INDIAN INSTITUTE OF TECHNOLOGY, BOMBAY

DEPARTMENT OF PHYSICS

Synopsis of the thesis entitled

MANY BODY EFFECTS IN HOMOGENEOUS AND INHOMOGENEOUS ELECTRON SYSTEMS

to be submitted by

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in partial fulfilment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

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The simplest manifestation of many body effects is seen in the electron gas system e.g. plasmons in a homogeneous system (an infinite jellium) and surface plasmons in an inhomogeneous system (a semi-infinite jellium). In this thesis we wish to study different many body effects. The first part of the thesis deals with the many body effects in a homogeneous system and the second part with the interactions of an inhomogeneous system with external charge or atom.

Part I : Developing a theory for frequency and wavevector dependent dielectric function amenable to numerical computations has been an interesting and challenging task. Due to the constraints set by the numerical aspect, however, most of the work is limited to theories accurate in the long wavelength or high frequency limits. Due to the exchange-correlation - hole around each electron there is a modification of the mean Hartree field; one refers to the difference between the effective field and the mean Hartree field via the so called local field correction, $G(q,\omega)$. Assuming that the hole is bound rigidly to the electron, most theories obtain a static $G(q)$. In general, the motion of the hole is very complex and requires a frequency dependent local field. Experimental observations on X-ray and electron energy loss spectra at large momentum transfers cannot be explained by a static $G(q)$, and developing a theory giving a complex, frequency dependent local field incorporating the dynamic and dissipative effects seems essential. In this thesis, we suggest several approximations which take into account the dynamic correlations in the electron gas and in particular we calculate the damping of long wavelength plasmons. We use the equation of motion (EOM) method for Wigner distribution functions. The EOM for the one particle distribution function $f^{(1)}$ contains the two particle distribution function $f^{(2)}$ and so on. We truncate the hierarchy of equations by approxi-ting for $f^{(2)}$ in the EOM for $f^{(1)}$ as,

$$f^{(2)}_{k\sigma k'\sigma'}(r,r',t) = f^{(1)}_{k\sigma}(r,t)f^{(1)}_{k'\sigma'}(r',t)\ \frac{1}{n^2}\ C^{(2)}(r,r',t),$$

where,

$$C^{(2)}(r,r',t) = \sum_{\substack{k\sigma \\ k'\sigma'}} f^{(2)}_{k\sigma k'\sigma'}(r,r',t).$$

This type of decoupling has proved useful for classical liquids. Different approximations for $C^{(2)}$ now lead to various results obtained by other workers. Thus, we have here, a simple and methodical approach giving the earlier results.

For an improved treatment, $C^{(2)}(r,r',t)$ is related to the irreducible density-density correlation function $D^{(2)}$, which in turn is related to a time ordered correlation function $\pi(r,t;r',t')$. We write an integral equation for π in the presence of a weak external potential ϕ_e and retains terms only to linear order in ϕ_e. Making an ad-hoc SSTL[1] - like approximation for the vertex function occurring therein, we obtain a frequency dependent $G(q,\omega)$. In the $\hbar \to 0$ limit, this result reduces to one obtained by Singwi et al[1], who neglected the frequency dependence and obtained a static $G(q)$. We retain the frequency dependence and carry out explicit calculations for $G(q,\omega)$ in the $\hbar \to 0$ limit. The $G(q,\omega)$ is split into two terms - one, a static local field obtained earlier by STLS[2] and the other a complex, frequency dependent part. The imaginary part of G has a frequency dependence controlled by the coupling between the excitation modes of the system. This feature was obtained earlier by Sharma et al[3], who used the Mori formalism. Such a mode coupling feature had not been noticed in any of the earlier mean field approaches. We present explicit calculations for damping coefficient Γ, in the long wavelength limit[4]. The result for the $r_s \longrightarrow 0$ limit compares fairly well with an earlier perturbative calculation[5] in the same limit. The damping in metallic density range ($1.8 \leq r_s \leq 5.6$) however is much smaller. We also present $G(q,\omega)$ for finite q and ω. Many of the predicted limiting features are noted. Although the experimentally observed double peak structure in the energy loss spectra is not present, the present results do show a shift in the peak towards experimental result. A defect in the present theory is that the static and high frequency limits of $G(q,\omega)$ are the same. This could be due to the ad-hoc nature of the approximation for the vertex function.

We improve upon the above approximation by using linear response theory to obtain the vertex function. Γ calculated in this case has values much higher than in the former case. The mode coupling feature is retained here too. To understand the content of this approximation we also develop a response function corresponding to $D^{(2)}$ in the presence of an external field, and then from its EOM obtain $G(q,\omega)$. Also, a similar expression for $G(q,\omega)$ is obtained by extracting $C^{(2)}$ from an EOM for $f^{(2)}$. These two additional approaches indicate that our theory includes higher order correlations. This gives rise to the mode coupling term which was not obtained in any of the previous EOM approaches such as that of Aravind et al[6]. This, along with the improvement in damping coefficient values, and the simple systematic approach are the positive aspects of our theory.

The equilibrium value of $f^{(2)}$ is unknown and earlier workers[6] have used ansätze satisfying certain requirements for it. We use the EOM method and obtain an expression for $f^{(2)eq}$ which differs from the ansätze[6]; however numerical calculation is not attempted because of difficulties in handling heavy computational work.

Part II : Here we study the semi-infinite jellium, a representative of metal with a planar surface, in the presence of an external perturbation. To circumvent difficulties arising from the inhomogeneity, we work mainly within the frame work of the model Hamiltonian approach. We first study the dynamic image potential $V(z,v)$ i.e. the interaction between an incoming charged particle and the metal surface. Earlier workers assumed that the particle moves at a constant speed. We incorporate the acceleration of the particle and calculate V(z,v) using both, the model Hamiltonian[7] and the microscopic dielectric response approach[8]. The results do not show much improvement over the earlier self-consistent calculation by Ray and Mahan[9], but we are able to show for the first time how the local speed of the particle enters the self-consistent scheme. Using the model Hamiltonian approach and assuming that an uniformly moving atom or molecule is approaching a metal surface, we also calculate the dynamic van der Waals interaction W(z,v). We find that due to the large mass of the incoming particle, its velocity is too small to have any significant effect on W(z,v) at any distance of importance. We also calculate the single loss probability $\bar{P}_{1a}$, for a molecule approaching a metal surface with an uniform layer (coverage less than unity) of adsorbed molecules. A typical calculation shows that $\bar{P}_{1a}$ is almost zero. However a reduction in the excitation frequency of the adsorbed molecules ($\lesssim$ 0.1 eV) can yield a finite $\bar{P}_{1a}$.

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