Thermodynamic properties of fermionic systems (Sodium, Potassium and Lithium): Isothermal compressibility and magnetic susceptibility as a function of Landau parameters

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Abstract

Isothermal compressibility and magnetic susceptibility are thermodynamic properties (response functions) that characterize the behavior of materials subjected to changes in pressure and magnetic field. These thermodynamic properties can be expressed in terms of Landau parameters. The Landau parameters depend on the interaction between the particles in the system and can be calculated from Fermi liquid theory. The first term in this series, F_0^(s,a), is the most important for describing the thermodynamic properties of fermionic systems at low temperatures and moderate densities. However, for denser systems or at higher temperatures, the higher order terms, F_1^(s,a), and F_2^(s,a), can have a significant influence on the behavior of the system and modify predictions based on F_0^(s,a) alone. The results of the theoretical model were used to determine the thermodynamic properties of sodium (Na), potassium (K) and lithium (Li) and compare with experimental results reported by other authors. It was shown that the isothermal compressibility of sodium (Na) is 1.45 and potassium (K) is 1.08, while the magnetic susceptibility of sodium (Na) is 1.58 and potassium (K) is 1.83. and of lithium (Li) is 3.33.

Keywords*:* Isothermal compressibility; magnetic susceptibility; Landau parameters.

1. Introduction

Thermodynamics, as a part of physics, deals with studying energy transformations and the laws governing them. Within thermodynamics, various properties of physical systems are studied under different external conditions, such as temperature, pressure or magnetic field, among others. Response functions, such as isothermal compressibility and magnetic susceptibility, are thermodynamic properties that indicate how the volume or magnetization of a material changes when applying changes in pressure or magnetic field respectively. These thermodynamic properties are of great interest for studying materials since they provide information on their structural, thermal, mechanical and magnetic properties[1], [2].

Materials' isothermal compressibility and magnetic susceptibility can be studied using various physical theories, such as Quantum Mechanics, Statistical Thermodynamics and Landau's theory of Fermi Liquids. The latter theory, also known as phenomenological theory, is important because its results can be directly contrasted with experimental results. Thus, it allows describing the behavior of interacting fermion systems (Fermi liquids) by non-interacting fermion systems (Fermi gases), introducing interactions in effective particles called quasi-particles. The theory is based on the idea that elementary excitations near the Fermi level can be treated as quasi-particles that retain the

properties of the original fermions but have a different effective mass and spin. Landau's theory of Fermi liquids allows one to calculate fermionic systems' thermodynamic and transport properties such as electrons in metals, superconducting materials and nuclear material[2]–[6].

In the case of fermionic systems, such as metals, the interaction functions or Landau parameters are denoted by$F_l^{s,a}$, where *s* and *a* indicate whether the function is symmetric or antisymmetric underspin or particle momentum exchange, respectively. These functions can be expanded into a Legendre Polynomial series, where the coefficients are called Landau parameters$F_l^{s,a}$, where l is the index of the corresponding spherical harmonic. The first term of this series, $F_0^{s,a}$, is one of the most important parameters for describing the thermodynamic properties of fermionic systems at low temperatures and moderate densities. However, for denser systems or at higher temperatures, the higher-order terms, $F_1^{s,a}$, y $F_2^{s,a}$, can have a significant influence on the behavior of the system and modify predictions based on system performance alone$F_0^{s,a}$[3], [4], [7]–[9].

This research presents a theoretical study of the isothermal compressibility and magnetic susceptibility of alkali metals (sodium, potassium and lithium) as a function of interaction functions.$F_0^{s,a}$, $F_1^{s,a}$, and$F_2^{s,a}$. The Fermi liquid theory is used, which is an approach to treat interacting fermionic systems at low temperatures, where the excitations of the system are considered to be quasi-particles with an effective mass and momentum-dependent energy. Analytical expressions for the above thermodynamic properties are obtained regarding the interaction functions and compared with experimental results reported by other authors. It is shown that the inclusion of higher order terms improves the agreement between theory and experiment and allows explaining some anomalies observed in these metals[3], [4], [6]–[8].

