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MAGNETIC PROPERTY (KNIGHT SHIFT) CALCULATION OF LIQUID ALKALI METALS USING MODEL PSEUDOPOTENTIAL

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ABSTRACT

In this work, the charge density incorporated in the Model pseudopotential was used with the structure factor derived via the charged hard sphere (CHS) model to calculate Knight shift of liquid alkali metals. The calculated values are in perfect agreement with the experimental values. The results showed that the charge density and Model pseudopotential can be used effectively to predict theoretically experimental values of Knight shift of any liquid metal.

Keywords: ***Knight shift, Structure factor, Form factor, Dielectric function, Charge density, Model pseudopotential.***

1.0 INTRODUCTION

Knight [1] discovered that the nuclear magnetic resonance (NMR) of ^{63}Cu occurs at about a quarter percent higher frequency in metallic copper that in CuCl salt, this observation was named Knight shift. The Knight shift K, measures the magnetic hyperfine field at the nucleus produced by the conduction electrons which are polarized in a magnetic field. Knight shift are often dominated by the Pauli term and, in its simplest form, can be written as $K=\langle a \rangle \chi_p$. Here χ_p is the conduction electron Pauli spin susceptibility which depends on the density of states at the Fermi level, $N(E_F)$, and $\langle a \rangle$ is an average magnetic hyperfine coupling constant associated with the wave function character at the nucleus, for conduction electrons at the Fermi surface. The Knight shift therefore provides, through $\langle a \rangle$, insight into the wave-function character associated with $N(E_F)$ [2].

Knight shift serves as a powerful probe of condensed matter systems. Knight shift of metals and alloys is very important because it probes changes in electronic properties such as density of states or

wave function behaviour of conduction electrons in the vicinity of the resonant nucleus.

2.0 LITERATURE REVIEW

Previously, Bari and Jani [3] and Aditya [4] have used model pseudopotential to calculate the Knight shift of liquid metals but the results obtained are not very close to the experimental values.

Kumar and Durga [5] used Harrison's [6] first principle pseudopotential technique which is a branch of orthogonalized plane wave (OPW) formalism in conjunction with the hard sphere technique of Ashcroft and Langreth [7] to study the Knight shift of Cu-Sn alloy. The study reveals that for Cu-Sn, $(K\%)_{th}$= 0.497 against $(K\%)_A$= 0.26 and $(K\%)_B$= 0.73. The Knight shift of Cu-Sn alloy shows linear function with respect to solute concentration supporting Kaeck's [8] assumption.

Chakrabarti *et al.* [9] used Harrison's [6] first principle pseudopotential technique to study the Knight shift of the two alkali metals (sodium and potassium). The calculated values of Knight shift for sodium and potassium are 0.075% and 0.301%.

There is need to improve on previous calculated values of knight shift of liquid alkali metals. In this paper, Knight shift of liquid alkali metals will be calculated differently by using the charge density which is incorporated in the model pseudo potential proposed by Pandya *et al.*,[10] with the structure factor derived via the charged hard sphere model. The calculated values of Knight shift are in perfect agreement and very close to the experimentally determined values, the experimental values for any liquid metal can be predicted theoretically using this model potential.

3.0 AIM AND RESEARCH PROBLEMS

The aim of this work is to calculate the magnetic property (Knight shift) of liquid alkali metals using Model pseudopotential method.

Research problems: to calculate the Knight shift of liquid alkali metals in a simplified way and reduce cost of computation; to use an approach that will improve on previously calculated values of Knight shift of liquid alkali metals by other researchers.

4.0 MATERIALS AND METHOD

The material that was used in this work are Code Blocks C++ program package and computer. The model pseudo potential [10] in this work is given as:

$$W_{ion}(r) = \sum_{n=1}^{2} B_n e^{-(r/na)} \qquad r < R_c \qquad (1)$$

the Pseudopotential of the electron has this form when it is inside the core radius R_c and r is the electron distance from the nucleus.

$$W_{ion}(r) = -\frac{Z_s}{r} \qquad r > R_c \qquad (2)$$

the Pseudo potential of the electron has this form when it is outside the core radius R_c and r is the electron distance from the nucleus.

