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The Comparative Study of Superconducting State Parameters for Noble Metals Using Non Local Pseudopotentials

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Abstract - *In the present study, theoretical computations of superconducting state parameters [Electron Phonon coupling strength (λ), Coulomb pseudopotential (μ*), Transition temperature (Tc), Isotope effect exponent (α) and Effective interaction strength (N_0V)] have been carried out using first principles pseudopotentials for noble metals. The two sets of non local pseudopotentials, obtained with Kohn-Sham and Lindgren approximations for conduction band-core exchange are used, while exchange due to conduction electrons are studied through Hubbard and Singwi exchange-correlation functions respectively. The present study confirms that Lindgren approximation is more effective than Kohn-Sham approximation for the computation of physical properties based on form factors and energy wave number characteristic [F(q)] particularly at small q (q<2kf), which is in agreement with assertion made by Moriarty.*

Keywords: *First principle pseudopotentials, superconducting state parameters, noble metals.*

I. Introduction

In the past as well as in the recent years, local and nonlocal pseudopotentials are used as one of the most powerful techniques to study many physical properties of metals, liquid metals, alloys and metallic glasses [1]-[4]. The pseudopotential theory is found to be very easy conceptually and less complicated computationally, at the same time it generates good results which are comparable with those generated by lengthy, tedious and computationally complicated first principle methods. Recently, it has also been observed that, the pseudopotential theory (local and nonlocal) is also applied to complex state of the matter-superconductivity with good degree of success [5], [6]. In the last decades, it has been observed that using BCS theory and McMillan formalism SSPs are studied with different forms of local pseudopotentials. It has been observed that the philosophies involved in the determination of pseudopotential parameters, are different. It has been also found that different forms of exchange and correlation are involved in computation without noticing their effects, on pseudopotential form factors for $q \leq 2k_f$, which is important region for study of SSPs [5], [6]. In our opinion, such studies are not sufficient because they do not explain, which form of exchange and correlation is used for conduction electron, is proper. The validity of any pseudopotential form factors can be judged by its ability to predict not only the high q dependent properties but also the physical properties computed with the help of form factors depending on the low value of q. The study of superconductivity requires form factors for the low value of q (particularly, $q \leq 2k_f$).

The main objective of the present study is to throw some light in this area. The system we have selected for the study of superconducting state parameters (SSPs) [Electron Phonon coupling strength (λ), Coulomb pseudopotential (μ*), Transition temperature (Tc), Isotope effect exponent (α) and Effective interaction strength (N_0V)]. In case of transition metals (Noble metals) of the periodic table, treatment of the d- electrons complicates the picture in comparison with simple metals. During

literature serve, we observed that, the comprehensive study of properties of transition metals (static, dynamic and electronic) using local and nonlocal pseudopotentials is very rare. The main reasons for above facts are as follows:

Local model pseudopotentials are very easy at the same time require a lot of adjustable parameters in comparison with first principle or nonlocal pseudopotentials [1], [2].

In the present communication, we use nonlocal pseudopotentials due to Moriarty, to compute SSPs. The philosophy involved, in the computation of nonlocal pseudopotentials for noble metals by Moriarty is different, particularly, for the conduction band core exchange potential and free electron exchange approximation [7], [8].

Present paper is organized as follows:

In section-2, we describe theory for calculating SSPs with necessary expressions. Section-3 is devoted for results and discussion. Finally, we conclude our paper with some concluding remarks.

I.1. Theory

In the present study, we have used non local pseudopotential due to Moriarty [7], [8].

The non-local pseudopotential is given by,

$$\langle k+q|w|k\rangle = \langle k+q|w_0|k\rangle + \sum_d \frac{\langle k+q|V_d|V_d|k\rangle}{(k^2-E_d)} \quad (1)$$

The electron-phonon coupling strength λ is computed using [5]

$$\lambda = \frac{12m^*Z^*}{M\langle\omega^2\rangle}\int_0^1 x^3\,[V(x)]^2\,dx \quad (2)$$

In above equation, m* is effective mass, M is mass of ion, $x=q/k_f$, where k_f is the Fermi wave vector, V(x) is a screened pseudopotential form factors and $\langle w^2\rangle$ is an averaged square of phonon frequency.

There are two ways to find $\langle w^2\rangle$,

(1) $\langle w^2\rangle = (w_L^2+w_T^2)/2$

(2) $\langle w^2\rangle = (k_B\Theta_D)^2$. Where, k_B is Boltzmann constant and Θ_D is Debye temperature at zero degree K. In the present calculation, we have used 2nd approach.

Coulomb pseudopotential is given by [5],

$$\mu^* = \mu/(1+\mu \ln k_f^2/k_s^2\Theta_D) \quad (3)$$

Where, μ is taken from Gajjar et al [5].

