The crystalline metal is regarded as a collection of ions arranged in a periodic lattice and immersed in a more or less uniform sea of conduction electrons. The physical properties of these systems are governed by the nature and the arrangement of the ions, and by the distribution of the conduction electrons in the periodic lattice. In the presence of external perturbing fields, the ions get displaced and the conduction electrons redistribute themselves in response to the external field and the field produced by the displacement of the ion cores. The ion cores get polarized if the outermost electrons are liable to be excited under the action of the external field.

In most of the studies of the metallic systems it is assumed that the ion cores are rigid and the core polarization effects are neglected. This seems to be true in simple metals where the separation between core and conduction electrons is clear and the outermost shells of the core are completely filled. The system of transition metals poses the problem where such a separation is not clear. The adiabatic approximation is generally observed for the relative motion of the ions and electrons. Under this approximation it is assumed that the ionic and electronic motions are separable as the electrons because of their lighter mass move much faster than the ions.
Such an approximation is found to be invalid in explaining many physical properties such as superconductivity where the electron-ion correlated motion plays the dominant role.

The present thesis is devoted to the study of thermal and electronic properties of transition metals. We precisely investigate here, the dynamical response of the metallic system to the weak magnetic and thermal perturbing fields. The core and conduction electrons in transition metals are separated on the basis of model band structures and other available informations. The core polarization effects are completely neglected and the response of the conduction electrons to the perturbing magnetic and thermal fields is mainly studied. In studying the response to the thermal field, the adiabatic approximation is taken to be valid. In the first four chapters, the investigations on the magnetic response function are presented and in the last chapter the calculations for phonon frequencies are presented.

The magnetic linear response function or the generalized dynamical magnetic susceptibility $\chi(q, \omega)$ of a sample of aggregated matter is defined by the equation

$$M(\mathbf{q}, \omega) = \chi(q, \omega) H(\mathbf{q}, \omega)$$  \( (1.1) \)

$\chi$ here in general a tensor (diagonal for a cubic substance such as nickel), relates the overall response $\langle M \rangle$ of the system to the perturbing magnetic field $H$ with wavevector $\mathbf{q}$ at
frequency $\omega$. For isotropic materials $M$ and $H$ are parallel vectors and the susceptibility is then a scalar quantity. For static magnetic fields, the corresponding magnetic susceptibility $\chi(q,0)$ is called the static magnetic susceptibility.

The quantum theory of the static magnetic susceptibility $\chi(0,0)$ of simple metals has been put forward by many authors through the use of pseudopotential formalism. Attention has recently been focused on the response function of a metallic system to a spatially and time-varying magnetic field as this can be directly compared with the neutron inelastic scattering measurements. The formal functional forms of dynamical spin and orbital susceptibilities are rigorously obtained but their explicit evaluation for a realistic multiband system is still awaited. Considerable progress has been made in recent years in the understanding of ferromagnetic metals in terms of the itinerant electron model. Izuyama, Kim and Kubo have shown that the spin waves which arise naturally from the Heisenberg model may also be obtained from this model. Doniach used the formalism due to Izuyama, Kim and Kubo to calculate the spin susceptibility of paramagnetic palladium in the random phase approximation in a one-band itinerant electron model. A more searching test of the itinerant model is the comparison of the predicted and measured differential cross-section for the inelastic scattering of neutrons. This was done by Lowde and Windsor who in their comprehensive paper gave a detailed
analysis of their measurements on the magnetic response function of nickel. Their calculation was based upon a one-band model and the interference between partial susceptibilities arising from the various bands was neglected. These authors used the free electron and tightbinding approximations. In the free electron approximation the role of overlap matrix elements in the expressions for the unenhanced susceptibility function is completely ignored. In the tightbinding approximation the contribution of all the five d-subbands is explicitly evaluated but the effects of an s-like band are neglected. For the inelastic scattering cross-section, Thompson$^{10}$ discussed scattering by Stoner single particle modes at low temperatures for a short-range interaction using a single band model for ferromagnetic metal.

Yamada and Shimizu$^{11}$ evaluated dynamical spin susceptibility for a multiband system and calculated it in the two-band model scheme for ferromagnetic nickel. Gillan$^{12}$ and Sokoloff$^{13}$ calculated the spin susceptibility in multi-band and one band model, respectively but both the authors took a simplified view of the form factors. Gupta and Sinha$^{14}$ calculated the static susceptibility of paramagnetic chromium using augmented plane-wave band structure calculations. Cooks and Wood$^{15}$ also calculated the static susceptibility function of ferromagnetic nickel using realistic band structure calculations. Rath and Freeman$^{16}$ recently studied the static susceptibility of scandium
using augmented plane-wave band structure calculations. Mori calculated the static paramagnetic susceptibility of nickel, palladium and platinum taking into account the energy band effects. Diamond in his comprehensive paper formally worked out the theory of exchange enhanced generalized dynamical susceptibility of strong paramagnetic transition metals but the numerical calculations are carried out for palladium only in the static case. Lipton computed dynamical susceptibility of palladium using an interpolation scheme which incorporates both the s and d-like band effects but neglected the wavevector dependence of the matrix elements assuming them to be equal to unity. Hayashi and Shimizu derived the generalized susceptibility for a single band model of d-electrons and for a two band model of d and s-electrons and applied it to calculate the impurity screening and induced spin density of ferromagnetic nickel using effective mass approximation for energy bands.

