Study of Variation of Superconducting Transition Temperature With Electron-Phonon Coupling And Coulomb Pseudo Potential in Alkali Metals Using Orthogonalised Plane Wave Pseudopotential method.

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ABSTRACT

By using Orthogonalised Plane Wave Pseudopotential we studied variation of superconducting transition temperature T_c with electron-phonon coupling (λ) and Coulomb Pseudopotential (μ^*) of alkali metals. Unique opportunity taken to this method to investigate alkali metal for the purpose. Although the superconducting properties of the alkali metals are highly anomalous, these properties can still be understood within a conventional BCS framework where the electron pairing arises through the electron phonon interaction.

***Key words**: OPW, Pseudopotential, Superconductivity, Transition Temperature, Alkali Metals, Electron-Phonon Coupling*

I. INTRODUCTION

Superconductivity is a state of metals below a certain critical temperature [1]. Superconductivity has completed a fascinating long Journey of more than hundred years since it was discovered by Kamerlingh Onnes in 1911 in Hg [2]. It became a rare example among the numerous scientific developments of the twentieth century where the inventive excitement of invention has not just been retained but indeed has continued to grow so long after the original event. The backbone of this journey is a series of spectacular, completely unanticipated experimental discoveries and each of new invention brings up a new twist leading to a new challenge. This phenomenon is not fully understood till date and we have a large number of unresolved questions; thus one would find themselves with numerous possible avenues of study for a superconducting state.

BCS theory, extended to take into account the fact that the effective interaction between electrons mediated by phonons is believed to describe the superconductivity of all elements at ambient pressure, and of thousands of superconducting compounds. In 1976 Roberts [3] lists several tens of thousands of superconducting alloys and compounds, almost all with critical temperatures below 20K, believed to be described by BCS theory.

Cs was reported as, first alkali metal with superconducting properties under high pressure J. Wittig; W. Buckel and W. Weber [4]. A. Rodriguez-Prieto and A. Bergara, [5] in the proceedings of the Joint 20th AIRAPT - 43rd EHPRG Meeting, June 27 - July 1, 2005 in Karlsruhe, Germany, proposed that these two results, that Li becomes superconducting under pressure and that Tc increases rapidly with pressure, are quite remarkable and confirm that at elevated densities the electronic structure of Li deviates markedly from that of a free electron gas, the anticipated Fermi surface becoming highly non-spherical.

Alkali metals became attention-grabbing systems and studied by employing different techniques especially for its role in superconductivity – one of its most fascinating property.

II. METHODOLOGY :

Orthogonalzed Plane Waves (OPW) were introduced by Herring [6] in 1940; the method enabled first quantitative calculations of materials properties in 1959 [7]. Very general approach for construction of basis functions for valence states: exploits the idea that core states and valence states are essentially distinct and can be separated.

The Pseudopotential method [8, 10] is one of the simplest tools to study various physical and chemical properties of materials. The use of Pseudopotentials [10, 11, 12], in conjunction with plane waves, can dramatically reduce the magnitude of this problem. To realize the objective to investigate Variation of Superconducting Transition Temperature (T_c) With Electron-Phonon Coupling (λ) And Coulomb Pseudo Potential (μ^*) in Alkali Metals, Here, the formulation will be based on the Orthogonalized Plane Wave (OPW) Pseudopotential method. The Orthogonalised Plane Wave (OPW) method proposed by Harrison [11] in 1966 has been termed as Harrison's First Principle (HFP) pseudopotential technique and is used in our earlier work [13].

The First principle method expanded the states in Orthogonalised Plane Waves, plane waves with terms added to make them orthogonal to the core state, as the true band state must be. The matrix elements of the pseudopotential were defined to be the matrix elements of the Hamiltonion between the OPW's.

The present form of OPW is mainly due to the work of Philips and Kleinmann[11], Antoncick [14], Harrison [8, 15-20] and by Cohen and his co-workers [21-23].

a. MCMILLAN FORMULISM FOR TRANSITION TEMPERATURE (T_c)

The study of the relation between microscopic theory and observed superconducting transition temperature T_c was made by McMillan [24] on the basis of the famous gap equations given by Eliashberg [25], which are extensions of original BCS theory of Bardeen-Cooper-Schrieffer [26].