Rice[10]applied the Fermi-Landau theory of liquids to calculate theoretical estimates of the compressibility and magnetic susceptibility in terms of the Landau parameters $F_0^{s,a}$for sodium and potassium. These calculations were compared with reported experimental values. In another study, Brinkman and co-workers[11]obtained exact summation rules for the coefficients of the Legendre Polynomial expansion of the Landau interaction function. Landau parameters for sodium and potassium were determined by comparing with experimental values. Dunifer[12], [13]reports on a study of spin waves in high-purity sodium and potassium foils at cryogenic temperatures (1.4-10°K). Using Fermi Liquid theory, expressions for the magnetic susceptibility were obtained in terms of the parameters $F_0^{s,a}$, $F_1^{s,a}$.Lai[9], [14]presents a theoretical method for calculating the magnetic susceptibility in liquid metals. This approach combines Fermi Liquid theory with Pseudo-potential Perturbative theory to examine the role of electronic exchange corrections to paramagnetism in a simple liquid metal. The resulting prediction of spin susceptibility is quite accurate. Ashcroft[15]reports that a simple calculation of single metals' compressibility, binding energy and density yields good agreement with the experiment. Band structure effects are included in Perturbation Theory, using electron-ion interaction fitted to experimental data. Mace[12], [16]reports on spin-wave measurements on sodium and potassium metals with quasi-free electrons. A transmission microwave spectrometer operating at a frequency of 80 GHz was used. The theoretical calculations are fitted to experimental values obtained using the microwave transition technique. This allows a simple comparison of theory with experiment, obtaining values for B_0, B_1 and B_2, the first three parameters characterizing the many-body spin interaction. Edema [17],in this

work, the magnetic susceptibility of quasi-particles in metals was calculated using the Landau theory for Fermi liquids modified with the electron density parameter.
Therefore, this paper presents the compressibility$(k/k^0)$and magnetic susceptibility(χ/χ^0)in terms of the Landau Theory's re-normalized parameters, including the first three dominant orders of the Legendre Polynomial expansions. These determined expressions determine the response functions of some alkali metals such as Na, K and Li.

2. Theoretical model

2.1. Landau's Theory for Fermi Liquids

When calculating the partition function at low temperatures, only excited states very close to the ground state are generally taken. These excited states are elementary excitations or quasi-particles with defined energy and momentum. The energy spectrum of a Fermi liquid is similar to that of a Fermi ideal gas, and its ground state corresponds to occupying all states with momentum less than$|\vec{k}| < k_F$[4]–[7].
In order to apply Landau's Fermi Liquid theory to a system, the elementary excitations (quasi-particles) must be well-defined at low energies. This requires that the width$\Delta k$of the momentum of the elementary excitations is smaller than their energy. This width is determined by the interaction between quasi-particles, which in Landau's theory of Fermi Liquids is parameterized by the so-called Landau parameters[4], [6], [7].
The number of excitations is characterized by the shift of the distribution function from its value in the ground state [7].

$$\delta n_{k\sigma} = n_{k\sigma} - n^0_{k\sigma} \tag{2.1.1}$$

2.1.1 Quasi-particle interaction energy

For a system such as an ideal gas, there is a simple linear relationship between the energy of a specific state and the distribution function[6], [18].

$$E = E_0 + \sum_k \frac{k^2}{2m}\delta n_k \tag{2.1.2}$$

The relationship between the energy E of a state and the distribution function$n_{k\sigma}$becomes more complex when the interaction between the particles is considered. This relationship can be expressed as a functional of the form$E[n_{k\sigma}]$. If$n_{k\sigma}$is close to the equilibrium distribution function $n^0_{k\sigma}$,this functional can be expanded into a Taylor series[4], [6], [7].

