ISSP Workshop/Symposium 2007 on FADFT

The Electron Self-Energy in the Green's-Function Approach: Beyond the GW Approximation

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◎ Thanks to Professor Hiroshi Yasuhara for enlightening discussions for years

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Outline

Preliminaries

- One-particle Green's function G and the self-energy Σ
- Hedin's theory: Self-consistent set of equations for G, Σ, W, Π, and Γ

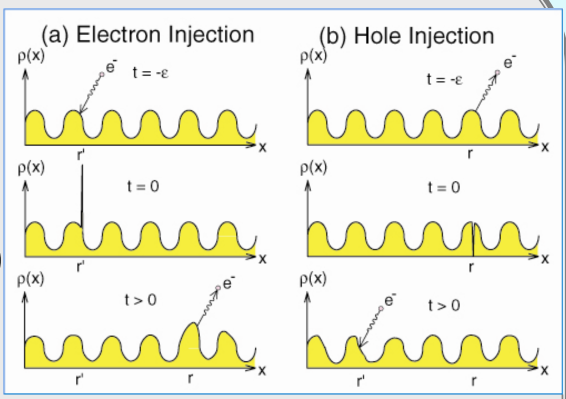
One-Electron Green's Function

$G_{\sigma\sigma'}(\boldsymbol{r},\boldsymbol{r}';t)$

Inject a bare electron with spin σ' at site $\boldsymbol{r}'$ at t=0; let it propage in the system until we observe the propability amplitude of a bare electron with spin σ at site $\boldsymbol{r}$ at t (>0)

→ Electron injection process

$$\langle \psi_\sigma(\mathbf{r},t)\psi^+_{\sigma'}(\mathbf{r}')\rangle$$



Reverse process in time: Pull a bare electron with spin σ out at site $\boldsymbol{r}$ at t=0 first and then put a bare electron with spin σ' back at site $\boldsymbol{r}'$ at t.

→ Hole injection process

$$\langle \psi^+_{\sigma'}(\mathbf{r}',-t)\psi_\sigma(\mathbf{r})\rangle \; (=\langle \psi^+_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r},t)\rangle)$$

$$\boxed{G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';t) \equiv -i\theta(t)\langle\{\psi_\sigma(\mathbf{r},t),\psi^+_{\sigma'}(\mathbf{r}')\}\rangle}$$

Spectral Representation

Complete Set diagonalizing H $\{|n\rangle\}$: $H|n\rangle = E_n|n\rangle$

$$G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\omega) \equiv \int_{-\infty}^{\infty} dt e^{i\omega t} G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';t) \equiv -i\int_0^{\infty} dt e^{i\omega t} \langle\{\psi_\sigma(\mathbf{r},t), \psi^+_{\sigma'}(\mathbf{r}')\}\rangle$$

$$= \sum_{nm} e^{\beta(\Omega-E_n)}(e^{\beta(E_n-E_m)}+1)\frac{\langle n|\psi^+_{\sigma'}(\mathbf{r}')|m\rangle\langle m|\psi_\sigma(\mathbf{r})|n\rangle}{\omega+i0^+ + E_m - E_n}$$

Spectral Function $A_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\omega)$

$$A_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\omega) \equiv -\frac{1}{\pi}\mathrm{Im}\, G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\omega)$$

$$= \sum_{nm} e^{\beta(\Omega-E_n)}(e^{\beta\omega}+1)\langle n|\psi^+_{\sigma'}(\mathbf{r}')|m\rangle\langle m|\psi_\sigma(\mathbf{r})|n\rangle\delta(\omega+E_m-E_n)$$

$$G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\omega) = \int_{-\infty}^{\infty} dE \frac{A_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';E)}{\omega+i0^+ - E}, \quad G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';t) = -i\theta(t)\int_{-\infty}^{\infty} dE\, e^{-iEt} A_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';E)$$

$$\int_{-\infty}^{\infty} dE A_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';E) = \delta_{\sigma,\sigma'}\delta(\mathbf{r}-\mathbf{r}'), \quad \lim_{\omega\to\infty} G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\omega) = \frac{\delta_{\sigma,\sigma'}\delta(\mathbf{r}-\mathbf{r}')}{\omega}$$

Thermal Green's Function

Thermal GF $G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\tau)$ $\quad -\beta < \tau < \beta$

$$G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\tau) \equiv -\langle T_\tau \psi_\sigma(\mathbf{r},\tau)\psi^+_{\sigma'}(\mathbf{r}')\rangle$$

$$\equiv -\theta(\tau)\langle\psi_\sigma(\mathbf{r},\tau)\psi^+_{\sigma'}(\mathbf{r}')\rangle + \theta(-\tau)\langle\psi^+_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r},\tau)\rangle$$

$$\psi_\sigma(\mathbf{r},\tau) \equiv e^{H\tau}\psi_\sigma(\mathbf{r})e^{-H\tau}$$

$$G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\tau) = \int_{-\infty}^{\infty} dE A_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';E)e^{-E\tau}[-\theta(\tau)f(-E)+\theta(-\tau)f(E)]$$

Fermi distribution function $f(E) = (1+e^{\beta E})^{-1}$

Antiperiodic function of period β $\quad G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\tau+\beta) = -G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\tau)$

$$G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\tau) = T\sum_{\omega_p} e^{-i\omega_p\tau}G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';i\omega_p)$$

Fermion Matsubara frequency $\omega_p = \pi T(2p+1)$

$$G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';i\omega_p) = \int_0^{\beta} d\tau\, e^{i\omega_p\tau}G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\tau) = \int_{-\infty}^{\infty} dE \frac{A_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';E)}{i\omega_p - E}$$

$G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';\omega)$ vs $G_{\sigma\sigma'}(\mathbf{r},\mathbf{r}';i\omega_p)$ analytic continuation on ω plane, $\omega+i0^+ \leftrightarrow i\omega_p$

Free Electron Gas

$$H=\sum_\sigma\int d\mathbf{r}\,\psi_\sigma^+(\mathbf{r})\left(\frac{p^2}{2m}-\mu\right)\psi_\sigma(\mathbf{r}),\quad \psi_\sigma(\mathbf{r})=\sum_{\mathbf{p}}u_{\mathbf{p}}c_{\mathbf{p}\sigma}\quad \text{Base: } u_{\mathbf{p}}=\frac{1}{\sqrt{\Omega_t}}e^{i\mathbf{p}\cdot\mathbf{r}}$$

$$H=\sum_{\mathbf{p}\sigma}\xi_{\mathbf{p}}c^+_{\mathbf{p}\sigma}c_{\mathbf{p}\sigma},\qquad \xi_{\mathbf{p}}\equiv \mathbf{p}^2/2m-\mu$$

$$\begin{aligned}G_{\mathbf{p}\sigma\mathbf{p}'\sigma'}(i\omega_p) &= -\int_0^\beta d\tau\langle c_{\mathbf{p}\sigma}(\tau)c^\dagger_{\mathbf{p}'\sigma'}\rangle e^{i\omega_p\tau}\\ &= -\int_0^\beta d\tau e^{(i\omega_p-\xi_{\mathbf{p}})\tau}\langle c_{\mathbf{p}\sigma}c^\dagger_{\mathbf{p}'\sigma'}\rangle\\ &= -\frac{e^{\beta(i\omega_p-\xi_{\mathbf{p}})}-1}{i\omega_p-\xi_{\mathbf{p}}}\delta_{\mathbf{p}\mathbf{p}'}\delta_{\sigma\sigma'}[1-f(\xi_{\mathbf{p}})] = \delta_{\mathbf{p}\mathbf{p}'}\delta_{\sigma\sigma'}G^{(0)}_{\mathbf{p}\sigma}(i\omega_p)\end{aligned}$$

$$G^{(0)}_{\mathbf{p}\sigma}(i\omega_p)\equiv\frac{1}{i\omega_p-\xi_{\mathbf{p}}}\qquad A_{\mathbf{p}\sigma\mathbf{p}'\sigma'}(E)\equiv\delta_{\mathbf{p}\mathbf{p}'}\delta_{\sigma\sigma'}A^{(0)}_{\mathbf{p}\sigma}(E)=\delta_{\mathbf{p}\mathbf{p}'}\delta_{\sigma\sigma'}\delta(E-\xi_{\mathbf{p}})$$

$G_{p\sigma}^{(0)}(i\omega_p)$: characterized by the first-order pole at ξ_p in the complex $i\omega_{\mathrm{p}}$ (=ω) plane

Equation of Motion

$$H=\sum_\sigma\int d\mathbf{r}\;\psi_\sigma^+(\mathbf{r})\left(-\frac{1}{2m}\nabla_{\mathbf{r}}^2+v(\mathbf{r})\right)\psi_\sigma(\mathbf{r})+\frac{1}{2}\sum_{\sigma\sigma'}\int d\mathbf{r}\int d\mathbf{r}'\;\psi_\sigma^+(\mathbf{r})\psi_{\sigma'}^+(\mathbf{r}')u(\mathbf{r},\mathbf{r}')\psi_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r})$$

$$\frac{\partial G(\mathbf{r},\mathbf{r}';\tau)}{\partial\tau}=-\delta(\tau)\langle\{\psi_\sigma(\mathbf{r}),\psi_\sigma^+(\mathbf{r}')\}\rangle-\langle T_\tau e^{H\tau}[H,\psi_\sigma(\mathbf{r})]e^{-H\tau}\psi_\sigma^+(\mathbf{r}')\rangle$$

$$\begin{aligned}&\frac{\partial G(\mathbf{r},\mathbf{r}';\tau)}{\partial\tau}+\delta(\tau)\delta(\mathbf{r}-\mathbf{r}')+\left(-\frac{1}{2m}\nabla_{\mathbf{r}}^2+v(\mathbf{r})\right)G(\mathbf{r},\mathbf{r}';\tau)\\ &\quad=\sum_{\sigma'}\int d\mathbf{x}\;u(\mathbf{r},\mathbf{x})\langle T_\tau\psi^+_{\sigma'}(\mathbf{x},\tau)\psi_{\sigma'}(\mathbf{x},\tau)\psi_\sigma(\mathbf{r},\tau)\psi_\sigma^+(\mathbf{r}')\rangle\\ &\quad=\int d\mathbf{x}\;u(\mathbf{r},\mathbf{x})\int_0^\beta d\tau'\delta(\tau-\tau')\langle T_\tau\psi_\sigma(\mathbf{r},\tau)\sum_{\sigma'}\psi^+_{\sigma'}(\mathbf{x},\tau')\psi_{\sigma'}(\mathbf{x},\tau')\psi_\sigma^+(\mathbf{r}')\rangle\\ &\quad=\int d\mathbf{x}\;u(\mathbf{r},\mathbf{x})\int_0^\beta d\tau'\delta(\tau-\tau')\langle T_\tau\psi_\sigma(\mathbf{r},\tau)\rho(\mathbf{x},\tau')\psi_\sigma^+(\mathbf{r}')\rangle\end{aligned}$$

