GWΓ Method for the Self-Energy of a Many-Electron System

In the last two decades, we have witnessed the power of quantum Monte Carlo (QMC) simulations that allow us to obtain virtually exact information on the static properties associated with the ground-state wave function of a quantum many-body system. However, QMC cannot be used to evaluate dynamical properties, because dynamics requires information on excited-state wave functions as well. Thus we need to develop an alternative algorithm for dynamics.

Four decades ago, Baym and Kadanoff proposed a conserving approximation scheme by formulating the dynamical problem in terms of an energy functional $\Phi[G]$ with G the full Green's function. The self-energy Σ is obtained by $\Sigma=\delta\Phi[G]/\delta G$. One can choose $\Phi[G]$ at one's disposal. Although it is found to be very useful in many cases, this scheme never provides the exact Σ, because no algorithm is known to give exact $\Phi[G]$.

In 1995, I developed a conceptually new scheme to obtain the exact Σ, named the self-energy revision operator theory [1]; instead of pursuing $\Phi[G]$, I paid attention to the exact functional relations between Σ and the vertex function Γ, obeying the microscopic conservation law. In particular, Γ is determined through the Bethe-Salpeter equation with an irreducible electron-hole interaction given by the functional derivative, $\delta\Sigma/\delta\Gamma$. Starting from an arbitrary input, both Σ and Γ are iteratively revised towards self-consistency through the functional relations. Note that 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 $\delta\Sigma/\delta\Gamma$ is not feasible, prompting me to invent an alternative scheme to revise Γ on a computer in an accurate and efficient way. Recently such a scheme is provided, giving an accurate enough result for Σ, in which the Ward identity is satisfied automatically [2,3]. This method allows us to obtain accurate results for the dynamical quantities, promising us to open a new dimension to the quantum many-body problems.

My calculation scheme is schematically shown in Figure 1, which indicates that this method may be regarded as an extension of the Hedin's GW method by including Γ that is determined self-consistently with Σ. Thus it is named the GWΓ method.

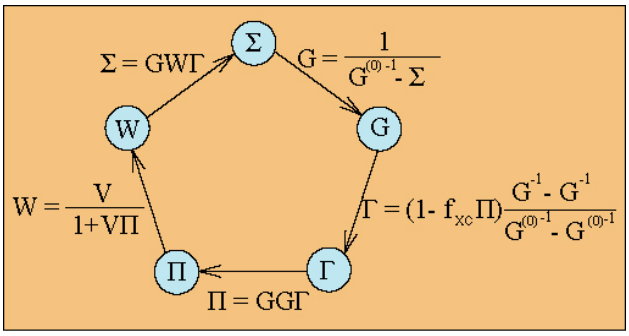

Figure 1: Schematic representation of my self-consistent calculation scheme for the self-energy Σ, where V is the bare Coulomb interaction, $G^{(0)}$ is the bare Green's function, Π is the polarization function, and f_{xc} is the exchange-correlation kernel appearing in the time-dependent density functional theory.

As an illustration, my method is implemented in the homogeneous electron gas at the density parameter $r_s = 4$ corresponding to sodium. The obtained single-electron spectral function $A(p,\omega)$ (which is given by $-\mathrm{Im}G(p,\omega)/\pi$) is shown in Figure 2. The main peak represents the structure of a quasiparticle. Its width is very sharp at and near the Fermi surface [Case (a)], indicating the existence of a well-defined quasiparticle. However, it is very broad far away from the Fermi surface [Case (b)]. In fact, its tail connects continuously with the plasmon-side band or the plasmaron (an entity composed of the real plasmon and the quasiparticle), implying a strongly decaying nature of the quasiparticle. Note that without Γ satisfying the Ward identity or the microscopic conservation law, this plasmaron peak

does not come to the right energy position.

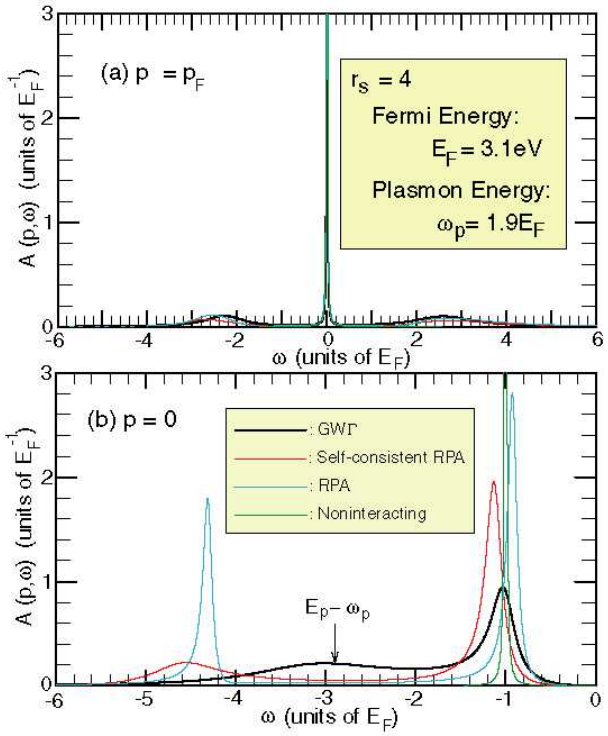

Figure 2: A(p,ω) for the homogeneous electron gas at the sodium density (a) at the Fermi surface (p=p_F) and (b) at the band bottom (p=0).

My result of A(p,ω) discloses the intriguing complexity of the single-electron spectral function even in such a simple system as the electron gas, urging us to make a more detailed analysis of the experimental data obtained by angle-resolved photoemission spectroscopy (ARPES) in various materials widely ranging from simple to transition metals.

References

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[3] Y. Takada, *Phys. Rev. Lett.* **87**, 226402 (2001).

Author

Y. Takada.