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Quantum information chemistry: exploring non-local entanglement phenomena

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This study explores the non-local phenomena arising from quantum entanglement (often referred to as non-locality). It investigates these phenomena through fundamental concepts of quantum information theory (QIT), particularly those involving quantum state superposition. The emergence of non-locality is discussed in connection with electron correlation from a chemical viewpoint, emphasizing both historical context and scientific significance. This phenomenon is analyzed using selected atomic and molecular test cases, providing insights into fundamental aspects of chemical systems and the processes they undergo. Ultimately, this work advances the emerging discipline of Quantum Information Chemistry (QIChem).

Keywords: Quantum information theory; quantum chemistry.

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1. Introduction

Quantum information theory (QIT) [1] is an interdisciplinary field at the junction of theoretical physics and computer science, examining how quantum mechanical principles can be harnessed for information processing, transmission, and storage beyond the scope of classical information theory. At its core, QIT leverages concepts such as superposition, entanglement, and uncertainty to develop new methods of encoding, manipulating, and communicating information, which lie beyond the reach of classical physics and traditional information theory.

Quantum information chemistry (QIChem) [2] is a nascent field that unites quantum information science and chemistry to examine and control chemical systems at the quantum scale. This interdisciplinary approach promises to reshape our understanding of chemical processes and spark innovations across various scientific and industrial domains. By leveraging concepts such as entanglement and superposition, QIChem offers new perspectives on the influence of quantum coherence in chemical dynamics [3].

The convergence of quantum science and chemistry is rapidly emerging as a driver of next-generation quantum technologies to advance the fundamental understanding of materials used in quantum information applications [4] for instance. Through entanglement, quantum computers promise to efficiently deliver accurate results for many important problems in quantum chemistry [5]. Chemists now sculpt molecular qubits whose engineered spin-lattice and spin–spin relaxation times rival those of solid-state color centers, offering synthetic tunability that could unlock scalable, application-specific quantum hardware [6]. Optically addressable spin-bearing molecules extend this paradigm by directly linking coherent spin states to photons, paving the way for room-temperature quantum sensors and networked quantum processors [7]. Across the broader chemical community, a growing agenda in quantum information science is identifying the problems—ranging from catalysis to materials discovery—where quantum algorithms promise transformative speed-ups [8]. Fundamental advances such as symmetry-protected rotational qubits in cold polyatomic molecules demonstrate that molecular degrees of freedom can store quantum information with built-in noise resilience [9], while comprehensive perspectives on quantum computing and chemistry chart the algorithmic and hardware milestones still needed to translate these concepts into practical devices [10]. Together, these developments showcase how the synergy between quantum science and chemistry is expanding the fundamental toolkit of both disciplines and laying the foundation for quantum computers, sensors, and communication systems built from tailor-made molecular building blocks.

In the following, we briefly discuss the development of electron correlation in quantum chemistry and the basic principles of quantum mechanics from which the non-local phenomenon of entanglement arises hierarchically. We then present illustrative examples of selected chemical aspects associated with non-locality: atomic electron correlation and the molecular dissociation process, both associated with entanglement phenomenon, the essence of QIChem.