Self-Energy

Dyson Equation

$$\left(i\omega_p+\frac{1}{2m}\nabla_{\mathbf{r}}^2-v(\mathbf{r})-\int d\mathbf{z}\,u(\mathbf{r},\mathbf{z})\langle\rho(\mathbf{z})\rangle\right)G(\mathbf{r},\mathbf{r}';i\omega_p)-\int d\mathbf{x}\,\Sigma(\mathbf{r},\mathbf{x};i\omega_p)G(\mathbf{x},\mathbf{r}';i\omega_p)=\delta(\mathbf{r}-\mathbf{r}')$$

$$\rho(\mathbf{x})[\equiv \textstyle\sum_{\sigma'}\psi_{\sigma'}^{+}(\mathbf{x})\psi_{\sigma'}(\mathbf{x})]\ ;\ \langle\rho(\mathbf{z})\rangle=\displaystyle\sum_{\sigma}G(\mathbf{z},\mathbf{z};-0^{+})=\sum_{\sigma}T\sum_{\omega_p}G(\mathbf{z},\mathbf{z};i\omega_p)e^{i\omega_p 0^{+}}$$

Self-Energy

$$\Sigma(\mathbf{r},\mathbf{x};i\omega_p)=-T\sum_{\omega_{p'}}\int d\mathbf{z}\int d\mathbf{y}\ u(\mathbf{r},\mathbf{z})G(\mathbf{r},\mathbf{y};i\omega_{p'})\Lambda(\mathbf{y},\mathbf{z},\mathbf{x};i\omega_{p'},i\omega_p)$$

Three-Point Vertex Function

$$\Lambda(\mathbf{y},\mathbf{z},\mathbf{x};i\omega_{p'},i\omega_p)=\int d\mathbf{y}'\int d\mathbf{x}'\int_0^\beta d\tau e^{i\omega_{p'}\tau}\int_0^\beta d\tau' e^{i(\omega_p-\omega_{p'})\tau'}\,G^{-1}(\mathbf{y},\mathbf{y}';i\omega_{p'})$$
$$\times\langle T_\tau\psi_\sigma(\mathbf{y}',\tau)\rho(\mathbf{z},\tau')\psi_\sigma^{+}(\mathbf{x}')\rangle_{\text{connected}}\,G^{-1}(\mathbf{x}',\mathbf{x};i\omega_p)$$

Density-Density Response Function

Density-Density Response Function

$$Q_{\rho\rho}(\mathbf{r},\mathbf{r}';i\omega_q)=-\int_0^\beta d\tau\ e^{i\omega_q\tau}\langle T_\tau\rho(\mathbf{r},\tau)\rho(\mathbf{r}')\rangle$$
$$=\sum_\sigma\int_0^\beta d\tau'\ e^{i\omega_q\tau'}\langle T_\tau\psi_\sigma(\mathbf{r}',-0^{+})\rho(\mathbf{r},\tau')\psi_\sigma^{+}(\mathbf{r}')\rangle$$
$$=\sum_\sigma T\sum_{\omega_p}e^{i\omega_p 0^{+}}\int d\mathbf{x}\int d\mathbf{y}\ G(\mathbf{r}',\mathbf{y};i\omega_p)\Lambda(\mathbf{y},\mathbf{r},\mathbf{x};i\omega_p,i\omega_p+i\omega_q)G(\mathbf{x},\mathbf{r}';i\omega_p+i\omega_q)$$

$$\Lambda(\mathbf{y},\mathbf{z},\mathbf{x};i\omega_{p'},i\omega_p)=\Gamma(\mathbf{y},\mathbf{z},\mathbf{x};i\omega_{p'},i\omega_p)$$
$$+\int d\mathbf{z}'\int d\mathbf{z}''\ Q_{\rho\rho}(\mathbf{z},\mathbf{z}';i\omega_p-i\omega_{p'})\,u(\mathbf{z}',\mathbf{z}'')\Gamma(\mathbf{y},\mathbf{z}'',\mathbf{x};i\omega_{p'},i\omega_p)$$

Polarization Function

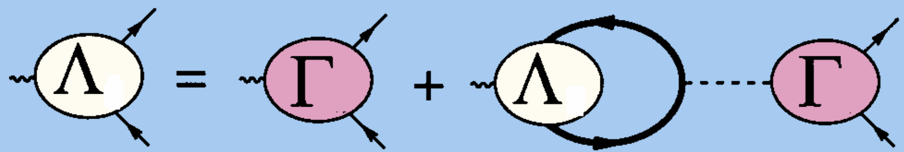
$$\Pi(\mathbf{r},\mathbf{r}';i\omega_q)$$
$$=-\sum_\sigma T\sum_{\omega_p}e^{i\omega_p 0^{+}}\int d\mathbf{x}\int d\mathbf{y}\,G(\mathbf{r}',\mathbf{y};i\omega_p)\Gamma(\mathbf{y},\mathbf{r},\mathbf{x};i\omega_p,i\omega_p+i\omega_q)G(\mathbf{x},\mathbf{r}';i\omega_p+i\omega_q)$$

$$Q_{\rho\rho}(\mathbf{r},\mathbf{r}';i\omega_q)=-\Pi(\mathbf{r},\mathbf{r}';i\omega_q)-\int d\mathbf{z}\int d\mathbf{z}'\ Q_{\rho\rho}(\mathbf{r},\mathbf{z};i\omega_q)u(\mathbf{z},\mathbf{z}')\Pi(\mathbf{z}',\mathbf{r}';i\omega_q)$$

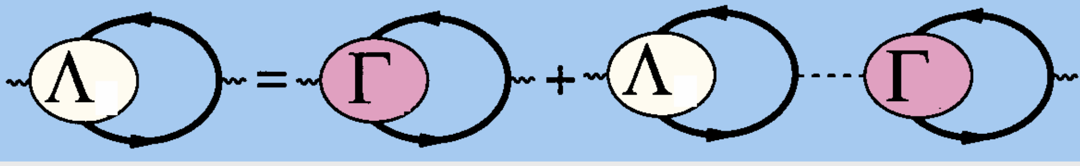
Polarization Function

$Q_{\rho\rho}$: Response to the external test charge
$-\Pi$: Response to the total (test+induced) charge

(1) $\Gamma\,(y,z,x;i\omega_{p'},\omega_p)$



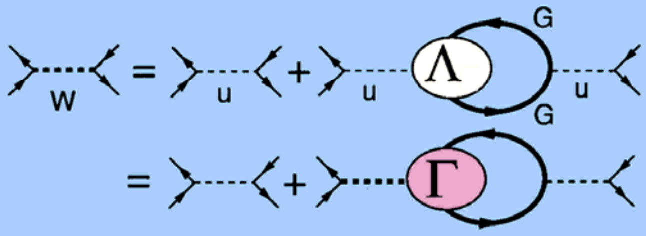
(2) $\Pi\,(r,r';i\omega_q)$



Effective Electron-Electron Interaction

W: (Direct Coulomb)+(Charge-Fluctuation mediated)

$$W(\mathbf{r},\mathbf{r}';i\omega_q)=u(\mathbf{r},\mathbf{r}')+\int d\mathbf{x}\int d\mathbf{y}\;u(\mathbf{r},\mathbf{x})Q_{\rho\rho}(\mathbf{x},\mathbf{y};i\omega_q)u(\mathbf{y},\mathbf{r}')$$
$$=u(\mathbf{r},\mathbf{r}')-\int d\mathbf{x}\int d\mathbf{y}\;W(\mathbf{r},\mathbf{x};i\omega_q)\Pi(\mathbf{x},\mathbf{y};i\omega_q)u(\mathbf{y},\mathbf{r}')$$



$$\int d\mathbf{z}\;u(\mathbf{r},\mathbf{z})\Lambda(\mathbf{y},\mathbf{z},\mathbf{x};i\omega_{p'},i\omega_p)=\int d\mathbf{z}\;W(\mathbf{r},\mathbf{z};i\omega_p-i\omega_{p'})\Gamma(\mathbf{y},\mathbf{z},\mathbf{x};i\omega_{p'},i\omega_p)$$

$$\Sigma(\mathbf{r},\mathbf{x};i\omega_p)=-T\sum_{\omega_{p'}}\int d\mathbf{z}\int d\mathbf{y}\;u(\mathbf{r},\mathbf{z})G(\mathbf{r},\mathbf{y};i\omega_{p'})\Lambda(\mathbf{y},\mathbf{z},\mathbf{x};i\omega_{p'},i\omega_p)$$
$$=-T\sum_{\omega_{p'}}\int d\mathbf{y}\int d\mathbf{z}\,G(\mathbf{r},\mathbf{y};i\omega_{p'})W(\mathbf{r},\mathbf{z};i\omega_p-i\omega_{p'})\Gamma(\mathbf{y},\mathbf{z},\mathbf{x};i\omega_{p'},i\omega_p)$$

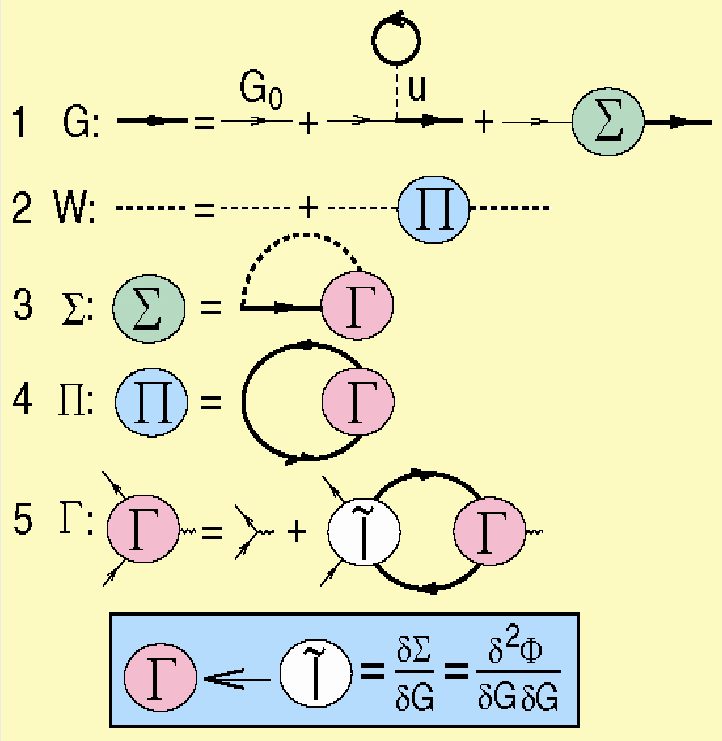
Hedin's Theory

L. Hedin: *Phys. Rev.* **139**, A796 (1965)

Philosophy

Rather than using the bare particle (G_0) and the bare interaction (u), we should describe physics in terms of real physical quantities like the quasi-particle (G) and the actual effective interaction (W).

