Impact of Fermi energy of liquid alkali metals (Li and Na) due to temperature variation.

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Abstract: In the present paper we have studied the temperature dependence of Fermi energy of simple liquid metals through the Harrison's first principle (HFP) pseudopotential technique. The structure factor needed for liquid metals has been taken from experimental measurements [X-ray and neutron diffraction].

The results have been compared with experimental data and theoretical values of other authors. Reasonable agreement has been obtained.

Key words: Fermi energy, pseudopotential and liquid alkali metals.

Introduction

Numerous calculation have been performed in the past decades for the band structure of metals using a variety of methods based on APW (augmented plane wave) and OPW (orthogonalised plane wave) method. A study of literature reveals that the Harrison's first principle method which is basically an OPW method has scarcely been used for the purpose except by Thakur (1980,a,b) and Singh (1988). Hence, we have persued this investigation with suitable choice of form factor $w(\mathbf{k},\mathbf{q})$ and structure factor $a(q)$.

Formalism

In the framework of conventional perturbation theory, the energy of a liquid metal is expressed as, [Harrison (1966)]

$$E(k)=\frac{\hbar^2k^2}{2m}+\langle\mathbf{k}|W|\mathbf{k}\rangle + \frac{2m}{\hbar^2}\sum_{q}{}'\frac{a(q)\left|N\langle\mathbf{k}+\mathbf{q}|w|\mathbf{k}\rangle\right|^2}{\left(|\mathbf{k}|^2-|\mathbf{k}+\mathbf{q}|^2\right)} \quad (1)$$

$a(q)$ is the liquid structure factor and is non-zero for a liquid. $\langle\mathbf{k}|W|\mathbf{k}\rangle$ are the matrix element for the crystal potential W. $N\langle\mathbf{k}+\mathbf{q}|w|\mathbf{k}\rangle$ are the screened form factor which we will assume to be local after evaluating the same at $k=k_F$ as done in pervious chapter and denoted by $w(q)$, m is the electronic mass and $\hbar=h/2\pi$, where h is the Planck's constant.

At the melting point, the above expression reduces to (Schneider and Stoll, 1967),

$$E(k) = \frac{\hbar^2 k^2}{2m} + \frac{2m}{\hbar^2}\sum_q^1 \frac{a(q)w^2(q)}{k^2 - |\mathbf{k}+\mathbf{q}|^2} - \frac{a(q)w^2(q)}{q^2} \qquad (2)$$

Replacing $\sum_q$ by $\frac{\Omega_0}{8\pi^3}\int d^3q$ and putting $k = k_F$, we obtain for the energy at the Fermi level,

$$E(k_F) = \frac{\hbar^2 k_F^2}{2m} + \Delta(k_F) - \Delta(0) \qquad (3)$$

where,

$$\Delta(k_F) = -\frac{m}{4\pi^2\hbar^2 k_F n} \int_0^\infty qa(q)w^2(q)\ln\left|\frac{2k_F+q}{2k_F-q}\right| dq$$

and $$\Delta(0) = \frac{m}{4\pi^2\hbar^2 n}\int_0^\infty a(q)w^2(q)dq \qquad (4)$$

Here n ($=\frac{1}{\Omega_0}$; Ω_0 is the atomic volume) is the number of atoms per unit volume related to the Fermi wave number k_F and valence Z by the relation,

$$n = \frac{k_F^3}{3\pi^2 Z} \qquad (5)$$

Here it has been assumed that $a(q)$ and $w(q)$ are isotropic.

Computation and Result

The Fermi energy $E(k_F)$ has been computed through equations (3). The computed result of the present computation has been given in Table 1 alongwith the computed result of pervious authors and the free electron data for comparison. The Fermi energy has been expressed in unit of $10^{-12} erg$, k_F is expressed as $A^{0^{-1}}$.

A perusal of Table 1 brings out the fact that the computed Fermi energy are in reasonable agreement with the results of pervious authors as well as with free electron Fermi energy. The Fermi energy $E(k_F)$ of the alkali metals has been theoretically investigated in this paper. As the previous data of these quantities are only for the higher temperature have been estimated for comparison. It has been observed through Table 1 that

the Fermi energies for the alkali metals computed by us are in fair agreement with the previous data and with the free electron Fermi energy E_F^0.

Temperature dependence

The temperature dependence of the Fermi energy $E(k_F)$ has been shown in Figs. 1 and 2 for **Li and Na** respectively. Qualitative agreement has been obtained in general.

Table-1

Computed Fermi energy of liquid metals (10^{-12} erg) and k_F ($A^{0^{-1}}$) with other theoretical and experimental data.

Metal Temp. (^{0}C)	k_F $A^{0^{-1}}$	$\in_{nl}$	$E(k_F)$ Present value	E^0_F Free electron Fermi energy	Schneider and stoll (1967)	Thakur (1980)
Li						
170	1.0926	H	7.8457	7.3238	-	7.3643
		C	7.9584	-	-	-
250	1.0514	H	7.7894	7.2789	-	-
		C	7.6584	-	-	-
Na						
105	0.8456	H	5.3354	4.9412	-	4.8493
		C	5.4857	-	-	-
200	0.8378	H	5.2145	4.8952	-	-
		C	5.2586	-	-	-