2. Historical overview of electron correlation and entanglement in quantum chemistry

Electron correlation, the deviation from mean-field (Hartree-Fock) approximations due to electron-electron interactions, has been a central challenge in quantum chemistry since the early days of quantum mechanics. In modern terms, electron correlation is fundamentally connected to the quantum mechanical phenomenon of **entanglement**, where electrons become inseparably linked at the quantum level, and the state of one electron cannot be described independently from others. In the **1920's** and **1930's**, foundational quantum chemistry approaches, such as Hartree-Fock theory, explicitly neglected electron correlation (and hence entanglement), simplifying computations but limiting their accuracy for correlated systems [11]. The entangled nature of electrons was implicitly recognized, but computational tools were insufficient to accurately describe these subtle quantum interactions. By the **1950's** and **1960's**, methods emerged to explicitly include correlation, most notably Configuration Interaction (CI). CI captures electron correlation by considering superpositions of electron configurations, inherently reflecting quantum entanglement between electrons in different orbitals [12]. Although entanglement was not explicitly discussed at that time, CI methods represented a significant step toward capturing quantum correlations more rigorously. In the **1960's** and **1970's**, Møller Plesset perturbation theory [13] provided systematic approaches to electron correlation, implicitly accounting for electron entanglement through corrections beyond the independent-particle approximation [14]. Nevertheless, entanglement as a physical concept remained mostly implicit or unexplored in quantum chemical literature. The **1970's** and **1980's** brought the groundbreaking development of Coupled-Cluster (CC) methods [15]. Coupled-Cluster approaches, particularly CCSD(T), explicitly describe electron correlation through clusters of electron excitations, implicitly capturing the highly entangled nature of electrons in correlated molecular systems. These methods quickly became the gold standard for quantum chemical accuracy due to their sophisticated treatment of correlation and the underlying entanglement it reflects. In the late **1980's** and **1990's**, Density Functional Theory (DFT) provided efficient ways to include electron correlation implicitly [16]. While DFT itself does not explicitly model electron entanglement, recent interpretations highlight that the underlying exchange-correlation functionals approximate entanglement effects indirectly. The recognition of entanglement as an explicit conceptual tool entered quantum chemistry prominently in the **1990's** and **2000's**, especially within strongly correlated and multireference methods. Complete Active Space Self Consistent Field (CASSCF) and multireference configuration interaction (MRCI) explicitly address strong electron correlation, where electrons become highly entangled and traditional single-reference methods fail [17]. Quantum information theory has increasingly provided frameworks to quantitatively measure entanglement, helping to guide methodological improvements and interpretation of correlation phenomena.

Recent developments (**2000's to present**) incorporate the concept of entanglement, notably through Density Matrix Renormalization Group (DMRG) and Quantum Monte Carlo methods, enabling accurate treatments of strongly correlated systems [18]. These methods utilize entanglement explicitly as a computational resource, providing improved descriptions of electron correlations that are difficult to handle classically. Moreover, quantum computing is beginning to emerge as a promising frontier for directly leveraging entanglement in simulations, potentially transforming our capability to treat complex correlated molecular problems [19].

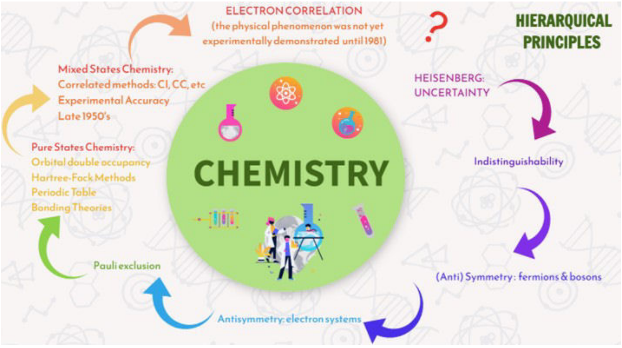

FIGURE 1. Highly correlated quantum chemistry methods already accounted for electron correlation and implicitly for entanglement with no explicit link to the physical phenomenon of non-locality.

Thus, throughout the historical evolution of quantum chemistry, the shift from implicit to explicit recognition of entanglement has profoundly influenced how electron correlation is understood and modeled, shaping modern theoretical and computational chemistry. In Fig. 1, we depict the state of the art of the quantum chemistry methods accounting for electron correlation without any explicit link to the entanglement phenomenon prior to its experimental verification in the late **1980's** and **1990's.**

