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Estimation of Time Evolution of Muon Spin Polarization in ^{14}N and ^{15}N Systems

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ABSTRACT

In muon spin rotation and relaxation (μSR) method, time evolution of muon spin polarization provides the information about local electronic and spin dynamic states of the material. Quantum simulation and estimated frequency of the simulated spectra help to interpret the observed polarization spectra. Based on spin dipole interaction between the muon and nearby nuclei (^{14}N, ^{15}N and proton) in zero field measurement case, muon spin polarization spectra and corresponding frequencies are estimated using the quantum simulation. The oscillation frequency increases with approaching the muon towards the nuclei. Variation of separation between frequency positions with changing distance between muon and nuclei indicates the distribution of the magnetic field at the muon site. This study will help to distinguish the origin of oscillation in zero field μSR spectra in the isolated system containing ^{14}N and ^{15}N nuclei (e.g., glycine with ^{14}N, glycine with ^{15}N).

Keywords: muon; muon spin rotation and relaxation; quantum simulation; spin dipole interaction.

1. INTRODUCTION

Muon spin rotation and relaxation (μSR) method has been used to understand the life, materials, fundamental and advanced science, science beyond standard model, etc. In this method, spin polarized muons (here positive muons) incident into sample decay to positrons along the preferential direction of muon spin at the time of decay and those positrons are collected by detectors installed around the sample. Based on the time evolution of muon spin polarization, the interested properties (local electronic and spin dynamic states) of the materials can be detected [1, 2]. The nature of polarization time spectra provides the information about the behavior of muon and its states, and magnetic behavior of its surrounding in the material under the experimental environments/conditions. In zero field measurement (ZF, without any external field), the oscillation in time spectra in non-magnetic materials was reported in various samples by different groups [3-5] which is ascribed to nuclear dipole interaction between the muon and nuclei nearby the muon site. Originally, the ZF oscillation in metal fluoride crystal were explained based on dipole interaction between muon and nearby spin-one-half nuclei [3]. Similar interpretation was used to explain the oscillation in three spin-one-half system in triangular geometry in superconducting material [4] and that in collinear geometry in sodium alanate [5]. But it is difficult to interpret the oscillating ZF spectra from complex macromolecules like biosamples, if there. To interpret the μSR spectra (regardless of oscillation) from biosamples and understand the life phenomena like electron transfer in proteins [6-8], detection of molecular oxygen in biosamples [9, 10], etc., we have started systematic study (both experimentally and theoretically) from amino acids and peptide bonds. The stopping sites in amino acids - histidine, methionine [11] glycine, triglycine [12], tyrosine, tryptophan, phenylalanine [13] and N-acetylglycine-N-methylamide [14] were studied using first-principles calculations. It is found that the potential energy surface for muonium in the amino acids depends on the termination of main chain of amino acids. The stopping site for muonium in histidine was found in the aromatic side chain however the stopping site in glycine, triglycine and methionine, muon stopping site was found near O of unsaturated C=O bond in main chain. The estimation of muon site supports to understand the μSR data.

Muon is a spin half elementary particle which has mass around 207 times of electron mass and 1/9 times of proton mass. Its gyromagnetic ratio is around three times higher than that of proton which makes it more sensitive to materials. Its bound state with an electron is called as muonium which is like a light isotope of H atom with similar chemical properties. The details about μSR technique can be found everywhere [1].

In this article, the muon spin polarization function is estimated when muon stopped near nitrogen isotopes (^{14}N and ^{15}N) in the gas phase amino acids (assuming that there are no other spin-one-half nuclei around). This quantum simulation will answer the question of how the frequency of ZF spectra changes with stopping of muon at different distances from the nuclei (^{14}N, ^{15}N) and proton. It will help to understand the origin of the oscillation in ZF spectra.

2. METHOD

Spin dipole interaction between spin-polarized positive muon (spin-half particle) and nearby nuclei with nuclear spin (Fig. 1) can be derived by solving the Schrodinger equation for the Hamiltonian,

$$\widehat{H} = \sum_{i>j} \frac{\mu_0 \gamma_i \gamma_j}{4\pi |\boldsymbol{r}_{ij}|^3} \left[\boldsymbol{S}_i.\boldsymbol{S}_j - 3(\boldsymbol{S}_i.\hat{\boldsymbol{r}}_{ij})(\boldsymbol{S}_j.\hat{\boldsymbol{r}}_{ij})\right] \quad (1)$$

where i and j are used for the muon spin and nuclear spin of the nuclei, $\mathbf{r}_{ij}$ is the vector joining the spins $\mathbf{S_i}$ and $\mathbf{S_j}$. γ_i and γ_j are gyromagnetic ratio of muon and nuclei, respectively.