$$E[n_{k\sigma}] = E_0 + \sum_k \varepsilon_k\, \delta n_{k\sigma} + O\left(\delta n^0_{k\sigma}\right) \tag{2.1.3}$$

Using Landau's expansion of the energy functional,andusing Landau's expansion of the energy functional results in

$$\Delta E[n] = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \delta n_{\vec{k}\sigma} + \frac{1}{2V}\sum_{\vec{k}\sigma\vec{\acute{k}}\acute{\sigma}} f_{\vec{k}\sigma,\vec{\acute{k}}\acute{\sigma}}\delta n_{\vec{k}\sigma}\, \delta n_{\vec{\acute{k}}\acute{\sigma}} \tag{2.1.4}$$

The energy density of the quasi-particles can be expressed as [4]–[6].

$$\tilde{\epsilon}_{\vec{k}} = \frac{\delta E[n]}{\delta n_{\vec{k}\sigma}} = \epsilon_{\vec{k}} + \frac{1}{V}\sum_{\vec{k'}\acute{\sigma}} f_{\vec{k}\sigma,\vec{k'}\acute{\sigma}}\delta n_{\vec{k'}\acute{\sigma}} \quad (2.1.5)$$

Landau Fermi's liquid theory is based on the equations (2.1.4) and (2.1.5). All Landau parameters are derived and obtained from these equations.

2.2. Isothermal Compressibility Expressions (k/k^0), in terms of Landau parametersF_0^s,F_1^s y F_2^s

Isothermal compressibility is the measure of how the volume of a material changes when pressure is applied at a constant temperature and is defined as [1], [2], [6].

$$k = -\frac{1}{V}\frac{\partial V}{\partial P}\Big|_{T,N} = \frac{1}{n^2}\left(\frac{\partial n}{\partial \mu}\right)_{T,N} \quad (2.2.1)$$

where $P$is the pressure, $V$the volume and$n$, $\mu$is the particle density and chemical potential, respectively.

Using Landau's expansion of the energy functional and Fermi's liquid theory, the relation can be expressed as[3], [6]:

$$\frac{\partial n}{\partial \mu} = \frac{(m^*/m)N(0)}{[1+\sum_{l=0}^{\infty} F_l^s\, P_l(cos\vartheta)]} \quad (2.2.2)$$

Replacing in (2.2.5)in (2.2.1)the result is

$$k = \frac{1}{n^2}\left(\frac{\partial n}{\partial \mu}\right)_{T,N} = \frac{1}{n^2}\left(\frac{N^*(0)}{1+F_0^s}\right) \quad (2.2.3)$$

Of[4], [6]$N^*(0) = \frac{m^*}{m}N(0)$and for a non-interacting system there is $k^0 = \frac{N(0)}{n^2}$by replacing we obtain.

According to [19], it is necessary that $N^*(0) = \frac{m^*}{m}N(0)$. In addition, for a non-interacting system, $k^0 = \frac{N(0)}{n^2}$. By replacing these expressions, the following relationship is obtained.

$$\frac{k}{k^0} = \frac{m^*/m}{[1+F_0^s]} \quad (2.2.4)$$

where$F_0^s$is the Landau parameter, which is defined as the first coefficient in the Legendre Polynomial expansion.

To express this relation in terms of higher order coefficients of the Legendre Polynomial, the expansion of the Landau energy functional and Fermi's liquid theory can be used in the expression(2.2.1)[6], [19].

$$\frac{\partial n}{\partial \mu} = \frac{(m^*/m)N(0)}{[1+\sum_{l=0}^{\infty} F_l^s\, P_l(cos\vartheta)]} \quad (2.2.5)$$

Substituting the expression (2.2.5) into the equation (2.2.1), the following result is obtained

$$k = \frac{1}{n^2}\frac{m^*/mN(0)}{[1+\sum_{l=0}^{\infty} F_l^s\, P_l(cos\vartheta)]} \tag{2.2.6}$$