3. Quantum chemistry: from uncertainty to non-locality and entanglement

Quantum chemistry is deeply rooted in foundational principles of quantum mechanics that form a natural conceptual hierarchy. At its core lies the **Heisenberg uncertainty principle**, which establishes fundamental limits on simultaneous measurements of complementary properties (*e.g.*, position and momentum). This intrinsic uncertainty shapes the probabilistic nature of quantum mechanics and determines the structure and behavior of quantum states [20]. Building upon uncertainty, quantum mechanics introduces the indistinguishability principle, which implies that identical quantum particles cannot be distinguished even in principle. This indistinguishability leads to symmetry requirements in the total wavefunction [21]. In particular, electrons, being fermions, possess antisymmetric wavefunctions under particle exchange, a condition encoded mathematically by the anti-symmetrization postulate and manifest physically as the antisymmetry principle [21,22]. The antisymmetry requirement directly results in the Pauli exclusion principle, which prohibits two electrons from occupying the same quantum state simultaneously. Pauli's principle profoundly influences atomic structure, chemical bonding, and molecular stability [23]. At the next level, Pauli exclusion naturally enforces constraints on double occupancy of orbitals and leads to electron correlation—the interplay between electrons beyond mean-field approximations. Electron correlation significantly modifies chemical behavior by accounting explicitly

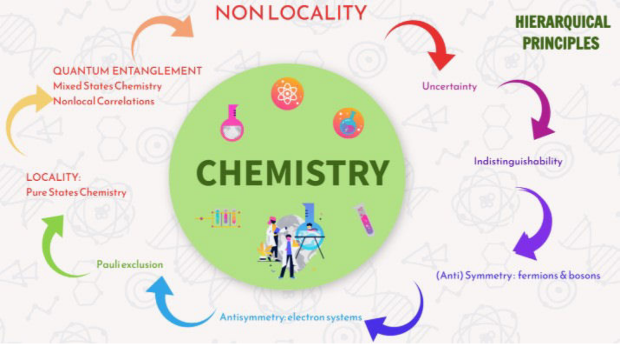

FIGURE 2. Basic principles of quantum mechanics from which the non-locality phenomenon arises with an explicit connection to the source of the uncertainty principle.

for electron-electron interactions, highlighting how electrons avoid each other due to mutual repulsion and quantum statistics [11,15]. Furthermore, correlation and Pauli exclusion together impose restrictions on electronic localization, leading to the concept of **locality**. Quantum-chemical models frequently exploit the near-local character of electron interactions—through approaches such as local correlation schemes and local-density functionals—yet the exact many-electron wavefunction itself is fundamentally non-local. It links electrons across spatially distant regions, exemplifying quantum non-locality [24] and giving rise to entanglement, the distance-defying quantum correlation. In strongly correlated, multireference systems such entanglement is especially pronounced, making it a cornerstone of modern theoretical chemistry and quantum information science [18,24].

Today, recognizing and explicitly treating entanglement is crucial for the accurate modeling and interpretation of complex chemical phenomena, including conical intersection-driven processes, charge-transfer reactions, and excited-state dynamics.

4. Non-local chemical phenomena

4.1. Correlation energy as an indicator of non-locality: helium-like systems

This study emphasizes the intrinsically quantum nature of correlation energy, derived purely from the wave function rather than any external Hamiltonian. We resolve longstanding ambiguity around correlation energy by associating it with the quantum concept of nonlocality, linking it to non-dynamic correlations that appear in states where the Slater rank exceeds one. By comparing correlation energy with quantum entanglement metrics, such as von Neumann and linear entropies, we demonstrate a close relationship between these phenomena.

Our findings show a direct one-to-one mapping between entanglement and correlation energy in helium-like systems across different nuclear charges (Z). We supply numerical evidence indicating a linear dependency between E_{corr} and quantum entanglement in helium isoelectronic atoms, using configuration-interaction wave functions that capture strong electron correlation. This outcome highlights the profound link between entanglement and correlation energy in atomic systems.

4.2. Electron correlation

In many-electron environments, electron correlation is a fundamental phenomenon intimately tied to quantum entanglement and nonlocality, rather than a mere artifact of numerical methods or variational bounds. Under the Hartree-Fock (HF) framework, electrons interact only via average fields, effectively assuming uncorrelated motion. As a result, the difference between the HF energy E_{HF} and the exact ground-state energy E_0 –referred to as correlation energy E_{corr}– captures the shortfall in HF's description:

$$E_{\text{corr}} = E_0 - E_{\text{HF}}, \tag{1}$$

where the maximum value of zero corresponds to an independent-particle state. Thus, this measure highlights the absence of explicit electron-electron interactions in the HF model.