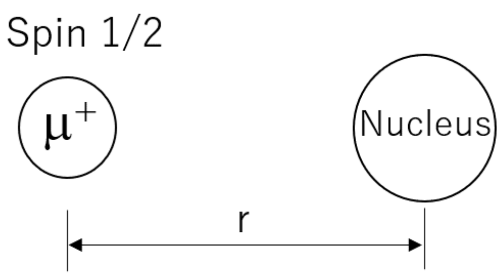

Fig. 1: Schematic diagram of muon stopped near nuclei at distance (r). Spin of muon, proton, ^{14}N and ^{15}N is 1/2, 1/2, 1 and 1/2, respectively.

The quantum simulation was performed using a Quantum code [15] which solves the time evolution of the muon spin using density matrix method. Spin evolution for muon due to its dipole interactions with nearby nuclei was estimated by solving the Hamiltonian matrix (Eq. 1) of order n (for two particle system, n = $2^2 \times 2^2$). For zero field case, using the averaged powder method along three axes, the polarization function (asymmetry) for simple model can expressed as the form of Eq. 2.

$$P(t) = \sum_i^n [A_i \cos(\omega_i t) + B_i \sin(\omega_i t)] \quad (2)$$

where A_i and B_i are coefficients of cosine and sine terms, respectively. The $\omega_i = 2\pi f_i = \frac{\mu_0 \hbar \gamma_{N_i} \gamma_\mu}{4\pi r^3}$ is precessional frequency. The μ_0 is permeability of free space, γ_μ and γ_{N_i} are gyromagnetic ratio of the muon and nearby nuclei, respectively. The r is distance between muon and nuclei N_i (Fig. 1). The values of γ_{14_N}, γ_{15_N}, γ_μ and γ_p used in simulation are 3.0776, -4.3172, 135.5 and 42.5764 MHz/T, respectively. All the coefficients of imaginary term, B_i, vanishes. The amplitudes of ω_i depends on the distance of muon from nearby H nuclei.

3. RESULTS AND DISCUSSIONS

From the solution of Schrodinger equation for two particle system, generally the polarization function (Eq. 2) contains 16 terms but in present geometry of the system, there are only four non-zero terms. So at each distance, we can observe only four frequency terms.

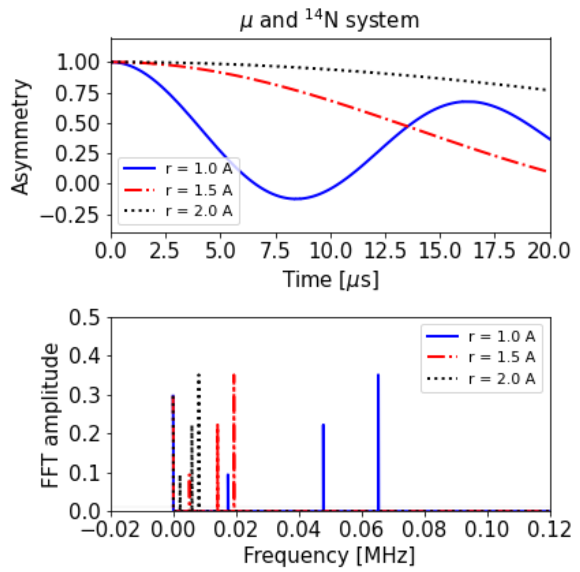

Fig. 2: Time evolution of muon spin polarization in ^{14}N system at different distances. Time spectra presented in upper panel and corresponding FFT in lower panel.

Figure 2 shows the time evolution of muon spin polarization in ^{14}N system at different distances (r = 1.0 angstrom(A), 1.5 A and 2.0 A) in upper panel and corresponding Fast Fourier Transform (FFT) in the lower panel. The initial asymmetry is normalized to 1. The oscillation frequency varies with distance of muon from the ^{14}N nuclei however the amplitudes of corresponding peaks remain consistence. The A_i and ω_i at d = 1.0 A are presented in Table 1. Similar pattern of frequency with distance is observed in time evolution of muon spin polarization in ^{15}N and proton system as shown in Fig. 3 and Fig. 4, respectively.