→ Closed set of equations determining G, W, Σ, Π, and Γ self-consistently.



Comparison with TDDFT

Hedin Theory vs. TDDFT

$$Q_{\rho\rho}(r,r';t) = -i\,\theta(t)\langle[\rho(r,t),\rho(r',0)]\rangle$$

1) $$Q_{\rho\rho} = -\frac{\Pi}{1+u\Pi}$$

2) Basic component in TDDFT: Π_0

$$Q_{\rho\rho} = -\Pi_0 + \Pi_0(u+f_{xc})\,Q_{\rho\rho}$$

Key quantity in TDDFT: f_{xc}

$$f_{xc} = \frac{\delta v_{xc}}{\delta n} = \frac{\delta^2 E_{xc}}{\delta n\,\delta n} \longleftrightarrow \tilde{\Gamma} = \frac{\delta\Sigma}{\delta G} = \frac{\delta^2\Phi}{\delta G\,\delta G}$$

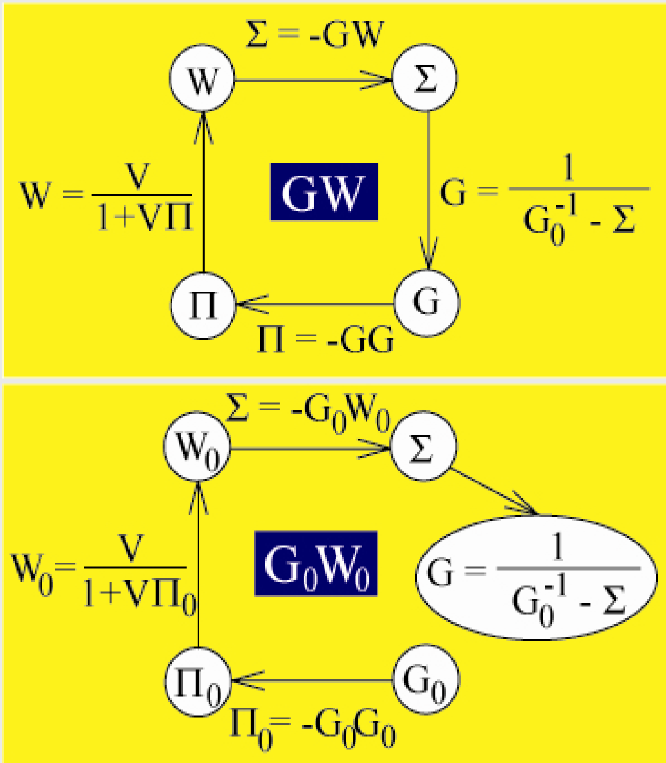
GW Approximation

In actual calculations, it is very often the case that Γ is taken as unity, neglecting the vertex correction altogether.

→GW approximation

Even the self-consistent iterative procedure is abandoned.

→G_0W_0 calculation



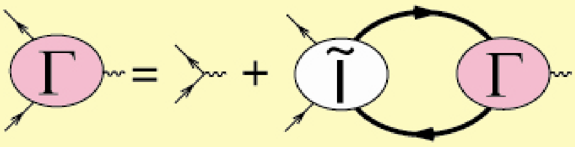
Part I. *GWΓ* Scheme

- Introducing “the ratio function”
- Averaging the irreducible electron-hole effective interaction
- Exact functional form for *Γ*
- An approximation scheme for *Γ*

Vertex Functions

Irreducible Electron-Hole Effective Interaction

$$\tilde{I} = \frac{\delta\Sigma}{\delta G} = \frac{\delta^2\Phi}{\delta G\,\delta G}$$



Scalar and Vector Vertex Functions: Γ and $\boldsymbol{\Gamma}$

Bethe-Salpeter Equation

$$\Gamma(p+q,p) = 1 + \sum_{p'} \tilde{I}(p+q,p;p'+q,p')G(p'+q)G(p')\Gamma(p'+q,p')$$

$$\boldsymbol{\Gamma}(p+q,p) = \boldsymbol{\gamma}(p+q,p) + \sum_{p'} \tilde{I}(p+q,p;p'+q,p')G(p'+q)G(p')\boldsymbol{\Gamma}(p'+q,p')$$

$$\mathbf{q}\cdot\boldsymbol{\gamma}(p+q,p) = \epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}} \qquad p=(\mathbf{p},i\omega_n)$$

Ward Identity

Those vertex functions satisfy the Ward identity, representing the conservation of local electron number:

$$q_0\Gamma(p+q,p) - \mathbf{q}\cdot\boldsymbol{\Gamma}(p+q,p) = G^{-1}(p+q) - G^{-1}(p)$$
$$= q_0 - \epsilon_{\mathbf{p}+\mathbf{q}} + \epsilon_{\mathbf{p}} - \Sigma(p+q) + \Sigma(p)$$

$$q_0 = i\omega_q = i2\pi Tq \;\; (q = 0, \pm1, \pm2, \pm3, \cdots)$$

In the GW approximation, this basic law is not respected.

Steps to Determine the Functional Form for Γ

1. Introducing "the ratio function": $R(p+q,p)$
2. Introducing "the average of the irreducible electron-hole effective interaction": $\langle \tilde{I} \rangle_{p+q,p}$
3. Exact relation between $R(p+q,p)$ and $\langle \tilde{I} \rangle_{p+q,p}$
4. Exact functional form for $\Gamma(p+q,p)$ in terms of $\langle \tilde{I} \rangle_{p+q,p}$
5. Approximation to this functional form

Ratio Function

1^0 Definition: Ratio between the scalar vertex and the longitudinal part of the vector vertex

$$R(p+q,p) \equiv \frac{\Gamma(p+q,p)\mathbf{q}\cdot\boldsymbol{\gamma}(p+q,p)}{\mathbf{q}\cdot\boldsymbol{\Gamma}(p+q,p)}$$

2^0 Represent the vertex functions in terms of R(p+q,p):

$$\Gamma(p+q,p) = \frac{G(p+q)^{-1} - G(p)^{-1}}{q_0 - (\varepsilon_{\mathbf{p+q}} - \varepsilon_{\mathbf{p}})/R(p+q,p)}$$

$$\mathbf{q}\cdot\boldsymbol{\Gamma}(p+q,p) = \frac{G(p+q)^{-1} - G(p)^{-1}}{-1 + R(p+q,p)q_0/(\varepsilon_{\mathbf{p+q}} - \varepsilon_{\mathbf{p}})}$$

3^0 Make an approximation through R(p+q,p), which automatically guarantees the Ward identity.

Average of the Irreducible EH Effective Interaction

1^0 Definition:

$$\langle \tilde{I} \rangle_{p+q,p} \equiv \frac{\sum_{p'} \tilde{I}(p+q,p;p'+q,p')G(p')G(p'+q)\Gamma(p'+q,p')}{\sum_{p'} G(p')G(p'+q)\Gamma(p'+q,p')}$$

2^0 Rewrite the Bethe-Salpeter equation using $\langle \tilde{I} \rangle_{p+q,p}$ as

$$\Gamma(p+q,p) = 1 - \langle \tilde{I} \rangle_{p+q,p}\Pi(q)$$

$$\mathbf{q}\cdot\mathbf{\Gamma}(p+q,p) = \varepsilon_{\mathbf{p+q}} - \varepsilon_{\mathbf{p}} - q_0 \langle \tilde{I} \rangle_{p+q,p}\Pi(q) - \sum_{p'} \tilde{I}(p+q,p;p'+q,p')[G(p'+q) - G(p')]$$

3^0 Accurate functional form for $\Gamma(p+q,p)$:

$$\Gamma(p+q,p) = \left[1 - \langle \tilde{I} \rangle_{p+q,p}\Pi(q)\right]\Gamma_{\mathrm{WI}}(p+q,p)$$

$$\Gamma_{\mathrm{WI}}(p+q,p) \equiv \frac{G(p+q)^{-1} - G(p)^{-1}}{\tilde{G}(p+q)^{-1} - \tilde{G}(p)^{-1}}$$

$$\tilde{G}(p)^{-1} \equiv G_0(p)^{-1} - \sum_{p'} \tilde{I}(p+q,p;p'+q,p')G(p')$$