Historically, Collins first linked correlation energy with an informational entropy distinct from the thermodynamic one [27], suggesting that E_{corr} may be proportional to an information-theoretic measure. As discussed below, an independent-particle state exhibits zero linear and von Neumann entropies of its one-particle density matrix, whereas nonzero quantum entropies and thus entanglement appear when electron correlation is introduced [28].

Numerous approaches beyond HF address this limitation. Full Configuration Interaction (FCI), for example, attempts to solve the Schrödinger equation exactly within a designated one-electron basis by summing over all possible Linear Combinations of Slater Determinants (LCSD). While exceedingly precise, FCI remains practical only for smaller systems due to its exponential growth in configurations as electron count rises.

In both FCI and other LCSD methods, correlation emerges strictly from the wave function, leaving the Hamiltonian unaltered. In earlier work, some regarded correlation as a byproduct of using an inadequate single-determinant wave function, prompting skepticism about its physical significance.

Distinguishing between non-dynamic (static) and dynamic correlation clarifies the concept further. Non-dynamic correlation considers scenarios where multiple determinants are inherently necessary (*e.g.*, bond-breaking), whereas dynamic correlation addresses short-range electron-electron interactions beyond mean-field approximations, as seen in coupled-cluster or multi-reference methods. In practice, both types often appear together, with LCSD methods explicitly targeting static correlation (when HF fails), while dynamic correlation is introduced through post-HF or density functional theory (DFT) strategies.

4.3. Non-locality and quantum entanglement

Recent perspectives have reframed electron correlation in the context of quantum information theory, identifying it as an entanglement phenomenon [28]. Within this framework, entanglement, a fundamental aspect of quantum mechanics, manifests non-dynamic correlation in electronic structures. We specifically examine helium-like atoms with nuclear charges from 1 to 10, showing that linear and von Neumann entropies track closely with electron correlation.

Even though we employ relatively compact one-electron bases to build full configuration interaction (FCI) wave functions, our data remain highly accurate regarding entanglement and exhibit large correlation energies. This connection between correlation energy and entanglement gives a compelling physical account of non-dynamic correlation, tying it to intrinsic quantum mechanisms rather than computational artifacts. Such a viewpoint enhances our understanding of how electrons behave quantum mechanically in atoms and molecules, linking established chemical notions with quantum information theory.

Let us remark that a configuration-interaction wavefunction (CI) accounts for quantum non-locality by superposing multiple Slater determinants whose excitations couple spatially separated regions, thereby embedding electron-electron correlations that violate classical locality. The richer (higher-rank) the excitation manifold, the more faithfully the CI description reproduces the entanglement structure mandated by the exact many-electron state.

4.4. Entanglement measures

A pure state of N identical fermions can be written as $|\Psi\rangle$, and the associated density matrix is $\rho = |\Psi\rangle\langle\Psi|$. This state is non-entangled (separable) if it can be represented by a single Slater determinant formed from N orthonormal one-particle states (*i.e.*, Slater rank equals one). Otherwise, it is termed entangled.

There are multiple methods for quantifying entanglement in an N pure -fermion state $|\Psi\rangle$. For instance, one technique relies on the single-particle reduced density matrix, derived by tracing out $N-1$ electrons from $\rho = |\Psi\rangle\langle\Psi|$. This reduced density matrix then becomes a straightforward way to evaluate the magnitude of entanglement within the system.