The Fourier transform of the model pseudo potential in q-space is given as:

$$W_{ion}(q)=4\pi a^3\rho\left[\frac{B_1H_1}{\left(1+a^2q^2\right)^2}+\frac{8B_2H_2}{\left(1+4a^2q^2\right)^2}\right]-\frac{4\pi Z_s\rho}{q^2}.\cos qR_c \qquad (3)$$

where Z_s, a, q, ρ are the effective number of valence electrons per atom, measure of the softness of the repulsive potential, wave vector and charge density. B_1,B_2 are coefficients of the Dirichlet series and H_1,H_2 are represented as the sum of the repulsive and the oscillatory contributions. The charge density ρ is obtained from squaring the radial wave function and the radial wave function is obtained from the solution of the Schrodinger equation in spherical polar coordinate.

$$\rho=\left|R_{nl}(r)\right|^2 \qquad (4)$$

Where $$R_{nl}(r)=-\left[\left(\frac{2Z}{na_0}\right)^3\frac{(n-l-1)!}{2n\{(n+l)!\}^3}\right]^{\frac{1}{2}}e^{-\frac{\rho}{2}}\rho^l L_{n+l}^{2l+1}(\rho)$$

where $L_{n+l}^{2l+1}(\rho), n, l, a_0, \rho$ are the associated Laguerre polynomial, principal quantum number, angular momentum quantum number, Bohr radius and unitless quantity.

$$a_0=\frac{4\pi\varepsilon_0\hbar^2}{\mu e^2}, \rho=\frac{2Zr}{na_0}$$

where $r, \varepsilon_0, \hbar, e$ are the electron distance from the nucleus, permittivity of free space, reduced Planck's constant and electronic charge.

$$B_1=\frac{Z_s}{R_c}\left[1-\frac{2a}{R_c}\right]e^{\frac{R_c}{a}}, B_2=\frac{2Z_s}{R_c}\left[\frac{a}{R_c}-1\right]e^{\frac{R_c}{2a}}$$

$$H_1=2-e^{(Y_1)\left[Y_1(1+X_1)-(1-X_1)\right]}\times\frac{\sin qR_c}{aq}+\left[2+Y_1\left(1+X_1\right)\right]\times\cos qR_c$$

$$H_2=2-e^{(Y_2)\left[Y_2(1+X_2)-(1-X_2)\right]}\times\frac{\sin qR_c}{2aq}+\left[2+Y_2\left(1+X_2\right)\right]\times\cos qR_c$$

where $X_1=a^2q^2, X_2=2^2a^2q^2, Y_1=\frac{R_c}{a}, Y_2=\frac{R_c}{2a}$

The Thomas Fermi dielectric constant [11] is used to screen the form factor in this work and given as:

$$\varepsilon(q)=1+\frac{k_o^2}{q^2}, k_o=0.815k_F\left(\frac{r_s}{a_o}\right)^{\frac{1}{2}}$$

where k_F is Thomas-Fermi wave vector

The structure factor derived via the charged hard sphere (CHS) model [12] is given as follows:

$$S(q)=\frac{S_0(q)}{\left[1+\rho\beta V(q)S_0(q)\right]} \qquad (5)$$

$$V(q)=\left[\frac{W^2(q)}{\phi(q)}\right]\left[\frac{1}{\varepsilon(q)}-1\right] \qquad (6)$$

where $\phi(q)=\frac{4\pi e^2}{q^2}$ and ε(q) is the dielectric function.

$$S_0(q)=\frac{1}{1-\rho C_0(q)} \quad (7)$$

$$\rho C_0(q)=\left(\frac{24\eta}{q^6}\right)Aq^3(\sin q-q\cos q)+Bq^2\{2q\sin q-(q^2-2)\cos q-2\}$$

$$+Cq\{(3q^2-6)\sin q-(q^2-6)\}+D\{(4q^2-24)q\sin q-(q^4-12q^2+24)\cos q+24\}$$

$$+\frac{E}{q^2-\gamma q^4\cos q}\begin{Bmatrix}6(q^4-20q^2+120)q\sin q\\-(q^6-30q^4+360q^2-720)\cos q-720\end{Bmatrix} \quad (8)$$

$$A=\frac{(1+2\eta)^2}{(1-\eta)^4}+\frac{Q^2}{4(1-\eta)^2}-\frac{(1+\eta)QK}{12\eta}-\frac{(5+\eta^2)^2}{60\eta} \quad (9)$$

$$B=6\eta M^2, C=\frac{K^2}{6}, D=\left(\frac{\eta}{2}\right)(A-K^2U), E=\frac{\eta K^2}{60}$$

$$Q=\frac{(1+2\eta)}{(1-\eta)}\left[1-\left\{\frac{1+2(1-\eta)^3K}{(1+2\eta)^2}\right\}^{1/2}\right]$$

$$M=\frac{Q^2}{24\eta}-\frac{(1+0.5\eta)}{(1-\eta)^2}, U=\frac{(1+\eta-\eta^2/5)}{12\eta}-\frac{(1-\eta)Q}{12\eta K} \quad (10)$$

