

# 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  $\Sigma$  and the vertex function  $\Gamma$ , obeying the microscopic conservation law. In particular,  $\Gamma$  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  $\Sigma$  and  $\Gamma$  simultaneously towards self-consistency through the relations, whereby the number of terms representing  $\Sigma$  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  $\Gamma$  on a computer accurately and efficiently. Recently a physically motivated and accurate enough prescription is given for  $\Gamma$  [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  $\omega$ . 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- $\omega$  side of the one-pair region, and extra contributions from multi-pair excitations outside of it.

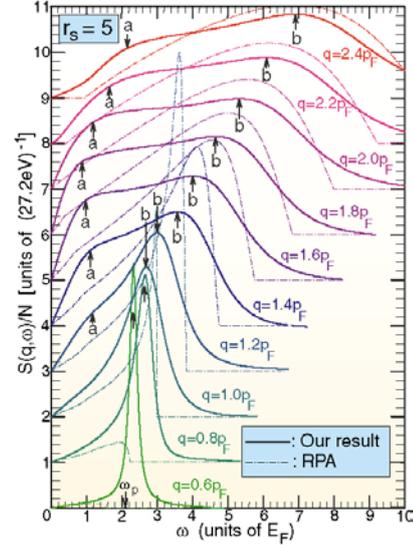


Fig. 1. Dynamical structure factor of the electron liquid at  $r_s=5$ . The value indicated by  $\omega_p$  is the plasmon energy at  $q=0$ . The excitonic effect manifests itself in the structure indicated by  $a$ .

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  $\omega$  is ascribed to the strong tight-binding nature of unoccupied 3d and 4f bands in Al, leading to the structure  $c$  in Fig. 2.

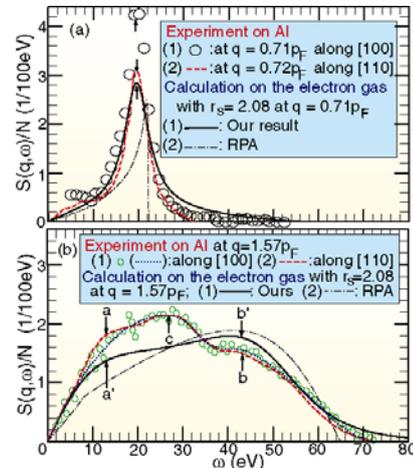


Fig. 2. Comparison between  $S(\mathbf{q}, \omega)$  of the electron liquid at  $r_s=2.08$  and the experimental one for Al metal.

## References

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- [3]Y. Takada and H. Yasuhara, *Phys. Rev. Lett.* **89**, 216402 (2002).

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