Transition temperature [5],

$$Tc = \frac{\Theta_D}{1.45}\exp\left[\frac{-1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right] \quad (4)$$

Isotope effect exponent [5],

$$\alpha = \frac{1}{2}\left[1-\left(\mu^*\ln\frac{\Theta_D}{1.45Tc}\right)^2\frac{1+0.62\lambda}{1.04(1+\lambda)}\right] \quad (5)$$

Effective interaction strength [5],

$$N_0V = \frac{\lambda-\mu^*}{1+\frac{12}{11}\lambda} \quad (6)$$

II. Results and Discussions

TABLE

SUPERCONDUCTING STATE PARAMETERS FOR NOBLE METALS:

Metals	SSPs	Model-1	Model-2	Others
Cu	λ	0.2886	0.1824	0.20
	μ*	0.1209	0.12097	0.10
	α	0.4922	0.4924	
	NoV	0.1328	0.0527	-0.20
Ag	λ	0.1585	0.09025	
	μ*	0.0702	0.0702	
	α	0.4975	0.4975	
	NoV	0.0772	0.2444	
Au	λ	0.3775	0.2373	
	μ*	0.0666	0.0666	
	α	0.4976	0.4977	
	NoV	0.2315	0.1404	

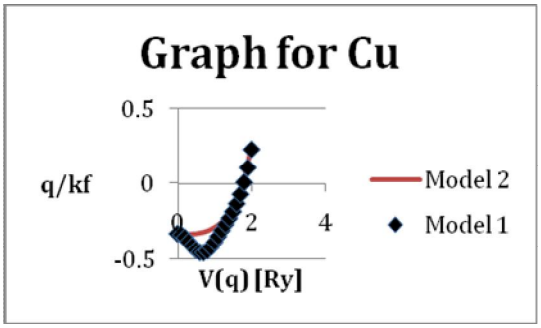

Fig. 1 Comparison of non local pseudopotential form factors for Cu.

The dotted and continuous lines represent results of Model 1 and Model 2 respectively.

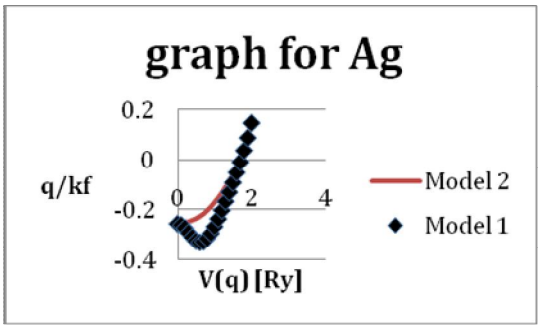

Fig. 2 Same as fig.1 for Ag.

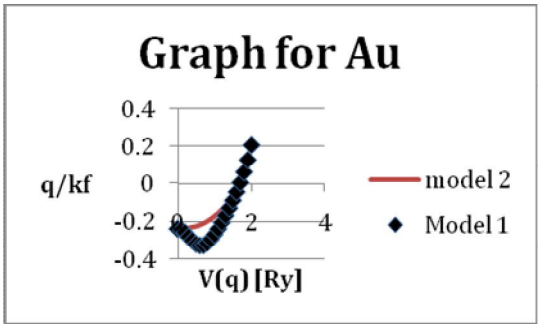

Fig. 3 Same as fig.1 for Au.

Moriarty [7], [8] has computed pseudopotential form factors using generalized pseudopotential theory. The quantities, which are required to calculate form factors, are calculated using 1st principle calculations. He has also computed resonance of d- position, using 1st principles and hybridization potential and ordinary potentials are computed using non local approach. The main difference in two sets of non local potentials is regarding the use of conduction band- core exchange potential and exchange due to conduction electrons. Non local form factors are plotted for Cu, Ag and Au in fig. 1, 2 and 3 respectively. He has used Kohn sham approximation and Hubbard forms of exchange and correlations. In all graphs, dotted lines show the behavior of the non local pseudopotentials computed by using Kohn-Sham approximations for conduction band-core exchange and exchange due to conduction electrons through Hubbard (we refer it as a Model-1), while continuous lines show the same, obtained by using Lindgren approximations for conduction band-core exchange and exchange due to conduction electrons through Singwi (Model-2). It is clear from all such graphs that 1st zero of both the potentials in case of all the metals are different, it is quite interesting to note that for low q region their values are differing appreciably. The computed results of SSPs due to both the potentials are displayed in table-1. It is interesting to note here all parameters, computed by two sets of form factors, are different. It is so because the 1st zero of both the pseudopotentials are different as well as their values for lower values for q are different, which has serious impact in the calculation of SSPs. Such effect has not been rigorously studied and pointed out in all previous studies. In our view, the conduction-core exchange and exchange due to conduction electrons are playing vital role in the computation of physical properties based on two different regions ($q \leq 2k_f$ and $q > 2k_f$). We must think to carry out the study with functions which works equally good in both the regions. The computed results for Cu are compared with [9] and we find that the non local pseudopotentials with Lindgren approximation for core potential generate results close to the results obtained using local pseudopotentials.

III. Conclusion

The present study supports the conclusion drawn by Moriarty that the difference between form factors calculated by using Kohn Sham and Lindgren free electron exchange approximation is fairly large at small q, but as q tends to $2k_f$ difference disappears. Thus it has serious effects on the calculation of physical properties depending on q ($q \leq 2k_f$). The reason behind this is Kohn sham potential did not depend sensitively upon metrics element or F(q) at small q. Thus, Lindgren approximation shows an improvement over the Kohn sham exchange. Looking to the success of the present approach, we would like to extend it for the study of SSPs for noble metal alloys and oxides using non local Pseudopotentials. Results are quite encouraging and will be published elsewhere.

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Author's Profile

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