Approximate Functional Form for Γ

1^0 Assume $\tilde{I}(p+q,p;p'+q,p') \approx \langle \tilde{I} \rangle_{p+q,p} \approx \bar{I}(q)$

$$\Gamma(p+q,p) = \frac{\Gamma_{\mathrm{WI}}(p+q,p)}{1+\bar{I}(q)\Pi_{\mathrm{WI}}(q)}$$

$$\Gamma_{\mathrm{WI}}(p+q,p) = \frac{G(p+q)^{-1} - G(p)^{-1}}{G_0(p+q)^{-1} - G_0(p)^{-1}}$$

$$\Pi_{\mathrm{WI}}(q) \equiv -\sum_{p} G(p+q)G(p)\Gamma_{\mathrm{WI}}(p+q,p)$$

2^0 Dielectric Function

$$\epsilon(q) \equiv 1 + V(\mathbf{q})\Pi(q)$$

$$= 1 + V(\mathbf{q})\Pi_0(q) \quad \text{: RPA}$$

$$= 1 + V(\mathbf{q})\frac{\Pi_0(q)}{1 - G_+(\mathbf{q})V(\mathbf{q})\Pi_0(q)} \quad \text{: Local Field Correction}$$

$$= 1 + V(\mathbf{q})\frac{\Pi_{\mathrm{WI}}(q)}{1+\bar{I}(q)\Pi_{\mathrm{WI}}(q)} \quad \text{: GW}\Gamma$$

Modified Lindhard Function $\Pi_{WI}(q)$

Rewrite $\Pi_{WI}(q)$:

$$\Pi_{WI}(q) \equiv -\sum_p G(p+q)G(p)\Gamma_{WI}(p+q,p)$$

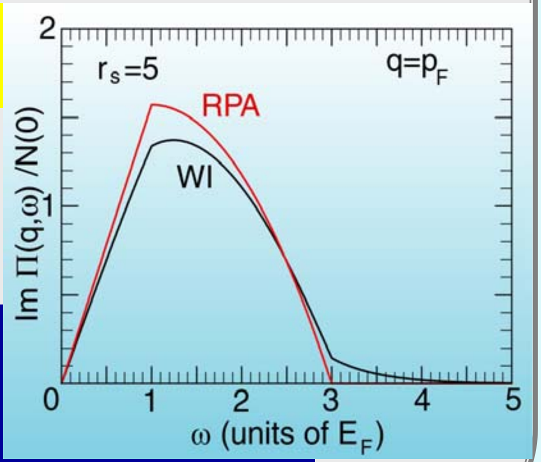
$$\Gamma_{WI}(p+q,p) = \frac{G(p+q)^{-1} - G(p)^{-1}}{G_0(p+q)^{-1} - G_0(p)^{-1}}$$

$\Pi_{WI}(q)$ is reduced to "the modified Lindhard function":

$$\Pi_{WI}(q) = 4\sum_{\mathbf{p}} n(\mathbf{p}) \frac{\varepsilon_{\mathbf{p+q}} - \varepsilon_{\mathbf{p}}}{\omega_q^2 + (\varepsilon_{\mathbf{p+q}} - \varepsilon_{\mathbf{p}})^2}$$

$$n(\mathbf{p}) = \lim_{\eta\to+0} T\sum_{\omega_p} G(p)e^{i\omega_p\eta}$$

$$\Pi_0(q) = 4\sum_{\mathbf{p}} \theta(p_F - |\mathbf{p}|) \frac{\varepsilon_{\mathbf{p+q}} - \varepsilon_{\mathbf{p}}}{\omega_q^2 + (\varepsilon_{\mathbf{p+q}} - \varepsilon_{\mathbf{p}})^2}$$



This function has been intuitively introduced and discussed by:
G. Niklasson, *PRB* **10**, 3052 (1974);
G. Vignale, *PRB* **38**, 6445 (1988);
C. F. Richardson and N. W. Ashcroft, *PRB* **50**, 8170 (1994).

Approaches to the Average Irreducible EH Interaction

◎ **Definition:**

$$\langle\tilde{I}\rangle_{p+q,p} \equiv \frac{\sum_{p'} \tilde{I}(p+q,p;p'+q,p')G(p')G(p'+q)\Gamma(p'+q,p')}{\sum_{p'} G(p')G(p'+q)\Gamma(p'+q,p')}$$

◎ **Condition to be satisfied** (Compressibility sum rule):

$$\lim_{\mathbf{q}\to\mathbf{0}} \left[1 - \langle\tilde{I}\rangle_{p+q,p}\Pi(q)\right]\Big|_{|\mathbf{p}|=p_{\mathbf{F}},\,\omega_q=0} = \frac{\kappa}{\kappa_0}$$

◎ **Approximation schemes:**

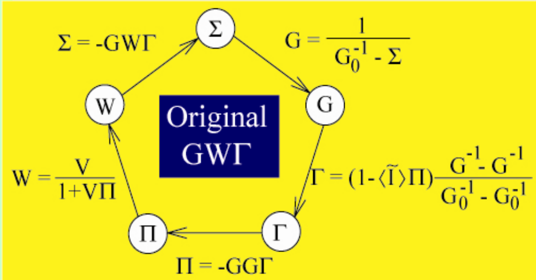
- Apply perturbation theory from both weak- and strong-coupling limits
- Borrow some useful accurate results obtained by QMC
- Adopt physical arguments, leading to the concept of "local field correction" $G_+(\mathbf{q},\omega)$ or "the exchange-correlation kernel" $f_{xc}(q,\omega)$ appearing in the TDDFT.

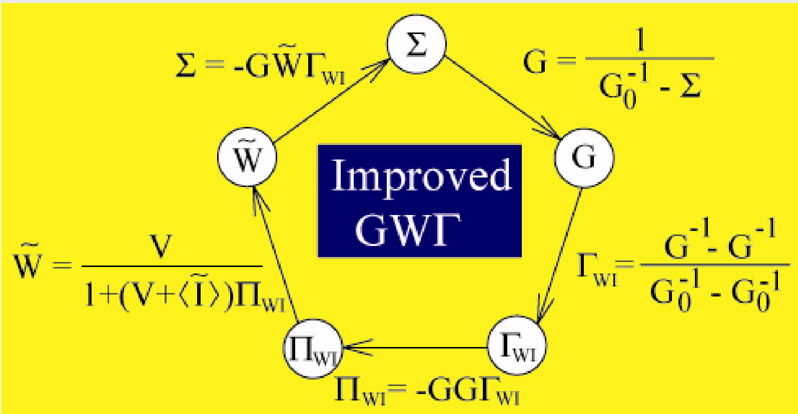
GWΓ Scheme

◎ Original GWΓ scheme [YT, PRL87, 226402 (2001)]:

(1) Time consuming in calculating Π;

(2) Difficulty associated with the divergence of Π at r_s=5.25 where κ diverges in the electron gas.





Part II. Illustrations

- Localized limit: Single-site system with both electron-electron and electron-phonon interactions
- Extended limit: Homogeneous electron gas

Single-Site Problem

◎Hamiltonian :

$$H = Un_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow) + \omega_0 a^\dagger a + \sqrt{\alpha}\omega_0(n_\uparrow + n_\downarrow)(a + a^\dagger)$$

◎Thermal Green's function:

$$\boxed{G_\sigma(\tau) = -\langle T_\tau c_\sigma(\tau) c_\sigma^+ \rangle} \quad n_\sigma = c_\sigma^+ c_\sigma, \ \ c_\sigma(\tau) = e^{\tau H} c_\sigma e^{-\tau H}$$

The result for $A(\Omega)$ at $T \ll 1$: (Exact result)

$$A(\Omega) = e^{-\alpha} \sum_{\ell=0}^{\infty} \frac{\alpha^\ell}{\ell!} \left[f_0(\mu+\alpha\omega_0)\delta(\Omega-\ell\omega_0+\mu+\alpha\omega_0) + f_1(\mu+\alpha\omega_0)\delta(\Omega-\ell\omega_0+\mu-U+3\alpha\omega_0) \right.$$
$$\left. + f_1(\mu+\alpha\omega_0)\delta(\Omega+\ell\omega_0+\mu+\alpha\omega_0) + f_2(\mu+\alpha\omega_0)\delta(\Omega+\ell\omega_0+\mu-U+3\alpha\omega_0) \right]$$

$$f_0(\Omega) = \frac{1}{1 + 2\exp(\Omega/T) + \exp[(2\Omega - U + 2\alpha\omega_0)/T]}$$

$$f_1(\Omega) = \exp(\Omega/T) f_0(\Omega) \qquad f_2(\Omega) = \exp[(2\Omega - U + 2\alpha\omega_0)/T] f_0(\Omega)$$

$$\frac{\langle N_\sigma \rangle}{N} = \int_{-\infty}^{\infty} d\Omega f(\Omega) A(\Omega)$$

$$\boxed{G(\omega) = \int_{-\infty}^{\infty} d\Omega \frac{A(\Omega)}{\omega + i0^+ - \Omega}}$$

Single-Site Hubbard Model

Exact Result for the thermal Green's Function

$$G_{\uparrow\uparrow}(\tau) = -\theta(\tau)\langle c_\uparrow(\tau) c_\uparrow^+ \rangle + \theta(-\tau)\langle c_\uparrow^+ c_\uparrow(\tau) \rangle$$
$$= -\theta(\tau)\left[e^{\tau(\mu-\varepsilon_0)} \langle (1-n_\downarrow)(1-n_\uparrow) \rangle + e^{\tau(\mu-\varepsilon_0-U)} \langle n_\downarrow (1-n_\uparrow) \rangle \right]$$
$$+\theta(-\tau)\left[e^{\tau(\mu-\varepsilon_0)} \langle n_\uparrow (1-n_\downarrow) \rangle + e^{\tau(\mu-\varepsilon_0-U)} \langle n_\uparrow n_\downarrow \rangle \right]$$

$$\boxed{G_{\uparrow\uparrow}(i\omega_p) = \int_0^\beta d\tau e^{i\omega_p \tau} G_{\uparrow\uparrow}(\tau)}$$

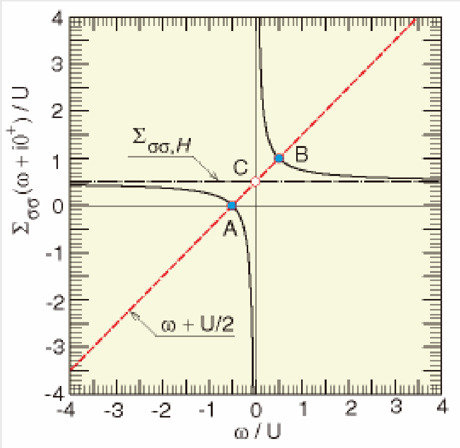
$$= \langle (1-n_\downarrow)(1-n_\uparrow) \rangle \frac{1 + e^{\beta(\mu-\varepsilon_0)}}{i\omega_p - \varepsilon_0 + \mu} + \langle n_\downarrow (1-n_\uparrow) \rangle \frac{1 + e^{\beta(\mu-\varepsilon_0-U)}}{i\omega_p - \varepsilon_0 - U + \mu}$$

$$\boxed{= \frac{1 - \langle n_\downarrow \rangle}{i\omega_p - \varepsilon_0 + \mu} + \frac{\langle n_\downarrow \rangle}{i\omega_p - \varepsilon_0 - U + \mu}}$$

Self-Energy for the Single-Site Hubbard Model

At half filling (Electron-hole symmetric case):

$$G(i\omega_p) = \frac{1}{2}\frac{1}{i\omega_p + U/2} + \frac{1}{2}\frac{1}{i\omega_p - U/2} \qquad \Sigma(\omega + i0^+) = \frac{U}{2} + \frac{U^2}{4}\frac{1}{\omega + i0^+}$$



On-shell value: poles of $G(\omega)$ → Two solutions of $\omega+U/2=\Sigma_{\sigma\sigma}(\omega)$;
On the other hand, there is only single solution in the mean-filed approximation.

