

Accurate Dynamic Structure Factor of the Homogeneous Electron Liquid

The electron liquid, an assembly of N electrons embedded in a uniform positive background, has been studied to clarify the nature of electron correlation in metals, putting aside the influence of the periodic ion potential. This simplified model poses us a tough problem, but after the struggles lasting longer than half a century, accurate knowledge of its almost all static properties is now acquired by a number of sophisticated methods including quantum Monte Carlo simulations over the entire region of metallic densities $1.88 < r_s < 5.6$ where r_s is the conventional density parameter.

As for dynamical properties, on the other hand, our knowledge is still not enough in spite of all previous efforts to go beyond the random-phase approximation (RPA) in an attempt to explain the double-peak structure in the dynamical structure factor $S(\mathbf{q}, \omega)$ observed in light metals like Al. Among approximation schemes, the Baym-Kadanoff (BK) conserving one formulated in terms of the full Green's function G is most suitable for the evaluation of $S(\mathbf{q}, \omega)$. Accuracy of the result depends critically on the choice of the energy functional $\Phi[G]$, but the result will never become exact, since no algorithm is known to give the exact $\Phi[G]$.

A conceptually different scheme is developed to obtain the exact $S(\mathbf{q}, \omega)$ [1]; instead of pursuing $\Phi[G]$, we pay attention to the exact functional relations between the self-energy Σ and the vertex function Γ , obeying the microscopic conservation law. In particular, Γ is determined by the Bethe-Salpeter equation with an irreducible electron-hole interaction given by the functional derivative, $\delta\Sigma/\delta G$. Starting from an arbitrary input, we iteratively revise both Σ and Γ simultaneously towards self-consistency through the relations, whereby the number of terms representing Σ generated in this iterative process rapidly increases, eventually covering all terms derivable from the exact $\Phi[G]$ when the self-consistency is achieved.

In a numerical algorithm, however, the functional differentiation $\delta\Sigma/\delta G$ is not feasible. Thus we need to invent an alternative scheme to revise Γ on a computer accurately and efficiently. Recently a physically motivated and accurate enough prescription is given for Γ [2], enabling us to obtain the result of $S(\mathbf{q}, \omega)$ [3] that is most accurate among all existing ones.

Throughout the metallic-density region, qualitative features of $S(\mathbf{q}, \omega)$ remain the same; a typical example at $r_s=5$ is given in Fig. 1. Besides a broad peak b located at almost the same position in the RPA, there appears a clear shoulder a accompanied by a steepened slope of the linear term in $S(\mathbf{q}, \omega)$ for small ω . The peak b , being identified as “the center of gravity” of one-pair excitations, is transformed continuously into the plasmon peak as $|\mathbf{q}|$ decreases.

The shoulder a is well developed particularly for $1.4 < |\mathbf{q}|/p_F < 2$ and the slope is surprisingly enhanced over the RPA value accordingly. These features imply inseparable coupling between one- and multi-pair excitations in the one-pair excitation region, attractive electron-hole multiple scattering (excitonic effect) on the low- ω side of the one-pair region, and extra contributions from multi-pair excitations outside of it.

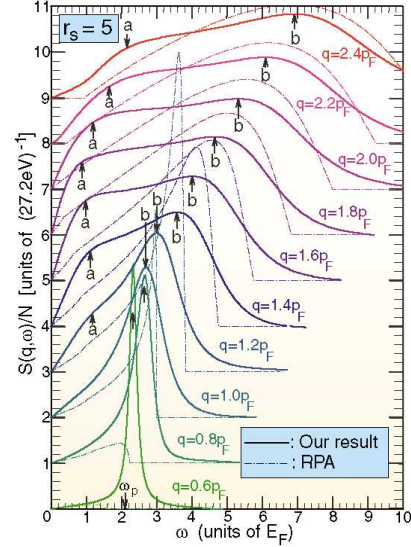


Fig. 1. Dynamical structure factor of the electron liquid at $r_s=5$. The value indicated by ω_p is the plasmon energy at $q=0$. The excitonic effect manifests itself in the structure indicated by a .

Since accurate knowledge of $S(\mathbf{q}, \omega)$ of the electron liquid is now available, we have compared it with the experimental one for Al, a metal regarded as most electron-liquid-like with $r_s=2.08$, in order to see how the band effects modifies the actual structure of $S(\mathbf{q}, \omega)$. The result of comparison is shown in Fig. 2, which leads us to conclude that the electron-liquid model applies well to Al on the whole and especially so for $\omega < E_F$ ($\sim 11\text{eV}$). The discrepancy from the model at higher ω is ascribed to the strong tight-binding nature of unoccupied 3d and 4f bands in Al, leading to the structure c in Fig. 2.

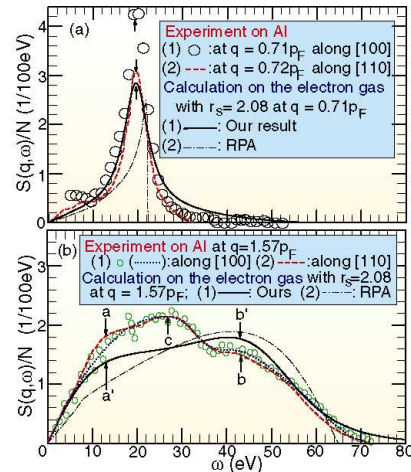


Fig. 2. Comparison between $S(\mathbf{q}, \omega)$ of the electron liquid at $r_s=2.08$ and the experimental one for Al metal.

References

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