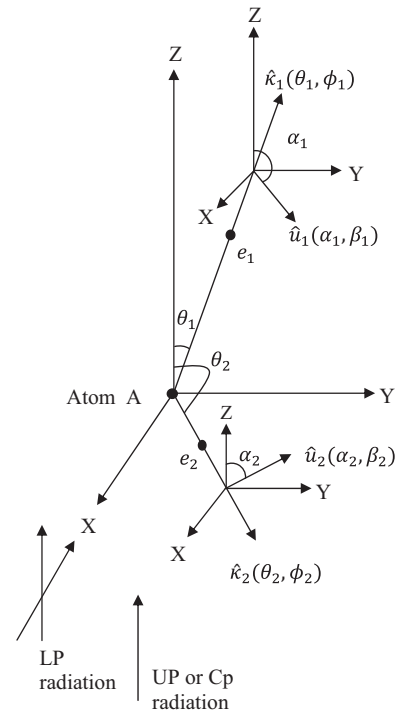


Fig. 1. Two electrons are emitted simultaneously after photoabsorption.

photon ( $\nu_r$ ) whose entanglement properties we want to investigate. The propagation vector of the  $i$  ( $= 1, 2$ )th electron is  $\vec{k}_i = (k_i, \theta_i, \phi_i)$  so that its kinetic energy can be written as  $\varepsilon_i = \hbar^2 k_i^2 / 2m$ . Here,  $\mu_i$  ( $= \pm 1/2$ ) is the projection of the spin angular momentum of  $i$ th electron along its spin quantization direction  $\hat{u}_i = (\alpha_i, \beta_i)$ . These two electrons before their ejection were an integral part of the atom A. If  $A^{2+}$  denotes the residual dication, then our one step DPI process can be represented by

$$h\nu_r (|l_r| = 1, m_r) + A |0\rangle \rightarrow A^{2+} |f\rangle + e_1 (\vec{k}_1; \mu_1 \hat{u}_1) + e_2 (\vec{k}_2; \mu_2 \hat{u}_2). \quad (1)$$

here  $E_r = h\nu_r$  and  $|l_r| = 1$  are, respectively, the energy and the angular momentum of the absorbed photon in the electric dipole (E1) approximation. The state of polarization of the photon is represented by the parameter  $m_r$ . Where,  $E_0$  and  $E_f$  are the energies of the atom A in the bound electronic state  $|0\rangle$  and the residual dication  $A^{2+}$  in the bound electronic state  $|f\rangle$  respectively. The polar axis of our space (or photon) frame of reference shown in Fig. 1 is in the direction of the electric vector of the linearly polarized ( $m_r = 0$ ) radiation present in the process (1); if the ionizing radiation is circularly polarized ( $m_r = \pm 1$ ) or unpolarized, its direction of incidence then defines the polar axis of the photon frame.

Here  $\rho_0 = |0\rangle\langle 0|$  and  $\rho_r = |m_r\rangle\langle m_r|$  are the respective density operators of the target atom A before DPI and of the ionizing radiation. The incident photon and the atom are not correlated before the interaction between the two takes place. This means the density operator of the combined (atom + photon) system of Eq. (1) can be written by the direct product

$$\rho_i = \rho_0 \otimes \rho_r. \quad (2)$$

Here  $F_p$  is the photoionization operator in the E1 approximation. Then the density operator of the combined ( $A^{2+} + e_1 + e_2$ ) system in Eq. (1) after DPI becomes

$$\rho_f = K_p F_p \rho_i F_p^\dagger. \quad (3)$$

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