The linear entropy of ρ_r given by

$$S_L[\rho_r] = 1 - Tr\left(\rho_r^2\right), \tag{2}$$

provides a practical quantitative measure for the entanglement of the density matrix. Specifically,

$$\xi_L[\rho_r] = N\left[S_L[\rho_r] - \frac{N-1}{N}\right], \tag{3}$$

which is normalized to the interval [0,1]. This quantity is zero precisely when the state $|\Psi\rangle$ has Slater rank 1 and is therefore separable.

Accordingly, the linear entanglement measure of the single-particle reduced density matrix ρ_r for fermionic systems can be expressed in terms of natural spin orbitals via Löwdin's spectral decomposition:

$$\xi_L\left[\rho_r\right] = 1 - \frac{1}{2N}\sum_i^M\sum_{\gamma=\alpha}^{\beta} n_i^\gamma, \tag{4}$$

where M is the dimension of the basis set. It is worth noting that closed-shell atomic systems are frequently characterized by a doubly occupied density matrix, *i.e.*,

$$\rho_r = \sum_i^M \left(n_i^\alpha + n_i^\beta\right)\left|\chi_i(\mathbf{r})\right|^2 ,$$

with $0 \leq n_i^\alpha + n_i^\beta \leq 2$ and

$$\sum_i^M \left(n_i^\alpha + n_i^\beta\right) = 1.$$

For a pure state of N identical fermions, von Neumann entropy of the single-particle reduced density matrix $\rho_r = Tr_{2,3,\ldots,N}\left(|\Psi\rangle\langle\Psi|\right)$, obtained by tracing out $N-1$ particles, is defined as

$$S_{vN}\left[\rho_r\right] = -Tr\left(\rho_r \ln \rho_r\right). \tag{5}$$

This measure quantifies the degree of entanglement in the N-fermion state $|\Psi\rangle$ through

$$\xi_{vN}\left[\rho_r\right] = S_{vN}\left[\rho_r\right] - \ln N, \tag{6}$$

which is nonnegative and vanishes exactly when $|\Psi\rangle$ has Slater rank 1, making it separable. The term $\ln N$ reflects the fact that, even in the separable case, the single-particle reduced density matrix has nonzero entropy.

As in the linear entropy case, this von Neumann entanglement measure can be written in terms of the natural occupation numbers:

$$\xi_{vN}\left[\rho_r\right] = \sum_i^M \left(n_i^\alpha + n_i^\beta\right)\ln\left(n_i^\alpha + n_i^\beta\right) - \ln N. \tag{7}$$

4.5. Entanglement: helium-like systems

In our investigation of the helium isoelectronic series, spanning from $^-$ to Ne^{+7}, we employed highly correlated electron densities from the work of López-Rosa *et al.* [29]. These densities derive from configuration interaction (CI) wave functions that systematically vary the nuclear charge Z. The CI computations utilized a $[3s, 3p, 2d]$ STO basis set, ensuring accurate capture of electronic behavior by distributing electrons across the K-shell and inter-shell regions.

We began our analysis by examining how the correlation energy E_{corr}, evolves as nuclear charge increases through the helium series. Figures 3 and 4 illustrate this trend along with

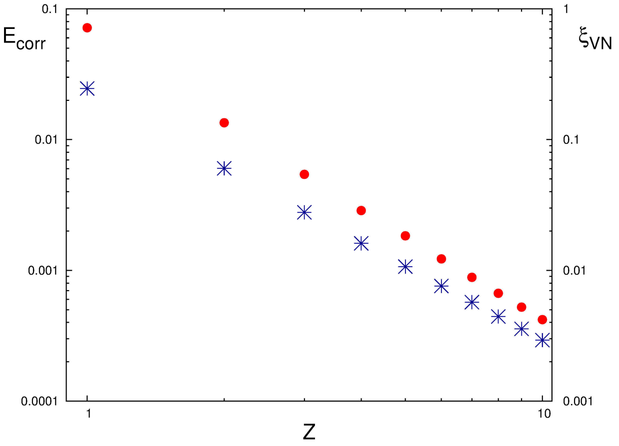

FIGURE 3. Dependence of the correlation energy, $E_{\rm corr}$ (dots), and linear entanglement ξ_L (stars) of the ground-state helium-like atoms on the nuclear charge $Z \in [1, 10]$.