Temperature dependence of Fermi energy of Li

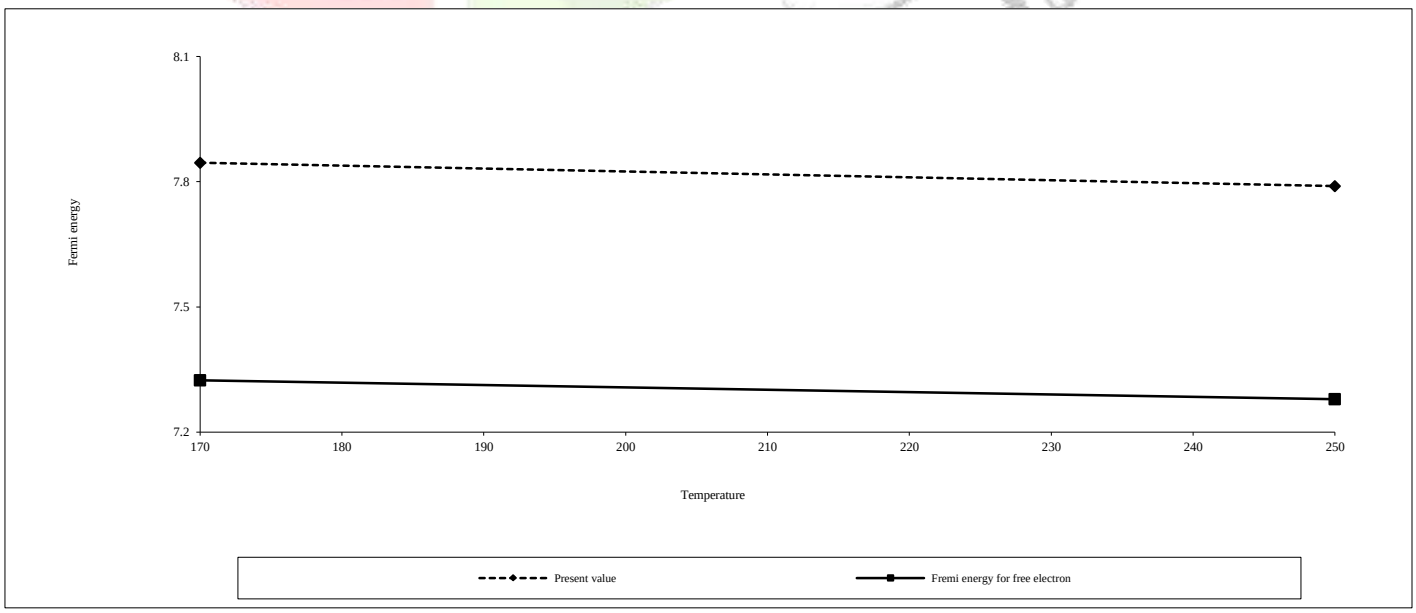

Fig.1

Temperature dependence of Fermi energy of Na

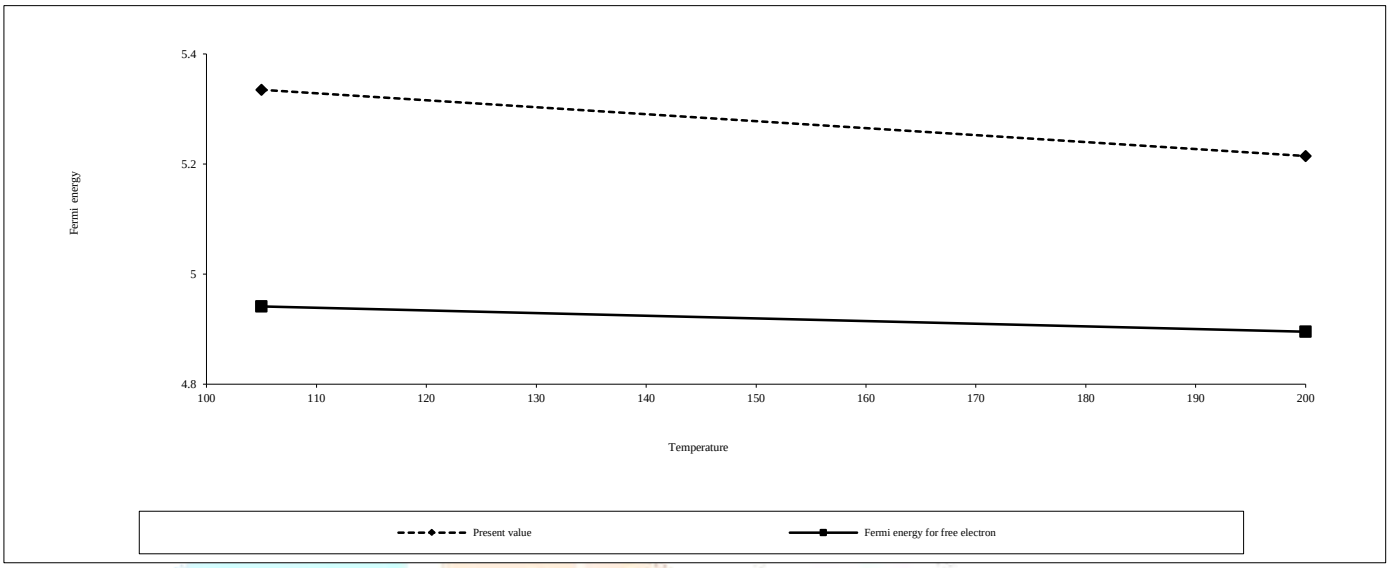

Fig. 2

Conclusion

From the above mentioned facts it may be concluded that the HFP technique can be successfully used for the computation of the **Fermi energy** of liquid metals provided suitable input parameters are used. However, as various approximations are involved within the framework exact reproduction of the experimental data is neither expected nor desired.

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