Most of the above authors have calculated the static or dynamical magnetic susceptibility using some simplifications at one stage or the other. In fact it is a prohibitively difficult task to include the realistic multiband structure and actual crystal wavefunctions in the evaluation of the dynamical spin susceptibility as this demands heavy computational efforts. Earlier a non-interacting band model scheme was proposed for the s and d-conduction electrons in a transition metal by Prakash and Joshi and was successfully
applied to investigate the dielectric screening, phonon frequencies and effective ion-ion potential of noble and transition metals\textsuperscript{22-26}. Hanke and Bilz\textsuperscript{27}, and Hanke\textsuperscript{28} justified the above model in the Wannier representation neglecting s-d hybridization which exists only in the small region of momentum space and much below Fermi energy.

In view of the computational simplicity we develop in chapter 2, the formalism for the dynamical magnetic susceptibility of Bloch electrons in the non-interacting band model scheme. The density matrix approach is adopted and the explicit expressions are obtained for the spin and orbital susceptibilities. The free electron approximation for s-electrons and tightbinding approximation for d-electrons is used while evaluating the various contributions to the susceptibility function. The explicit expressions are obtained for the various contributions arising from the intra and interband transitions of electrons in s and d-bands under the action of perturbing magnetic field.

In chapter 3, the formalism developed in chapter 2 is applied to calculate the susceptibility function for paramagnetic Ni, Pd, Pt and ferromagnetic Ni. In the non-interacting band model scheme it is found that paramagnetic Ni, Pd and Pt have s- and one d-subband partially filled, and the other four d-subbands are completely filled. In ferromagnetic Ni all the majority spin d-subbands are completely filled, while s-band
is partially filled. Two minority d-subbands and minority s-band are partially filled. Other minority d-subbands are completely filled. The atomic configurations taken up for Ni, Pd and Pt are (3d)$^9$ (4s)$^{0.6}$, (4d)$^9$ (5s)$^{0.6}$ and (5d)$^{9}$ (6s)$^{0.6}$, respectively. The number of electrons per atom assigned to the s-and d-subbands is determined by the ratio of the volume occupied by the bands. The diagonal part of the susceptibility matrix is evaluated for paramagnetic Ni, Pd, Pt and ferromagnetic Ni. The susceptibility is calculated for the field wavevector $q$ along three principal symmetry directions $[100]$, $[110]$ and $[111]$ and the anisotropy is found to be quite small except in the vicinity of $q = 0$. Therefore further calculations are extended only for the field wavevector $q$ along $[100]$ direction. The susceptibility function is studied as a continuous function of momentum and energy transfer. The exchange enhancement of the susceptibility function is also studied. The scattering function is calculated from the imaginary part of the unenhanced and exchange enhanced susceptibility function and compared with the neutron inelastic scattering data. The agreement is found to be reasonably good. In all the three metals Ni, Pd and Pt, the intraband part of susceptibility dominates for small values of wavevector while the interband part becomes comparable for higher values of momentum transfer. The susceptibility functions for Ni, Pd and Pt are also intercompared. The magnitude of the susceptibility decreases
as one goes from 3d to 5d metal. The contribution of the
minority spin (\(\downarrow\)) bands in case of ferromagnetic Ni is found
to be much larger than the contribution of the majority spin
(\(\uparrow\)) bands. The susceptibility in the ferromagnetic phase of
Ni is also found to be higher than that in the paramagnetic phase.

The temperature dependence of dynamical and static
magnetic response function is again an important quantity.
Rivier and Zuckermann\(^{30}\) emphasized the importance of temperature
variation of the spin susceptibility of metals and alloys in
order to explain other physical properties. Doniach and
Engelburg\(^{31}\), and Shimizu et al.\(^{32}\) have shown that the temperature
dependent static susceptibility can explain the specific heat
data at finite temperatures. It is well known that the resistivity
shows \(T^2\)-law at low temperatures and \(T\)-law at high temperatures.
Mill and Lederer\(^{33}\) calculated the resistivity of d-band metals
taking Izuyama et al.\(^{8}\) dynamical transverse susceptibility at
low and high temperatures in the itinerant electron model. It
has been observed that for nearly magnetic metals and alloys\(^{34-35}\)
at high temperatures, the resistivity departs from \(T\)-law and
have negative slope. The first improvement was done by Kaiser
and Doniach\(^{36}\) who used a low temperature expansion for the
spin susceptibility in the calculation of resistivity and then
Rivier and Zlatic\(^{37}\) calculated resistivity in the high
temperature limit. Jullien et al.\(^{38}\) have explained the essential
features of the paramagnon resistivity of nearly magnetic
metals using full temperature dependent dynamical susceptibility. Considering the importance of $\chi(q, \omega, T)$ it looks interesting and worthwhile to extend the formalism developed in chapter 2, to the investigation of the temperature dependence of the dynamical response function. The actual calculations which we present in chapter 4, are however limited in the non-interacting band model scheme. In this chapter, the formalism for the imaginary part of the temperature dependent dynamical magnetic susceptibility is developed starting from the temperature dependent Fermi distribution function. Kramers-Kronig relations are used to calculate the real part of the susceptibility. The susceptibility is studied as a continuous function of momentum and energy transfer, and temperature for Ni, Pd and Pt. It is found that susceptibility decreases with the increase of temperature. The effect of temperature on the $q$ and $\omega$ dependence of susceptibility is in general to broaden its peaks and to decrease its magnitude. It is also shown that the itinerant electron model explains ferromagnetism in Ni which is due to the spatial localization of the 3d-band resulting in large density of states at the Fermi surface.