Double-Site Hubbard Model at Half Filling

Hamiltonian

$$H = -t\sum_\sigma (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) - \mu \sum_{i\sigma} n_{i\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

$$c_{\pm\sigma} \equiv \frac{1}{\sqrt{2}}(c_{1\sigma} \pm c_{2\sigma})$$

One-electron Green's function

$$G_\pm(i\omega_p) = -\int_0^\beta d\tau\, e^{i\omega_p\tau}\langle T_\tau c_{\pm\sigma}(\tau)c_{\pm\sigma}^\dagger\rangle$$

$$= \frac{1}{4}\left(\sqrt{1+\gamma} \mp \sqrt{1-\gamma}\right)^2 \frac{1}{i\omega_p \mp t - \sqrt{U^2/4+4t^2}} + \frac{1}{4}\left(\sqrt{1+\gamma} \pm \sqrt{1-\gamma}\right)^2 \frac{1}{i\omega_p \mp t + \sqrt{U^2/4+4t^2}}$$

where $\gamma = U/\sqrt{U^2+16t^2}$

Self-Energy of the Doble-Site Hubbard Model

Self-energy

$$G_\pm(i\omega_p) = \frac{i\omega_p \mp 3t}{(i\omega_p \mp t)^2 - 4t^2 - U^2/4} \qquad G_\pm^{(0)}(i\omega_p) = \frac{1}{i\omega_p \pm t}$$

$$G_\pm(i\omega_p) = \frac{1}{i\omega_p \pm t + \mu - \Sigma_\pm(i\omega_p)}$$

$$\boxed{\Sigma_\pm(i\omega_p) = \frac{U}{2} + \frac{U^2}{4}\frac{1}{i\omega_p \mp 3t}}$$

cf. Self-energy of the One-site Hubbard Model

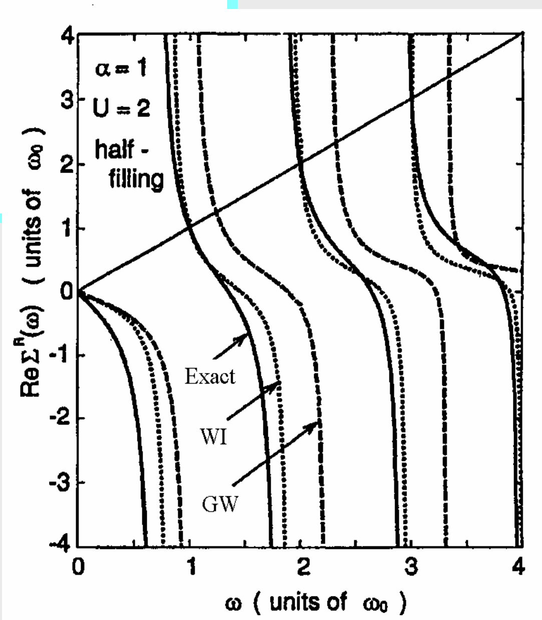
$$\boxed{\Sigma(i\omega_p) = \frac{U}{2} + \frac{U^2}{4}\frac{1}{i\omega_p}}$$

Self-Energy of the Single-Site H-H Model

Self-energy at half filling with U=$2\alpha\omega_0$

$$G(i\omega_p) = \frac{1}{i\omega_p + \mu - \Sigma(i\omega_p)} \qquad G^R(\omega) = \frac{1}{\omega + i0^+ + \mu - \Sigma^R(\omega)}$$

$$\Sigma^R(\omega) = \omega\left[1 - \frac{e^\alpha}{1 + \sum_{\ell=1}^{\infty}\frac{\alpha^\ell}{\ell!}\frac{(\omega+i0^+)^2}{(\omega+i0^+)^2 - \ell^2\omega_0^2}}\right]$$



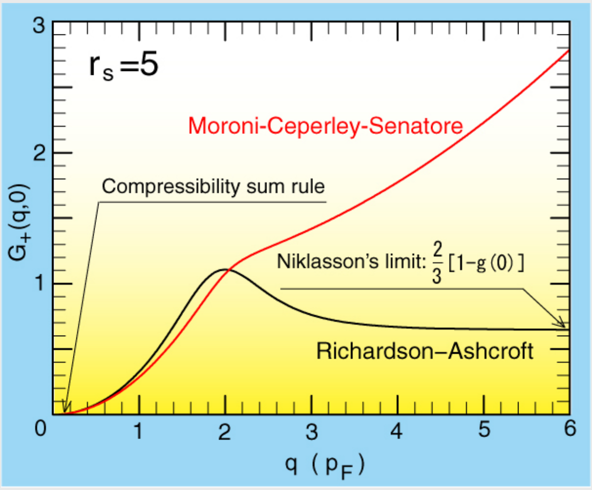
Inclusion of Γ_{WI} gives correct excitation energies, while *GW* does not.

Application to the Electron Gas

Choose $\bar{I}(q) \equiv -G_+(\mathbf{q})V(\mathbf{q})$ with using the modified local field correction $G_+(\boldsymbol{q}, i\omega_q)$ in the Richardson-Ashcroft form [*PRB* **50**, 8170 (1994)].

This $G_+(\boldsymbol{q}, i\omega_q)$ is not the usual one, but is defined for the true particle or in terms of $\Pi_{WI}(q)$.

Accuracy in using this $G_+(\boldsymbol{q}, i\omega_q)$ was well assessed by M. Lein, E. K. U. Gross, and J. P. Perdew, *PRB* **61**, 13431 (2000).

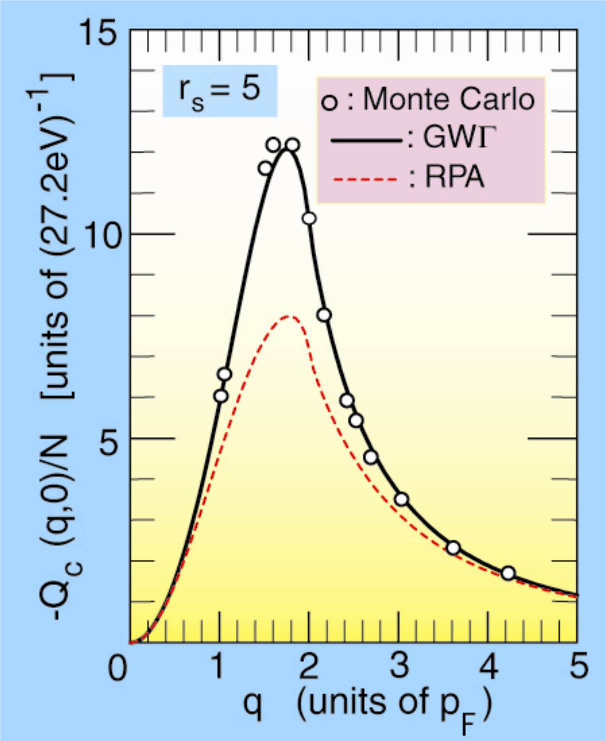


Accuracy Check for the GWΓ Scheme

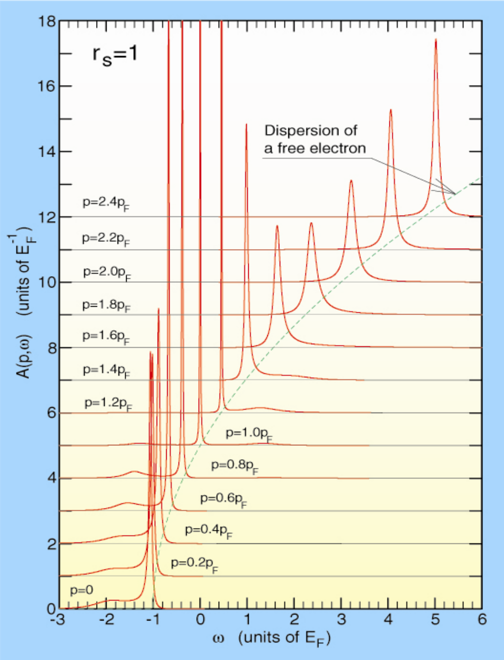
- Density Response Function $Q_c(\boldsymbol{q}, \omega)$

$$Q_c(\mathbf{q},\omega) = -\frac{\Pi(\mathbf{q},\omega)}{\varepsilon(\mathbf{q},\omega)}$$

- Monte Carlo data at ω=0: S. Moroni, D. M. Ceperley, and G. Senatore, *PRL* **75**, 689 (1995).