For Fermi gas, according to Dupuis (2010), the following is obtained

$$k^0 = \frac{N(0)}{n^2} \tag{2.2.7}$$

By using the first, second and third-order coefficients of the Legendre Polynomial, the following is obtained

$$\frac{k}{k^0} = \frac{m^*/m}{\left[1+F_0^s+F_1^s cos\theta+\frac{1}{2}F_2^s(3*cos\theta^2-1)\right]} \tag{2.2.8}$$

When making the angle $(\theta = 0)$, the expression is simplified and reduced to the following

$$\frac{k}{k^0} = \frac{m^*/m}{[1+F_0^s+F_1^s+F_2^s]} \tag{2.2.9}$$

When the angle$(\theta = 0)$, the expression reaches its maximum value. This occurs when two states of the quasi-particles, $(\vec{k},\sigma)$ y $(\overrightarrow{k'},\acute{\sigma})$, are parallel and in maximum equilibrium. As the angle varies, this parameter also undergoes small variations.

This means that by using the equation (2.2.9) to calculate the isothermal compressibility of sodium (Na), potassium (K) and lithium (Li), values can be obtained that are close to the theoretical and experimental values determined by other authors. However, if the terms$F_1^s = 0$ y $F_2^s = 0$, the expression reduces to the usual expression (2.2.4), suggesting that these terms are important for better approximation to the theoretical and experimental values.

2.3. Magnetic Susceptibility Values (χ/χ^0), in terms of Landau parametersF_0^s, F_1^sandF_2^s

The isothermal magnetic susceptibility is defined by [1], [9]:

$$\chi_T = \left(\frac{\partial M_z}{\partial H}\right)_{T,N} \tag{2.3.1}$$

where M_z is the density of magnetization defined in the direction of $\hat{e}_z$[19]

$$\partial M_z = -\frac{1}{V}\left(\frac{\partial E_0(H)}{\partial H}\right) = \frac{g\mu_B\hbar}{2}\left(\delta n_\uparrow - \delta n_\downarrow\right) \tag{2.3.2}$$

where g, μ_B and s_z are, respectively, the gyromagnetic radius, Bohr magneton and the *z*-component of spin.

Expanding this expression in terms of the Landau parameters using first, second and third-order coefficients of the Legendre polynomial expansion results in[9], [17], [19].

$$\partial M_z = \frac{g\mu_B\hbar}{2}\left(\mathrm{g}\mu_\mathrm{B}\mathrm{b}\frac{\hbar}{2}\frac{\mathrm{N}(0)}{1+F_0^a}\right)=\left(\frac{g\mu_B\hbar}{2}\right)^2\frac{\mathrm{N}(0)}{1+F_0^a}b \tag{2.3.3}$$

Substituting (2.3.3) into (2.3.1), the following expression is obtained.

$$\chi_T=\left(\frac{\partial M_z}{\partial H}\right)_{T,N}=\left(\frac{\mathrm{g}\mu_\mathrm{B}\hbar}{2}\right)\frac{N(0)}{1+F_0^a} \tag{2.3.4}$$

In most of the available literature, the term F_0^a is the only one included in the expression of magnetic susceptibility[6], [17]

$$\frac{\chi}{\chi^0}=\frac{m^*/m}{1+F_0^a} \tag{2.3.5}$$

whereF_0^a is the first coefficient of the Legendre Polynomial Expansion.