Eliasberg theory makes use of –

i. Coulomb repulsion μ given as–

$$\mu = N_f(0)|V_c| \tag{1}$$

where

$N_f(0)$ is single spin density of electronic states at Fermi surface.

ii. Electron-Phonon spectral function $\alpha^2(\omega)\, F(\omega)$ defined as–

$$\alpha^2(\omega)\, F(\omega) = N_f(0)\frac{\sum_{kk'}|M_{kk'}|^2\delta(\omega-\omega_q)\delta(\varepsilon_k)\delta(\varepsilon_{k'})}{\sum_{kk'}\delta(\varepsilon_k)\delta(\varepsilon_{k'})} \tag{2}$$

where

ω_q is phonon energy

ε_k is electron energy

q runs over wave number for phonons and $\vec{q} = \vec{k} - \vec{k'}$

k runs over band quantum number for electrons

$M_{kk'}$ is electron-photon coupling the matrix element

δ functions restricts the electrons to the Fermi surface

Using the above parameters

i. Zero-temperature Eliasberg theory determines the complex energy gap function $\Delta(\omega)$, and
ii. Finite-temperature Eliasberg theory determines the transition temperature T_c .

McMillan's [24] find T_c from the solution of the Finite-temperature Eliasberg theory, or more precisely, obtain approximate equation relating T_c to a small number of simple parameter.

By inverting Zero-temperature and thus using tunnelling conductance Eliasberg theory McMillan and Rowell [27] determine $\alpha^2(\omega)\, F(\omega)$and μ^*. T_c was determined from the interaction parameters $\alpha^2(\omega)\, F(\omega)$ and μ^*. Because the gap $\Delta(\omega)$ vanishes at T_c , this becomes a linear equation for infinitesimal function $\Delta(\omega)$. The condition that a nonzero solution exists determines the value of T_c .

The formula for superconducting transition temperature as a function of coupling constants for the electron-phonon and Coulomb interactions with an accuracy of ~1% was derived as –

$$T_c = \frac{\Theta_D}{1.45}\, exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\,\lambda)}\right] \tag{3}$$

McMillan used this Debye Θ for characteristic phonon frequency.

Dyne in 1972 introduced $\frac{\langle\omega\rangle}{1.20}$ in place of $\frac{\Theta_D}{1.45}$ and rewrites the equation as-

$$T_c = \frac{\langle\omega\rangle}{1.20}\, exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\,\lambda)}\right] \tag{4}$$

The formulation of McMillan has been re-analysed, particularly for the case of strong coupling superconductors, by Allen and Dynes [28], Nowotny [29] and Leavens [30].

III. COMPUTATION

Equation (4) is used in our present work for calculation of T_c of alkali metals. V-S form of screening observed to be most suitable for incorporating exchange and correlation effects [31-35] In our present investigation Vashishta – Singwi [36] form of screening is used with three different forms of eigenvalues of Herman-Skillman (HS)[37], Hafner (H)[38] and Clementi (C)[39].

we would like to emphasize the importance of involving a precise form for the pseudopotential. It must be acknowledged that although the eff ect of pseudopotential in strong coupling superconductor is large, yet it plays a decisive role in weak coupling superconductors i.e. those substances which are at the boundary dividing the superconducting and non-superconducting region. In other words, a small variation in the value of electron–ion interaction may lead to an abrupt change in the superconducting properties of the material under consideration.

In January 2018 impact of eigen values on λ is studied in earlier paper [40] and observed that with choice of appropriate eigenvalue SSP of alkali metal is reasonably reproducible by OPW pseudopotential.

b. Variation of T_c with λ of alkali metals:

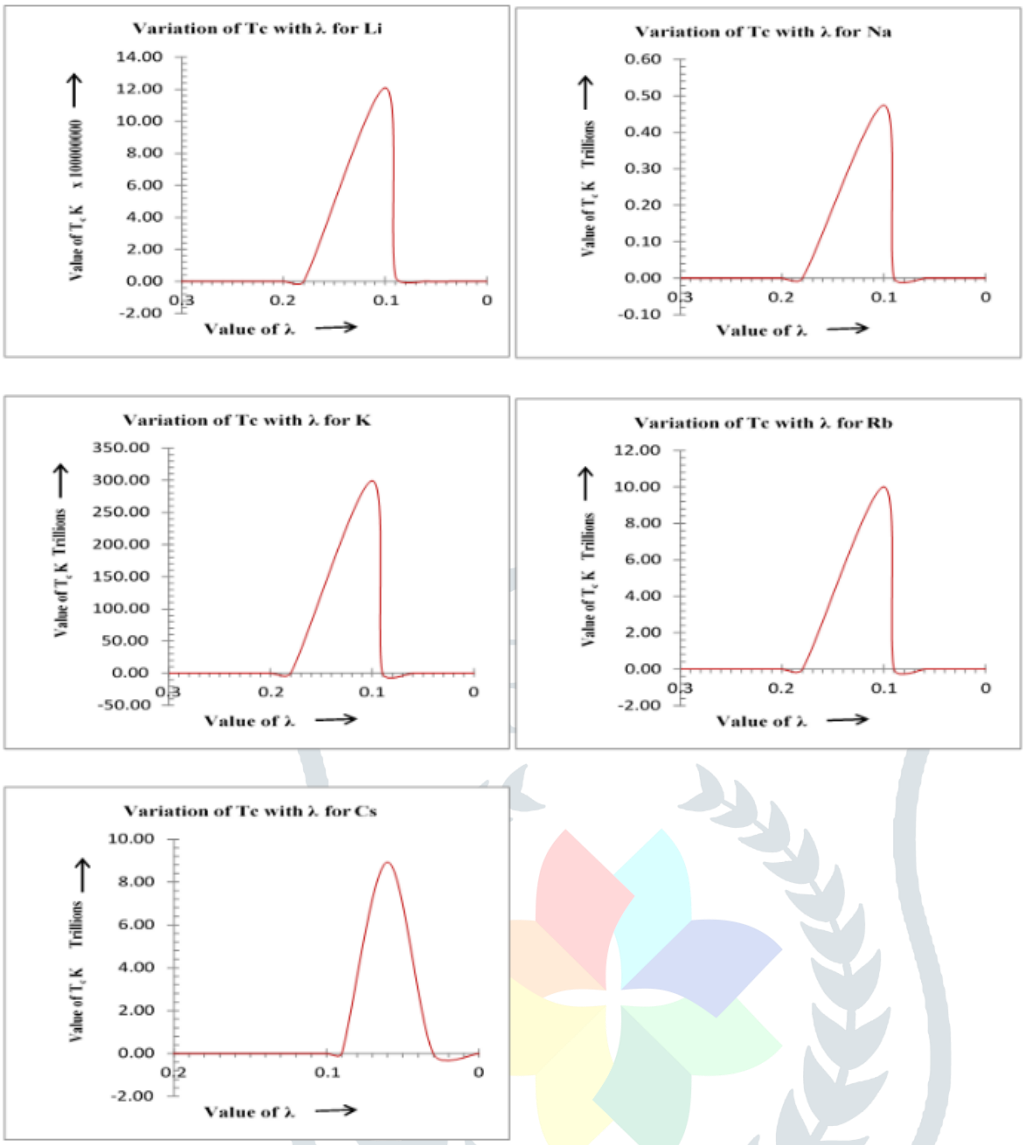

Fig 1: Variation of Tc of alkali metals with λ.

we have plotted variation of T_c with λ is plotted in figure 1 above. A steep increase in Tc for 0.18> λ > 0.09 in case of Li, Na, K and Rb is recorded. whereas Cs shows similar trend for 0.09> λ > 0.03.

Computed percentile influence of the various local field correction functions with respect to the V-S screening function on the Coulomb pseudopotential μ*, is tabulated in the Tables 1 below –

Table-1

μ* VS	μ*HS	μ*HS (%VS)	μ*H	μ*H (%VS)	μ*KL	μ*KL (%VS)
0.14132	0.13386	95%	0.14551	103%	0.13388	95%
0.13103	0.12289	94%	0.13507	103%	0.12990	99%
0.12396	0.11560	93%	0.12739	103%	0.12196	98%
0.12700	0.11771	93%	0.13033	103%	0.12425	98%
0.12697	0.11880	94%	0.13005	102%	0.12470	98%

Exchange correlation function of four different types Kleinmann-Langreth[41] , Vashishta–Singwi [36], Hubbard-Sham [42] and Shaw [43] are used in computation of μ^*.

c. Variation of T_c with μ^* of alkali metals:

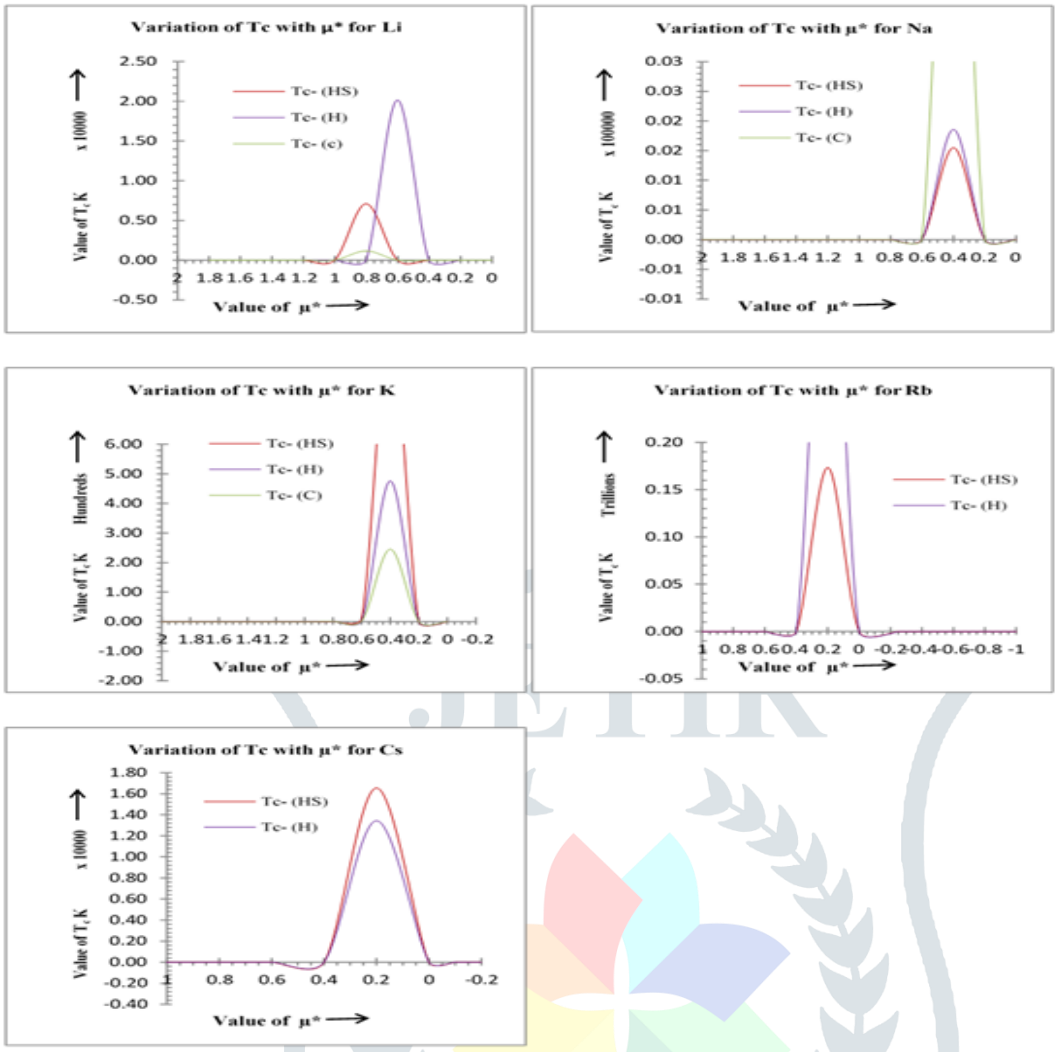

Fig 2: Variation of Tc of alkali metals with μ*

Figure 2, above, graphically elucidates the variation of Tc of alkali metals with Coulomb pseudopotential μ* . Local field correction functions of V-S form is used with three different forms of eigenvalues of Herman-Skillman (HS), Hafner (H) and Clementi (C).

IV. DISCUSSION AND RESULT:

We observe steep increase in Tc for 0.18> λ > 0.09 in case of Li, Na, K and Rb. whereas Cs shows similar trend for 0.09> λ > 0.03. Also

We observe that Tc shoots up in case of Li for the range 1 > μ* > 0.6 (with eigenvalues of HS &C) and 1> μ* > 0.6 (with eigenvalues of H), Na and K shows similar trend for 0.6 > μ* > 0.2 whereas similar shoots up in case of Rb and Cs is observed for 0.4 > μ* > 0 for all the three sets of eigenvalues.

The values of λ and Tc shows an appreciable dependence on the local-field correction functions, whereas for μ* a weak dependence is observed.

Our results are assenting to theoretical and experimental work on the subject in past. Thus, applicability of OPW pseudopotential technique and McMillan's formalism in study of SSP of binary alloys is also established from our present work. However, in the absence of experimental data, the presently computed values may be considered to form reliable data set, as their values are within the theoretical limits of the McMillan formulation. The comparison of presently computed results of the SSP with available experimental findings as well as with the theoretical work of other scholars by using different technique is highly encouraging, which confirms the applicability of the OPW pseudopotential method and V-S forms of the local-field correction and exchange functions is use in our present work reason because it satisfies the compressibility sum rule and

provides a better inter-ionic potential. V-S form of exchange correlation has been also examined by other researcher S. M. Rafique [31], J. Yadav et al. [32], J. Yadav et al. [33], S. K. Chakrabarti [34] and S. K. Chowdhary et al [35] with different-different superconducting systems. I believe a convincing outcome is presented leading some important insights. Also, in scarce of data for SSP of alkali metals our results and observed features might enrich data-sets for use in future research. Still, there is certainly much left to do.

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