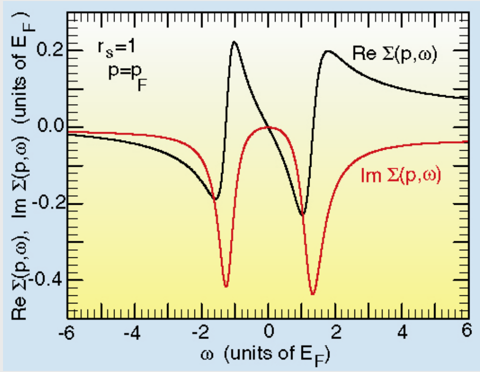


$A(p,\omega)$ and $\Sigma(p,\omega)$



$$A(\mathbf{p},\omega) = -\frac{1}{\pi}\,\mathrm{Im}G(\mathbf{p},\omega)$$

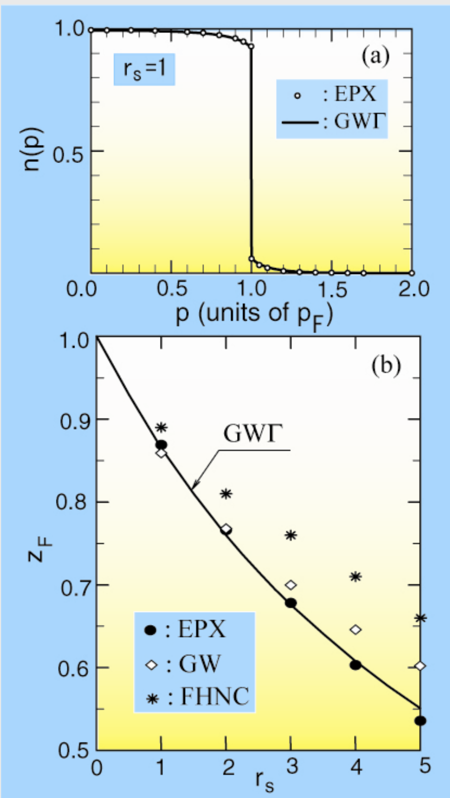
YT, *PRL* **89**, 226402 (2001); *Int. J. Mod. Phys.* B **15**, 2595 (2001).

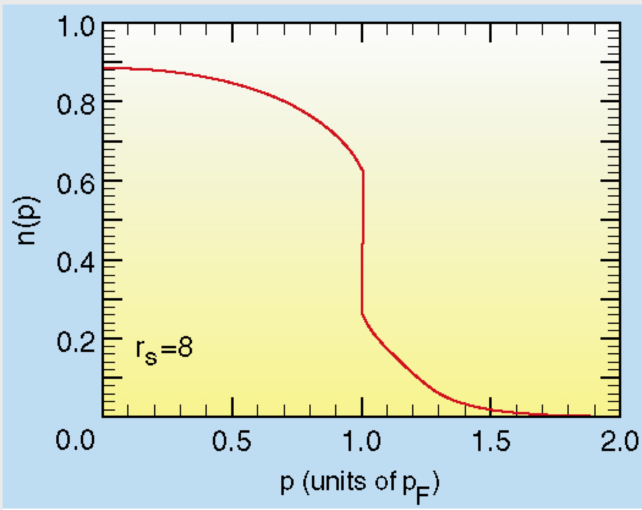


Note: This $\Sigma(\boldsymbol{p},\omega)$ is shifted by μ_{xc}.

- Nonmonotonic behavior of the life time of the quasiparticle (related to the onset of the Landau damping of plasmons)
- Plasmon satellites (Plasmaron)

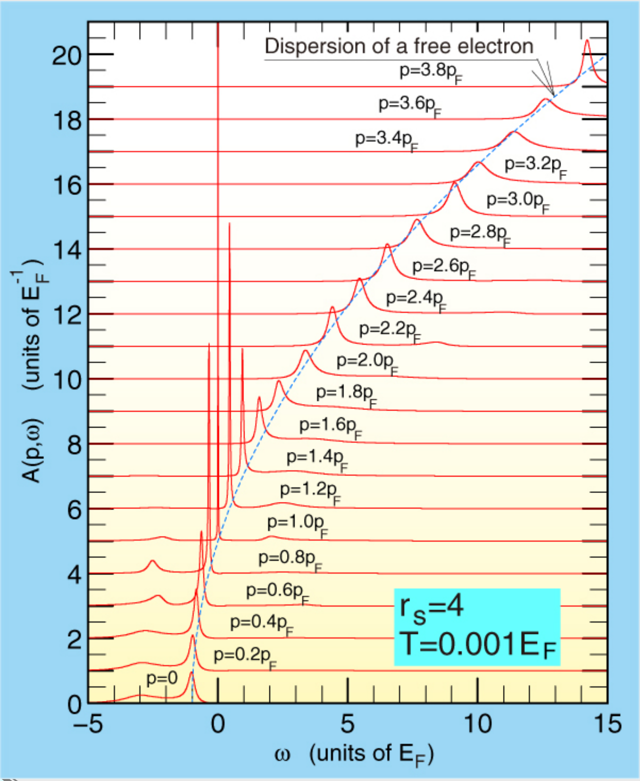
$n(p)$

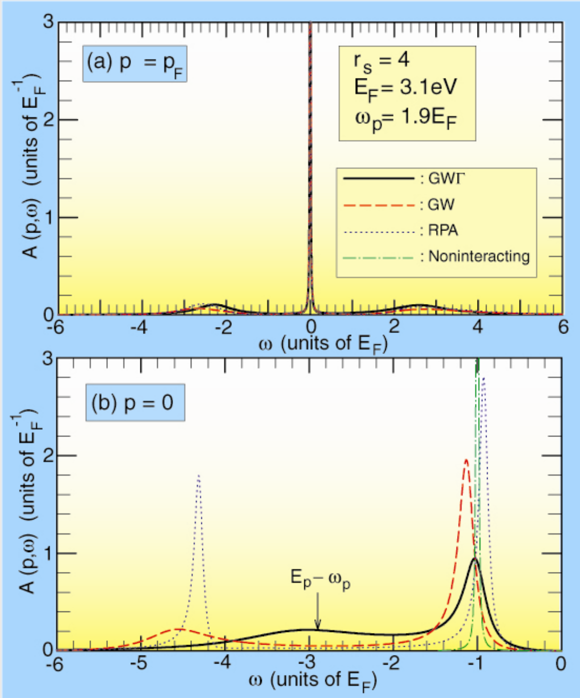




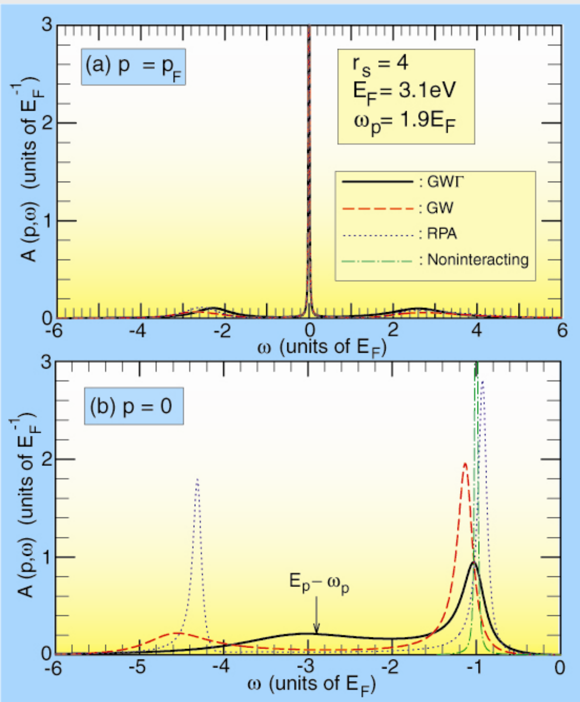
cf. EPX (Effective-Potential Expansion) data: YT & H. Yasuhara, *PRB* **44**, 7879 (1991).