To express the relationship (2.3.5) in terms of higher order coefficients of the Legendre Polynomial, the expansion of the Landau energy functional and the Fermi liquid theory can be used. In this way, the relation for the magnetization follows[17], [19].

$$\delta M_z=\left(g\mu_B\sigma\frac{\hbar}{2}\right)^2\frac{N(0)b}{1+\vec{\sigma}.\overrightarrow{\sigma'}\sum_{l=0}^{\infty}F_l^a\,P_l(cos\vartheta)} \tag{2.3.6}$$

Replacing(2.3.6) in (2.3.1) the following is obtained

$$\chi=\frac{\partial m}{\partial b}=\frac{(m^*/m)\chi_0}{1+\vec{\sigma}.\overrightarrow{\sigma'}\sum_{l=0}^{\infty}F_l^a\,P_l(cos\vartheta)} \tag{2.3.7}$$

Making use of the Legendre Polynomial Expansion

$$\sum_{l=0}^{\infty}F_l^a\,P_l(cos\vartheta)=F_0^a+F_1^a cos\theta+\frac{1}{2}F_2^a(3*cos\theta^2-1) \tag{2.3.8}$$

$$\frac{\chi}{\chi_0}=\frac{(m^*/m)}{1+F_0^a+F_1^a cos\theta+\frac{1}{2}F_2^a(3*cos\theta^2-1)} \tag{2.3.9}$$

It has been obtained for the magnetic susceptibility(χ/χ^0)an expression in terms of$F_0^a, F_1^a, F_2^a$and also has an angular dependence.

$$\frac{\chi}{\chi^0}=\frac{m^*/m}{1+F_0^a+F_1^a+\frac{1}{2}F_2^a} \tag{2.3.10}$$

When the angle $(\theta=0)$, the expression reaches its maximum value. This occurs when two states of the quasi-particle, $(\vec{k},\sigma)$ y $(\overrightarrow{k'},\acute{\sigma})$, are parallel and in maximum equilibrium. As the angle varies, this parameter also undergoes small variations.

In the expression obtained, (χ/χ^0)depends on the parameters $F_0^s, F_1^s$and$F_2^s$and has an angular dependence. By using equation (2.3.10) to calculate the magnetic susceptibility of sodium (Na), potassium (K) and lithium (Li), values are obtained that are close to the theoretical and experimental values reported by other authors. If the following terms are made to be$F_1^s = 0$and$F_2^s = 0$,the expression is reduced to the usual expression in(2.3.5)[17].

3. Results and discussion

3.1. Comparison between theoretical and experimental values of isothermal compressibility for sodium and potassium, and lithium

Table 1 presents experimental values of Landau parameters and effective mass for materials such as sodium and potassium, as reported by [11].

	Na	K
$m*/m$	1.24 ±0.02	1.21±0 .01
$A_0 = F_0^s$	0.10	0.15
A_1=F_1^s	-0.05±0.01	-0.030±0.005
$A_2 = F_2^s$	0.0± 0.005	…

Table1. Experimental values of Landau parameters for sodium (Na) and potassium (K), as well as the ratio of sodium (Na) to potassium (K),$\boldsymbol{m^*/\mathbf{m}}$were obtained through cyclotron resonance[11].

The values of the Laudau parameters presented in Table 1 are substituted into the formula (2.2.9) to obtain compressibility values for the materials sodium (Na) and potassium (K) shown in Table 2.

	m^*/m	F_0^s	F_1^s	F_2^s	$\frac{k}{k^0} = \frac{m^*/m}{1+F_0^s}$	$\frac{k}{k^0} = \frac{m^*/m}{1+F_0^s+F_1^s+F_2^s}$	Exp.[11]	Ter. [11]
Na	1.24	-0.1	-0.05	0.0	1.37	1.45	1.5	1.49
K	1.21	0.15	-0.03	0.0	1.05	1.08	1.0	1.08

Table2: Values of the isothermal compressibility obtained using the experimental data in Table 1 and the expression(2.2.9).

As can be observed in Table 2, the value of$(k/k^0)$for Na in the first approximation is 1.37, and 145 when higher order approximation terms are considered. On the other hand, for K(k/k^0)considering

terms in the first approximation is 1.05 and 1.08 in terms of a higher order of approximation is 1.08. According to Rice[10], the theoretical values of$(k/k^0)$for Na and K are (1.47) and (1.55) respectively. The results obtained by considering higher order approximation terms are close to the values reported by Rice who used Hubbard's theoretical approximation. Thus, it can be concluded that the values obtained with the proposed model determine the thermodynamic property $(k/k^0)$with good approximation and is consistent with reported theoretical and experimental values[10], [20].