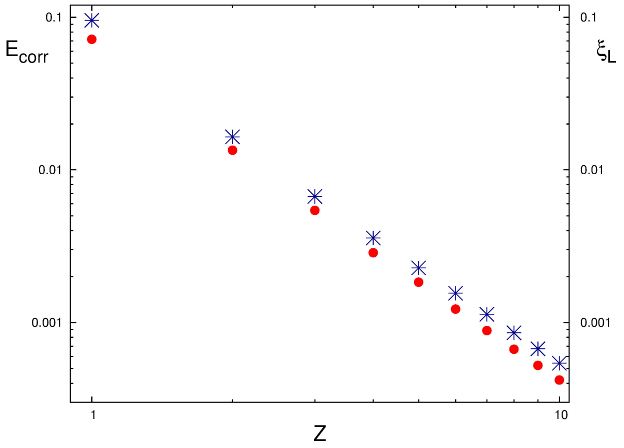

FIGURE 4. Dependence of the correlation energy, E_{corr} (dots), and the von Neumann entanglement, ξ_{VN}(stars) of the ground-state helium-like atoms on the nuclear charge Z.

the associated entanglement measures—namely, the linear and von Neumann entropies, respectively, for each system in the series. Both correlation energy and the entanglement measures exhibit a consistent decrease as nuclear charge rises, revealing a fundamental link between the quantum characteristics of these atoms and their electronic structures. This indicates that nuclear charge plays a pivotal role in shaping electron correlation and quantum entanglement throughout the series.

We investigated how two entanglement measures—linear and von Neumann entropies—relate to the correlation energy in the helium isoelectronic series, spanning nuclear charges from 1 to 10. By employing highly correlated configuration interaction (CI) wave functions, we observed a consistent pattern: both entanglement measures diminish as nuclear charge increases. This parallel decline underscores a profound link, as entanglement and correlation energy arise from the same underlying physical properties of atomic systems. Our findings indicate that in isolated atoms, entanglement can serve as a quantitative reflection of electron correlation energy, revealing a deep interplay between quantum entanglement and electron interactions. The results of this study are presented in Ref. [30].

4.6. The dissociation process of diatomic molecules

We investigate the quantum entanglement properties involved in the dissociation dynamics of selected homo- and heteronuclear diatomic molecules: H_2, He$\cdots$He, Li_2, Cl_2 and HCl, supported by detailed ab initio calculations of correlated molecular wavefunctions at various stages of bond breaking. Two principal scenarios are examined: (i) the united-atom limit, where the molecule behaves as a single quantum entity, and (ii) the asymptotic dissociation limit, in which the constituent atoms separate completely.

We also track how electronic entanglement evolves with the reaction coordinate, correlating it with key physical stages of the dissociation pathway. The results provide new perspectives on the complex interplay between quantum mechanical behavior and traditional chemical concepts, emphasizing how quantum entanglement responds to structural changes during chemical reactions.

Entanglement pervades composite quantum systems, particularly during dissociation. Yet, quantitative studies of entanglement in chemical processes remain relatively sparse. Here, we focus on how electronic entanglement changes throughout the dissociation of the H_2 molecule. By leveraging high-quality molecular wavefunctions derived through advanced ab initio methods, we use the von Neumann entropy of the single-particle density matrix to measure entanglement.

Our goal is to correlate changes in electronic entanglement with alterations in other key physical parameters, most notably the total energy, a crucial factor in bond cleavage. Examining the energy as a function of the interatomic distance R (the reaction coordinate) sheds light on distinct molecular configurations: a united-atom model at small R and a fully dissociated state at large R. We show that not only do energy values shift between these limits, but entanglement levels also vary, reflecting the close relationship between molecular structure and quantum mechanical properties.