Where $K=(24\eta\gamma)^{1/2}$ and $\gamma=\beta\left(\frac{Ze^2}{\varepsilon_0\sigma}\right)$

The dielectric function that will be used is that of the modified Hartree ε(q) and with the static dielectric function $\varepsilon_H(q)$ given as follows:

$$\varepsilon(q)=1+[1-f(q)][\varepsilon_H(q)-1] \quad (11)$$

$$\varepsilon_H(q)=1+\frac{me^2}{2\pi h^2k_FY^2}\left[1+\frac{(1-Y^2)}{2Y}\ln\left|\frac{1+Y}{1-Y}\right|\right]$$

where m is the ionic mass, h is Planck's constant, e is the electronic charge and Y=$\frac{q}{2k_F}$ or q.

The local field correction $f(q)$ due to Taylor [13] is used to incorporate the exchange and correlation among the conduction electrons in the dielectric screening and is given as:

$$f(q)=\frac{q^2}{4k^2{}_F}\left[1+\frac{0.1534}{\pi k_F}\right] \quad (12)$$

The Knight shift of liquid metals [14-16] given as:

$$K=\left(\frac{8\pi}{3}\right)\chi_p\frac{\gamma^2}{\beta}\left[1+2Z\int_0^\infty S(q)W(q)\left(\frac{q}{2K_F}\right)\ln\left|\frac{q+2K_F}{q-2K_F}\right|d\left(\frac{q}{2K_F}\right)\right] \quad (13)$$

where γ is an orthogonalization factor, β is a normalization factor taken to be unity. $S(q)$ is the structure factor and $W(q)$ is the screened form factor, χ_p is the conduction electron spin susceptibility, k_F is the Fermi wave vector and q is the wave vector.

5.0 RESULT AND DISCUSSION

The input parameters used in the calculation are given in Table 1 and the comparison between the calculated values of Knight shift of liquid alkali metals in this work and others previously calculated with the experimental values of Knight shift of liquid alkali metals are given in Table 2. The experimental values of Knight shift gotten from Seymour [17].

From table 2 the calculated Knight shift values in this work are in perfect agreement with the experimentally determined values and have a higher accuracy when compared with Bari and Jani, and Aditya values of Knight shift. The values of Knight shift increases from Li to Cs; in turn this means that the higher the charge density the lower the value of Knight shift and vice versa (since Li has the highest charge density among the alkali metals).

Table 1. Input Parameters Used in the Calculation of Knight Shift

Metals	Z	$X_p(x10^{-5})$	Υ^2	S(q)(a.u)	W(q)(a.u)	K_f(a.u)	r_c (a.u)
Li	1	5.000	66	0.0013	-7.64	0.58	1.66
Na	1	7.950	176	0.0009	-13.65	0.48	2.00
K	1	6.500	490	0.0006	-20.08	0.39	2.48
Rb	1	8.150	994	0.0014	-29.72	0.36	2.65
Cs	1	10.905	1620	0.0020	-32.46	0.33	2.87

Table 2: Comparing calculated values with Bari and Jani, Aditya and experimental values of Knight shift

Metals	Present work (K%)	Experimental value	Bari and Jani (K%)	Aditya (K%)
Li	0.027	0.026	0.0274	0.030
Na	0.115	0.116	0.1146	0.185
K	0.264	0.265	0.2399	0.252
Rb	0.663	0.662	0.5743	0.630
Cs	1.439	1.440	1.3416	1.037

6.0 CONCLUSION

From the result obtained it showed that the charge density incorporated in the model pseudo potential used in this work gave values that are in perfect agreement and very close to the experimental values of Knight shift of liquid alkali metals. The charge density can be effectively used to determine the variation of Knight shift across the liquid metals. This Model pseudopotential has improved previous results obtained and as a result can be used to predict theoretically experimental values of Knight shift of any liquid metal.

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