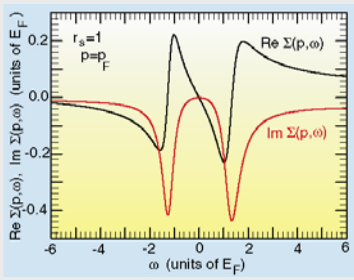
$A\ (p,\omega)$ at $r_s=4$

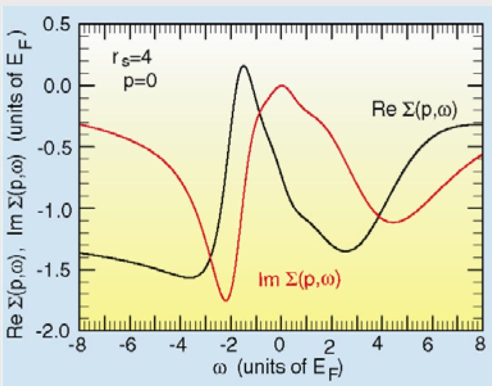




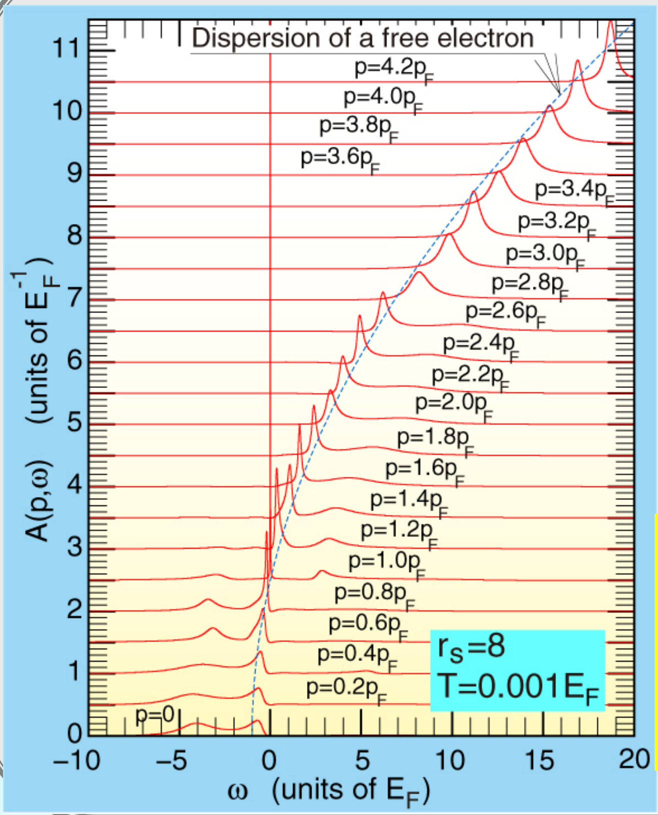
$\Sigma(p,\omega)$

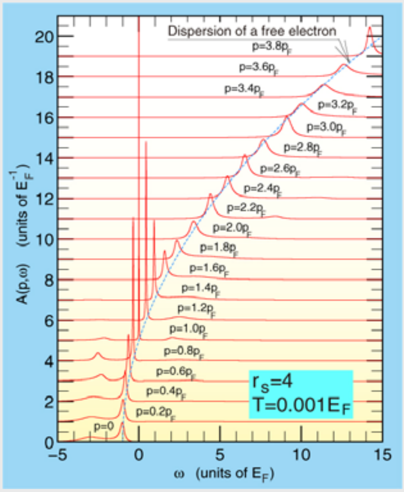






$A(p,\omega)$ at r_s=8

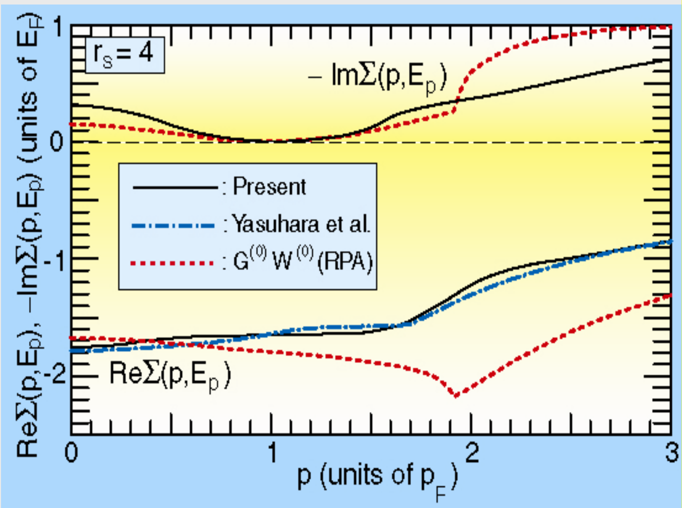




$m^*/m>1$ for $p<p_F$ ← correlation effect dominates;
$m^*/m<1$ for $p>p_F$ ← exchange effect dominates.

Quasiparticle Self-Energy Correction

ReΣ(*p*,*E*$_p$) and **ImΣ(*p*,*E*$_p$)**



- ReΣ increases monotonically.
  → Slight widening of the bandwidth
- ReΣ is fairly flat for $p<1.5p_F$
  → reason for success of LDA
- ReΣ is in proportion to $1/p$ for $p>2p_F$ and it can never be neglected at $p=4.5p_F$ where E_p=66eV. (←interacting electron-gas model)

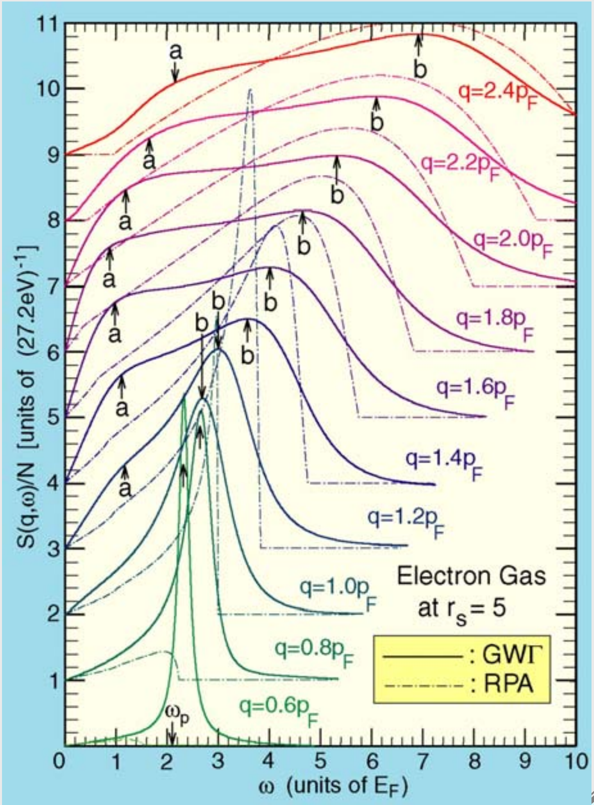
No abrupt changes in Σ(***p***,ω).

Dynamical Structure Factor

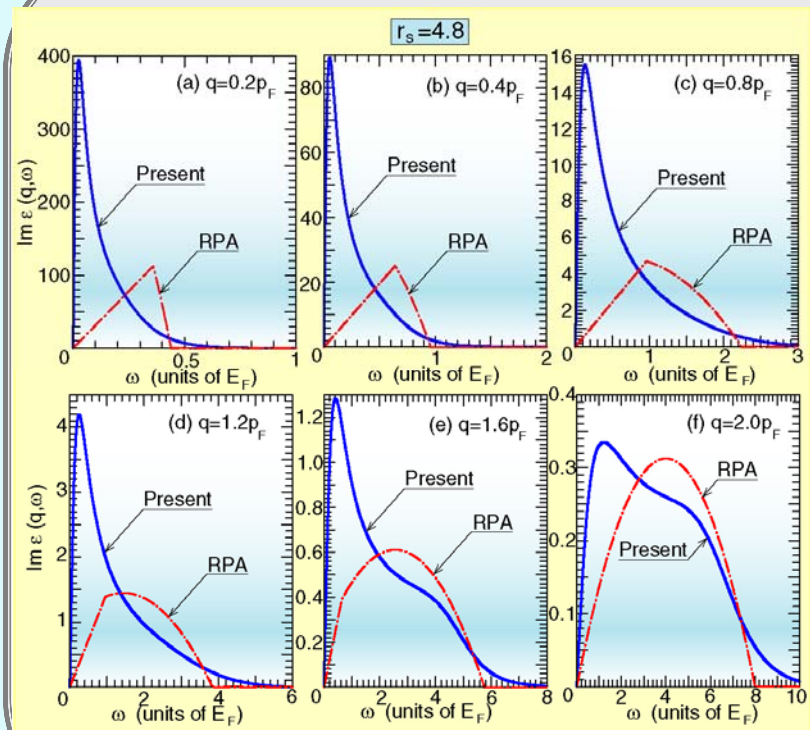
$$S(\mathbf{q},\omega) \;=\; -\frac{1}{\pi}\,\frac{1}{1-e^{-\omega/T}}\,\mathrm{Im}Q_c(\mathbf{q},\omega)$$

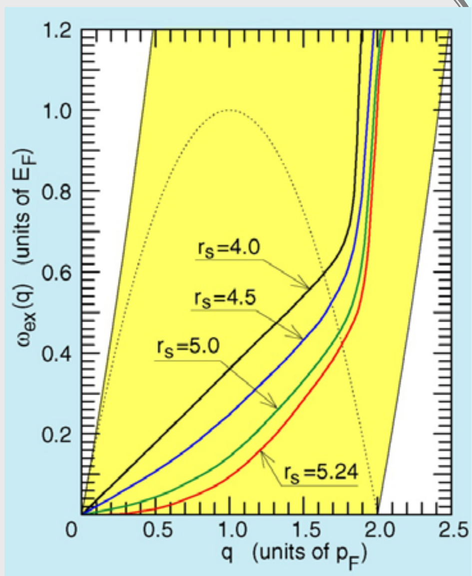
Although it cannot be seen in the RPA, the structure *a* can be clearly seen, which represents the electron-hole multiple scattering (or excitonic) effect.

YT and H. Yasuhara, *PRL* **89**, 216402 (2002).



Anomaly in the Dielectric Function



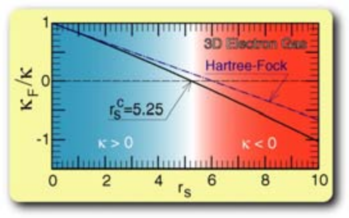


$$\varepsilon(\mathbf{q},\omega) \approx 1 + \frac{\kappa}{\kappa_F}\,\frac{q_{\mathrm{TF}}^2}{\mathbf{q}^2}\,\frac{\omega_{ex}(\mathbf{q})}{\omega_{ex}(\mathbf{q}) - i\omega}$$

Pole at $\omega = -i\,\omega_{ex}(\mathbf{q})$

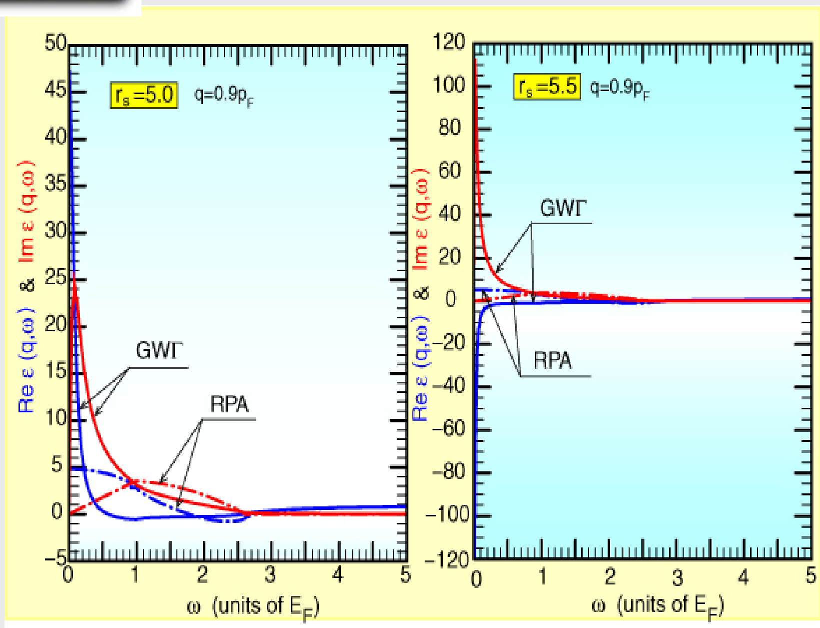
YT, *J. Superconductivity* **18**, 785 (2005).