Focusing on H_2 dissociation, we employ advanced computational chemistry techniques. The single-particle reduced density matrix, essential for von Neumann entropy calculations and electronic entanglement assessments, was obtained via Löwdin's natural orbital-based representation. We computed high-quality correlated molecular wavefunctions using quantum chemical configuration interaction singles and doubles (QCISD) and coupled cluster singles and doubles (CCSD). These rigorous post-Hartree–Fock methods adopt a variational framework rather than a perturbative approach, ensuring reliable convergence of energy values and more accurate depictions of electronic behavior.

In modeling these wavefunctions, we employed several basis sets– including Pople's 6-31G, 6-311G, 6-311++G

TABLE I. Von Neumann entropy [Eq. (4)] and the entanglement measure [Eq. (5)] at the united-atom representation ($R \rightarrow 0$) for the dissociation process of the homo- and hetero-nuclear diatomic molecules.

Molecular case		Atomic case		
Diatomic	vN-Entropy	Atom [a] (state [b])	vN-Entropy	ξ_{vN}
H_2	0,75303	He (S)	0,75135	0,05989
He$\cdots$He	1,58560	Be (S)	1,59482	0,19930
Li_2	1,90936	C (T)	1,88976	0,11760
Cl_2	3,56883	Se (D)	3,55398	0,04247
HCl	2,94390	Ar (S)	2,94179	0,05353

[a] von Neumann entropy of the united-atom representation ($R \rightarrow 0$), [b] Entropy at the dissociated atomic state of highest multiplicity.

TABLE II. Molecular and atomic energies, von Neumann entropy [Eq. (4)] and the entanglement measure [Eq. (5)] at the asymptotic regions ($R \rightarrow \infty$) for the dissociation process of the homo- and hetero-nuclear diatomic molecules.

	Energy		von Neumann Entropy					
Diatomic	Molecule	Atom [a]	Molecule	Atom (S) [b]	Atom (D)	Atom (T)	Tendency	ξ_{vN}
H_2	-0.999625	-1	1.38627	-	0	-	$\ln 2$	0.69312
He$\cdots$He	-5.805067	-5.805066	1.44477	0.75135	-	0.696763	1.44444 [c]	0.05815
Li_2	-14.86542	-14.86544	1.32974	-	1.32971	-	1.32971 (Li) [d]	0.23113
Cl_2	-919.2805	-919.3723	2.91664	-	2.88728	-	2.88728 (Cl) [d]	0.08343
HCl	-460.1171	-460.1862	2.99586	2.95282	-	-	2.95282 (Cl^-)[e]	0.10549

[a] Atomic energy at the dissociation limit ($R \rightarrow \infty$), [b] Notation stands for S-singlet state, T-triplet state, etc., [c] Entropy sum of the dissociated atomic states of helium, [d] Entropy of the dissociated atomic state of highest multiplicity, [e] Entropy of the dissociated atomic state for the anion of chlorine.

(d,p), and Dunning's cc-pVTZ and cc-pVQZ, chosen for their well-established capability to accurately capture the electron density in chemically significant regions. All electronic structure calculations were conducted with the Gaussian 03 software. The highest level of accuracy in this study was achieved through QCISD and CCSD methods using Dunning basis sets, as demonstrated by the numerical results in Tables I and II.

To investigate how the von Neumann entropy and electronic entanglement ξ_{vN} evolve during molecular dissociation, we have recorded their values, along with corresponding molecular and atomic energies, at two limiting conditions: the united-atom representation as $R \rightarrow 0$ (Table I) and the asymptotic limit as $R \rightarrow \infty$ (Table II).

In examining electronic entanglement in the H_2 molecule, Fig. 5 demonstrates how entanglement correlates with total energy across different interatomic distances R. Once R extends beyond 2Å, signifying molecular dissociation, both entanglement and energy display similar trends. This parallel offers valuable insights into entanglement dynamics, particularly near the united-atom regime ($R \rightarrow 0$), where the system resembles a helium-like atom, and in the asymptotic limit ($R \rightarrow \infty$), where the separated hydrogen atoms effectively lose their Coulombic interactions.