The calculation of orbital magnetic susceptibility of transition metals is also interesting but characteristically difficult. The difficulty lies in the evaluation of the overlap matrix elements where the derivative of the Bloch functions is involved. In the formalism developed in chapter 2,
the s-d hybridization effects are inherently ignored. Secondly, if one calculates the orbital contribution to the susceptibility function one finds that the contribution from the d-electrons which are represented by simple tightbinding wavefunctions is found to be zero. This of course does not seem feasible. The s-d hybridization effects are also quite important in transition metals as emphasized by Ehrenreich et al.\textsuperscript{39} Ziman\textsuperscript{40} and Harrison\textsuperscript{41}. Kubo et al.\textsuperscript{42} and Mori\textsuperscript{17} calculated the static orbital susceptibility in Ni, Pd and Pt with the aid of simplified energy bands and showed that orbital susceptibility makes a significant contribution to the total susceptibility function. However, Lowde and Windsor\textsuperscript{6} commented that the orbital part is only a few percent that of the spin part in metals like Ni and these authors completely ignored the calculations of orbital susceptibility.

In chapter 5, we have made an attempt to evaluate the dynamical spin and orbital susceptibilities of transition metals using the transition metal-model potential (TMMP) theory. The s-d hybridization effects are introduced in the TMMP through the nonlocality of the model potential\textsuperscript{43}. Ours is perhaps the first attempt to estimate the orbital part of the dynamical susceptibility of a transition metal. The tractable expressions are obtained for both the spin and orbital contributions to the susceptibility function by applying Shaw-Harrison\textsuperscript{44} model potential transformations to the Bloch
functions and these are used to calculate the spin and orbital susceptibilities of Al, Cu and V. These metals were chosen for this study because enough spectroscopic data are available for determining all the parameters of transition metal model potential required to compute the depletion hole contribution. To seek a relative comparison of susceptibility in these metals is also one of the aims of this investigations.

The susceptibility is separated into two parts: one due to the smooth part of the charge density and another due to the depletion hole charge density. The depletion hole contribution is found to be of the same order of magnitude as the free electron contribution. The orbital susceptibility as a whole is found to be about 10 to 80% that of spin susceptibility except at very small momentum transfer where the orbital susceptibility dominates over the spin susceptibility. The structural features of magnetic susceptibility are however dominated by the spin response rather than the orbital response. Both the spin and orbital contributions in case of Vanadium are found to be larger than those in Aluminium and Copper. The spin contribution in Aluminium is found to be more than that in Copper but the orbital contribution dominates in Copper. The limitations of the calculation are also discussed.

Harrison analyzed the problem of lattice dynamics of transition metals by generalizing the pseudopotential theory which explicitly includes the s-d hybridization for
transition metals. The theory was further extended by Moriarty\textsuperscript{45} to calculate the phonon frequencies and lattice stability of noble and alkaline earth metals. Animalu\textsuperscript{46} generated the transition metal-model potential (TMMP) by examining the spectroscopic data for a large number of 3d, 4d and 5d series of transition metals and used it to calculate the phonon frequencies of fcc and bcc transition metals. These authors used the free electron dielectric function modified by the exchange correlation corrections due to Hubbard\textsuperscript{47}. The calculated results were in agreement with the experiment for fcc metals. However, it could not be possible by this approach to explain the anomalies in the phonon frequencies of bcc transition metals. Since hcp structure is again a closed packed structure like fcc, therefore we found it interesting to extend the TMMP approach to investigate the phonon frequencies of hcp transition metals.

We calculate the phonon dispersion curves for Zn, Zr, Tl, Tb and Ho for which the experimental data through the neutron inelastic scattering measurements\textsuperscript{48-52} are also available. The bare ions are represented by TMMP and the exchange-correlation corrections due to Vashista\textsuperscript{53} and Singwi\textsuperscript{54} et al. are included in the Hartree dielectric function. The calculated phonon frequencies are all found to be real and in reasonably good agreement with the experimental values. This establishes the validity of the Animalu TMMP for hcp metals.
The limitations of the calculation are discussed and the relative comparison of phonon frequencies and the form factors for various metals is also carried out.

In the appendices, a few mathematical steps are elaborated for completeness.