3.2. Comparison between theoretical and experimental values of magnetic susceptibility for sodium (Na) and potassium (K) and lithium (Li).

Table 3 presents experimental values of the Landau parameters and the effective mass for materials such as sodium, potassium and lithium, as reported by[16].

	Na	K	Li
$m*/m$	1.24±0.02	1.21±0.01	2.30±0.20
$B_0 = F_0^a$	-0.21±0.05 [6] -0.215±0.02 [8]	-0.2±0.1 [6] -0.28±0.02 [8]	-0.23±0.03[16]
$B_1 = F_1^a$	0.01±0.03 [6] -0.005±0.04 [8]	0.1±0.2 -0.06±0.03	-0.08±0.05[16]
$B_2 = F_2^a$	0.0±0.05	0.01±0.05	0.0±0.05[16]

Table 3. Magnetic susceptibility values were obtained using (2.3.10) Landau parameters for Na, K and Li, and the m^*/m ratio was obtained by cyclotron resonance[16].

The values of the Laudau parameters presented in Table 3 are substituted in the formula (2.3.10) to obtain values for the magnetic susceptibility of some alkali metals such as Na, K and lithium, shown in Table 4.

	$\frac{m^*}{m}$	F_0^a	F_1^a	F_2^a	$\frac{\chi}{\chi^0} = \frac{m^*/m}{1+F_0^a}$	$\frac{\chi}{\chi^0} = \frac{m^*/m}{1+F_0^a+F_1^a+F_2^a}$	Exp. [11]	Ter. [11]
Na	1.24	-0.21	-0.005	0.0	1.56	1.58	1.74 ± 0.1 1.51 ± 0.06	1.47 1.41
K	1.21	-0.28	-0.06	0.0	1.68	1.83	1.58 ± 0.1 1.68 ± 0.25	1.55 1.45
Li	2.30	-0.23	-0.08	0.0	2.98	3.33	2.99[16]	3.1[16]

Table4: Values of$\boldsymbol{\chi/\chi^0}$for Na, K and Li obtained using experimental data from Table 3 and obtained using the expression (2.3.10).

As shown in Table 4, the value of $(\chi/\chi^0)$for Na is 1.56 in a first approximation and 1.58 when higher order terms are included. For K, $(\chi/\chi^0)$is 1.68 in a first approximation and 1.83 when considering higher-order terms. Finally, for the Li, $(\chi/\chi^0)$is 2.98 and 3.33 in a first and further approximation, respectively. According to Dunifer [12], [16], the theoretical values of$(\chi/\chi^0)$for Na, K and Li are 1.61, 1.71 and 2.99, respectively. Therefore, it is concluded that the values obtained with the higher order expressions are closer to thosevalues determined by Dunifer [12], [16] than those obtained experimentally using spin waves. Therefore, it is concluded that the values obtained with the proposed theoretical model are a good approximation and consistent with those reported by other theoretical models and experimental results.

4. Conclusions

Landau's Fermi liquid theory was applied to calculate thermodynamic properties such as isothermal compressibility and magnetic susceptibility of materials such as sodium (Na), potassium (K) and lithium (Li) using Landau's parameters with a higher order of approximation$F_0^{s,a}$, $F_1^{s,a}$and$F_2^{s,a}$.With experimental values reported by other authors, the isothermal compressibility of sodium 1.45 and potassium 1.08 was determined, as well as the magnetic susceptibility of sodium 1.58, potassium 1.83 and lithium 3.33. These results show that the proposed model accurately describes the studied materials' isothermal compressibility and magnetic susceptibility.

5. References

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