In the united-atom regime, the close agreement between the computed molecular *vN*-Entropy and that of a helium-like system highlights the high accuracy of our calculations, even in the challenging $R = 0$ region. As the internuclear distance increases, *vN*-Entropy rises steadily, eventually reaching a plateau in the dissociation limit. This plateau signifies the persistence of a finite degree of electronic entanglement, even as the atoms move far apart. Table I quantifies this behavior at small R, while Table II confirms that, at large R, the system's energy approaches twice the energy of an isolated hydrogen atom– further reinforcing the presence of residual entanglement at extended separations.

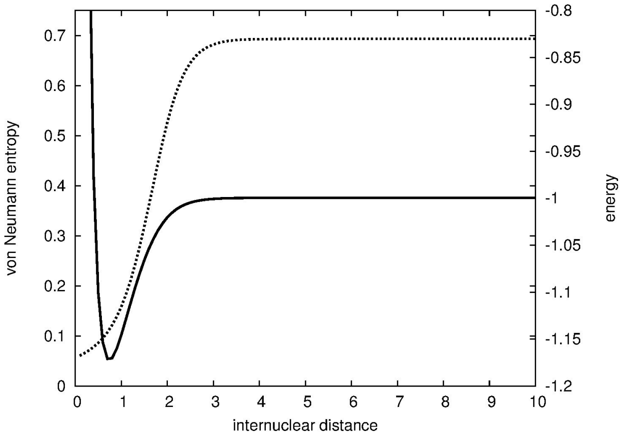

FIGURE 5. Entanglement (dotted line) and total energy (solid line) for the dissociation process of the hydrogen molecule.

An analysis of entanglement along the dissociation path of the hydrogen molecule reveals distinctive features at intermediate values of the interatomic distance. In the limit $R \to 0$ molecular entanglement diminishes, closely resembling the behavior of a unified atomic system. This decline aligns with the effectiveness of the Hartree–Fock approximation in describing atomic eigenstates, which suggests minimal entanglement in this limit. On the other hand, as $R \to \infty$ and the molecule dissociates, the entanglement behavior becomes molecule-dependent. Understanding this asymptotic behavior requires a detailed, system-specific analysis to capture the nuances of electronic interactions and their impact on entanglement. This study highlights the intricate relationship between molecular geometry, electron correlation, and quantum entanglement across the full range of the dissociation process. For the rest of the molecules (He$\cdots$He, Li_2, Cl_2 and HCl), we were able to show that the *vN*-Entropy fairly reproduces the united-atom entropy as well as the dissociated atomic species to a very large extent so as to represent the chemical features of each molecule, the mixture of states for several cases was clearly verified, as it may be observed from Tables I and II. The findings are presented in Ref. [31].

5. Concluding remarks

Entanglement is at the core of QIChem, a pervasive feature of composite quantum systems that becomes especially pronounced during dissociation, a process central to many chemical reactions. To illuminate how entanglement manifests across different electronic environments, we carried out two complementary analyses. First, using high-level configuration interaction (CI) wavefunctions for the helium isoelectronic series (nuclear charge Z = $1 - 10$), we monitored the behavior of two entanglement metrics—linear entropy and von Neumann entropy—alongside the correlation energy. All three quantities decrease smoothly as Z increases, showing that entanglement and correlation energy share a common electronic-structure origin and that, in isolated atoms, entanglement provides a quantitative gauge of electron correlation. Second, we turned to molecular systems and examined the evolution of electronic entanglement during the elementary dissociation of H_2 molecule. Employing configuration-interaction wavefunctions, we quantified entanglement with the von Neumann entropy of the single-particle density matrix and traced how it grows as the fragments separate. Together, these atomic- and molecular-scale studies demonstrate that entanglement captures the essential electron-interaction physics governing both correlation energies in tightly bound atoms and the delocalization–localization crossover that accompanies bond breaking in molecules, thereby underscoring its value as a unifying measure of electronic complexity in quantum chemistry.

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