English: Hyperfine Interactions in Lanthanide-organic Complexes for Quantum Information Processing

In this manuscript titled ”Hyperfine Interactions in Lanthanide-Organic Complexes for Quantum Information Processing,” we explore the intricate interplay between atomic physics and quantum computing, focusing on hyperfine interactions in lanthanide-organic complexes and their applications in quantum information processing. The work bridges multiple disciplines, including quantum computing, optimal control theory, nuclear structure, hyperfine interactions, f -elements, crystal field theory, and molecular magnetism.

We begin by examining the Hamiltonian of free lanthanide ions, deriving matrix elements that account for electronic structure, spin-orbit coupling, and hyperfine interactions. Utilizing hydrogen-like wavefunctions and Slater determinants, we ensure antisymmetry in multi-electron systems, adhering to the Pauli exclusion principle. The spin-orbit coupling is treated perturbatively, leading to fine- structure splitting, with matrix elements derived using angular momentum coupling schemes. Hyperfine interactions, including magnetic dipole and electric quadrupole contributions, are formulated to account for energy level splitting due to nuclear spin states, which are essential for precision spectroscopy and quantum information applications.

Transitioning to ligand field theories, we elaborate on how surrounding organic ligands influence the electronic structure of lanthanide ions in complexes. We contrast Crystal Field Theory (CFT), which models ligands as point charges, with Ligand Field Theory (LFT), which considers covalency and orbital overlap. The ligand field Hamiltonian is expressed through multipolar expansions, and matrix elements are derived using advanced angular momentum theory. Selection rules based on ligand symmetry are established, reducing the complexity of the problem. These concepts are crucial for understanding the electronic structure and spectroscopy of lanthanide-organic complexes used in quantum computing.

In exploring configuration interaction, we delve into the Judd-Ofelt theory and its generalizations, which describe electric dipole transitions in lanthanide complexes. We address how odd ligand field parameters facilitate configuration mixing between different parity states, such as $4f^n$ and $4f^{n-1}5d^1$, and how this mixing is essential for understanding the hyperfine Stark effect observed in experiments. Perturbation theory is employed to derive effective operators that account for these transitions, providing a theoretical framework for hyperfine-induced transitions in lanthanide complexes.

Relativistic corrections are addressed through the Dirac equation, providing a foundation for under- standing the hyperfine interaction and calculating hyperfine constants. We consider the finite mass, size, and magnetic characteristics of atomic nuclei, and how these nuclear properties influence the hyperfine structure in lanthanide ions. Calculations of hyperfine constants include corrections for finite nuclear charge and current distributions, using the Bohr-Weisskopf and Breit-Rosenthal corrections.

A significant portion of the work involves using electrons and muons as nuclear probes in hydrogen-like lanthanide ions, such as dysprosium. By calculating energy levels and hyperfine

constants for different isotopes and nuclear models, we demonstrate that muonic ions provide enhanced sensitivity to nuclear properties due to greater wavefunction penetration into the nucleus. Hyperfine anomalies are calculated, revealing the ability to discriminate between different nuclear models and isotopes, which is valuable

for designing qudits with desired properties.

Transitioning to quantum computing, we focus on the use of nuclear spins in lanthanide ions as qudits for quantum information processing. We provide an overview of qubits, qudits, and essential quantum concepts such as state representations, quantum gates, and critical timescales. We discuss the differences between qubits and qudits, illustrating how qudits, as d-level quantum systems, can represent more information and potentially offer advantages over qubits. The scaling of noise with the dimension of the Hilbert space is analyzed, and conditions under which qudits outperform qubits are derived.

We explore the dynamics of open quantum systems interacting with an environment under the Markovian assumption, employing the Lindblad equation to model these systems. Using perturbation theory on the Lindblad master equation, we study the effects of decoherence on quantum operations in qudits. Beyond the first-order approach, higher-order corrections are considered, revealing the nonlinearity of fidelity in open qudit systems and the necessity of accounting for these corrections in high-dimensional systems.

To address the implementation of quantum gates on nuclear spins, we employ optimal control theory to optimize gate generation and reduce gate times, thereby improving system performance. Techniques such as the rotating wave approximation, Givens rotation decomposition, and optimal control algorithms like GRAPE and MAGICARP are utilized to minimize the time and energy costs of implementing quantum gates in high-dimensional systems. These methods are crucial for overcoming the challenges associated with longer gate times and increased decoherence in qudits.

Finally, the manuscript explores the applications of the Prouhet-Thue-Morse sequence in quantum computing. This mathematical sequence is shown to have significant utility in error correction, the design of noise-resistant quantum memories, and the analysis of quantum chaos. Its properties allow for the construction of logical states that satisfy the Knill-Laflamme conditions for error detection and correction, providing robustness against certain types of errors and dephasing.

Overall, the manuscript presents a comprehensive study that bridges atomic physics and quantum computing, with a specific focus on hyperfine interactions in lanthanide-organic complexes for quantum information processing. The work provides theoretical insights into the complex interactions within these systems and practical considerations for advancing quantum computational technologies using lanthanide-based qudits.