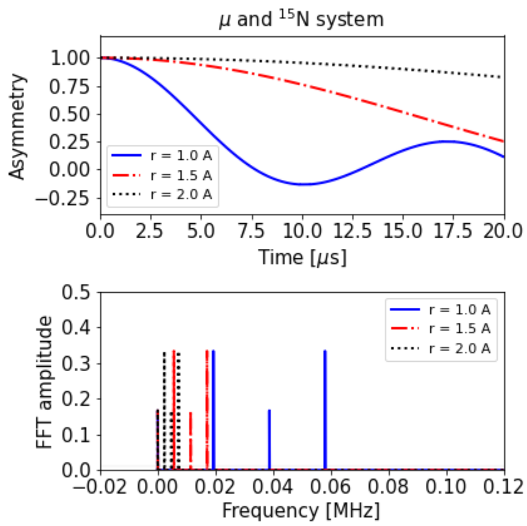

Fig. 3: Time evolution of muon spin polarization in ^{15}N system at different distances. Time spectra presented in upper panel and corresponding FFT in lower panel.

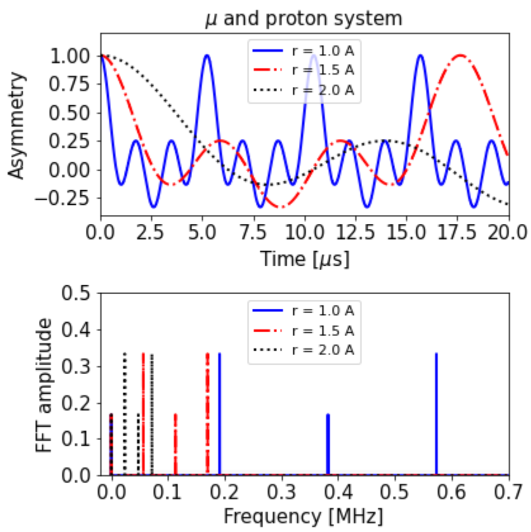

Fig. 4: Time evolution of muon spin polarization in H (proton) system at different distances. Time spectra presented in upper panel and corresponding FFT in lower panel.

Table 1: A_i and ω_i of μ–^{14}N, μ–^{15}N and μ–proton systems when muon at 1 A distance from respective nuclei.

$\mu - {}^{14}N$		$\mu - {}^{15}N$		$\mu - proton$	
A_i	ω_i	A_i	ω_i	A_i	ω_i
0.3333	0	0.1667	0	0.1667	0
0.0940	0.1101	0.3334	0.1218	0.3334	1.2009
0.2222	0.3007	0.1667	0.2435	0.1667	2.4018
0.3506	0.4108	0.3334	0.3653	0.3334	3.6028

Due to higher gyromagnetic ratio of proton with respective to ^{14}N and ^{15}N, the muon stopped near proton shows higher frequency. If the oscillation in ZF is originated from the interaction of muon with nearby hydrogen (proton), we can distinguish it from the frequency of the spectra. From above FFT, it is seen that when distance varies uniformly, the frequency separation between peaks is not uniform. For example, first peak at all distance is remains at zero however separation of, suppose, second third peak at 1.0 A, 1.5A and 2.0 A is not equal. It is obvious that the peak frequency position at zero remains consistent at same position however the peaks at higher frequency positions move differently. It may indicate the distribution of field at muon stopping site. If we observe the oscillating spectra in glycine ($C_2H_5NO_2$), then by comparing the frequency of observed spectra with estimated here, we can understand the origin of oscillation either from interaction between muon and isotopes of N or that between muon and proton.

4. CONCLUSIONS

Time evolution of muon spin polarization when muon stops nearby the spin nuclei like isotopes of nitrogen (^{14}N, ^{15}N) and proton were estimated using quantum simulation. The widening of field distribution at muon site is appeared when muon moves closer to those nuclei. It will help to understand the origin of oscillation in zero field μSR spectra from gas phase amino acids (e.g., glycine with ^{14}N, glycine with ^{15}N).

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