ε(q,ω) in the Negative-κ Region



$$\varepsilon(\mathbf{q},\omega) \approx 1 + \frac{\kappa}{\kappa_F}\frac{q_{\mathrm{TF}}^2}{\mathbf{q}^2}\frac{\omega_{ex}(\mathbf{q})}{\omega_{ex}(\mathbf{q}) - i\omega}$$

Pole at $\omega = -i\,\omega_{ex}(\mathbf{q})$



Part III. Comparison with Experiment

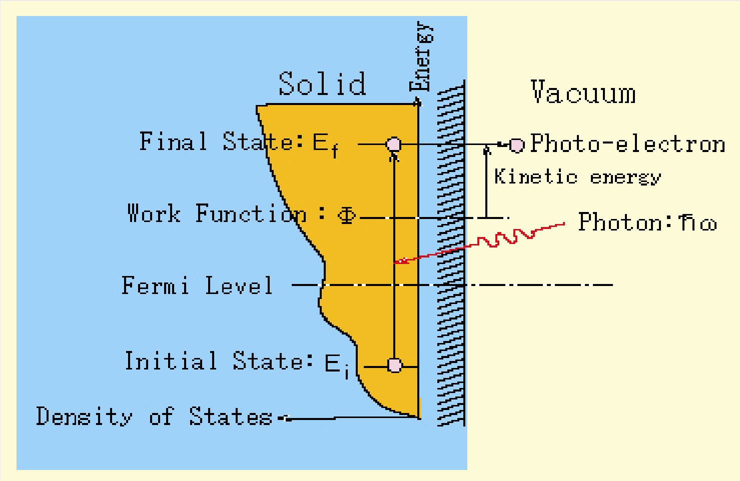
- ARPES and the problem of occupied bandwidth of the Na 3s band
- High-Energy Electron Escape Depth

ARPES

Angle-Resolved Photoemission Spectroscopy

Observation of photo electron ejected by soft x-ray（20–40eV）

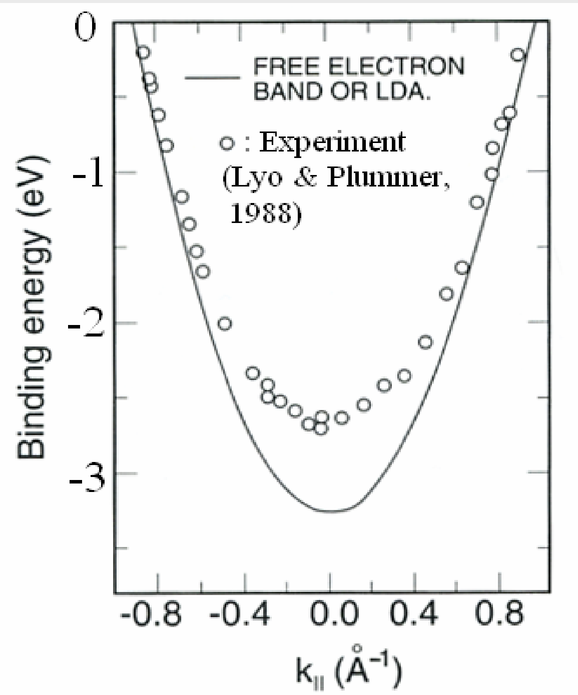
→ Direct observation of quasiparticle



Conventional assumption:
The final state is well described by "the free-electron model"

Lyo-Plummer's Experiment

Na (110) with photon energy ω = 16-66 eV



In-Whan Lyo & E. W. Plummer, *PRL* **60**, 1558 (1988)

$r_s = 4$

$E_F = 3.13$eV

Bandwidth narrowing by 18%

This is quantitatively reproduced by the GW approximation: regarded as Hallmark of GW

Yasuhara's Objection

H. Yasuhara, S. Yoshinaga, & M. Higuchi, *PRL* **83**, 3250 (1999)

Yasuhara claims that the final states of energies less than about 100 eV should be considered as "an interacting electron-gas model".

Based on this model, the bandwidth is not narrowed.

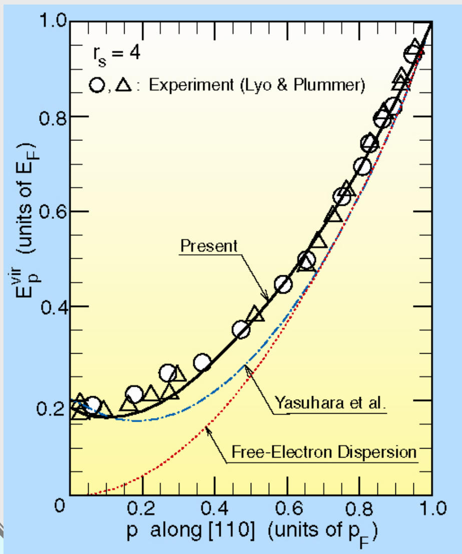
Yasuhara's calculation of the self-energy is not a self-consistent one, violating some sum-rules; an important question raised by Ku, Eguiluz, & Plummer, *PRL* **8**5, 2410 (2000).

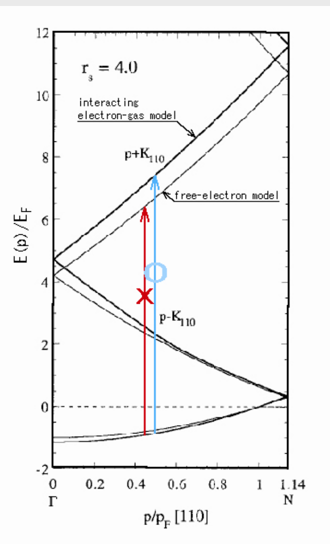
Compared my fully self-consistent result of $\boldsymbol{\Sigma(p,\omega)}$ with properly including the vertex corrections

Comparison with Experiment

Analysis of ARPES in terms of the interacting electron-gas model for the final state → The experimental data analyzed on the free-electron model should be compared with $\boldsymbol{E_p^{vir}}$, defined by

$$E_{\mathbf{p}}^{\mathrm{vir}} \equiv \varepsilon_{\mathbf{p}} + \mathrm{Re}\Sigma(\mathbf{p}, E_{\mathbf{p}}) - \mathrm{Re}\Sigma(\mathbf{p}+\mathbf{K}_{[110]}, E_{\mathbf{p}+\mathbf{K}_{[110]}})$$





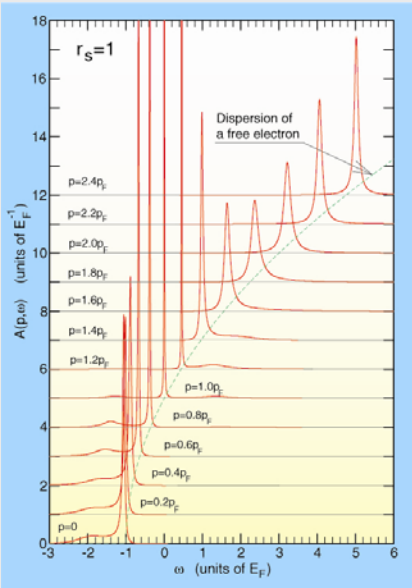
- Final state should be analyzed with using the interacting electron-gas model.
- Actual bandwidth of Na is not narrowed but slightly widened.
  → a clear indication of the flaw of GW.

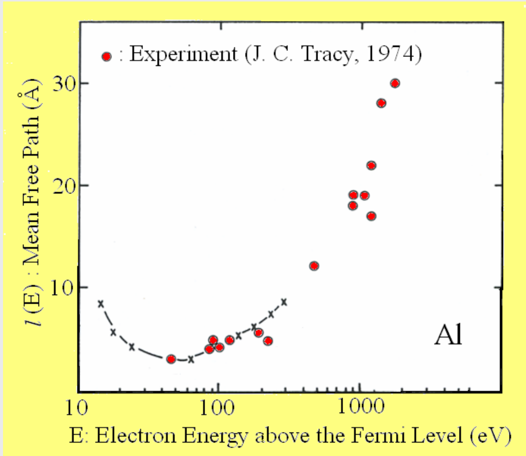
Electron Escape Depth

Inelastic electron mean free path: l

← Important in all kinds of surface electron spectroscopy

$$l_p^{-1} = -2\mathrm{Im}\Sigma(\boldsymbol{p},E_p)/v_p; \quad E=E_p$$





Interacting electron-gas model must be valid at least up to the region of minimum l_p.

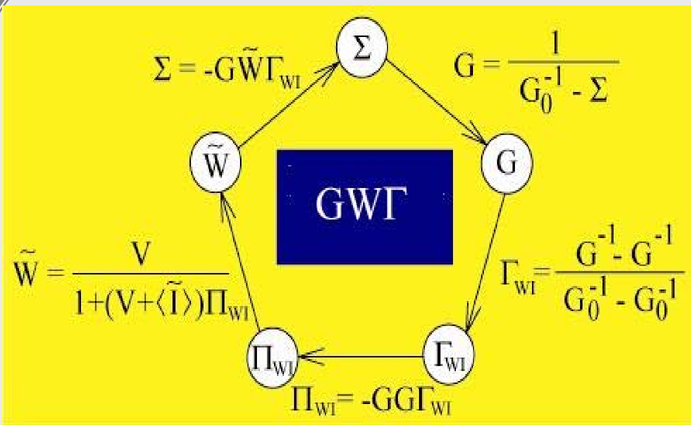
Summary

1^0 Suggested an useful functional form for the vertex function Γ.

2^0 Given an important message that ARPES should be not analyzed in terms of a free-electron model but an interacting electron-gas model.

3^0 Shown that the occupied bandwidth of sodium is not narrowed but slightly widened, which cannot be reproduced in the GW approximation.

Towards GWΓ in Real Solids



$$\Gamma_{\mathrm{WI}}(p+q,p)=\frac{G(p+q)^{-1}-G(p)^{-1}}{G_0(p+q)^{-1}-G_0(p)^{-1}}$$

$$\Pi_{\mathrm{WI}}(q)\equiv-\sum_p G(p+q)G(p)\Gamma_{\mathrm{WI}}(p+q,p)$$

$$\Pi_{\mathrm{WI}}(q)=4\sum_{\mathbf{p}} n(\mathbf{p})\,\frac{\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}}}{\omega_q^2+(\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}})^2}$$

$$n(\mathbf{p})=\lim_{\eta\to+0} T\sum_{\omega_p} G(p)e^{i\omega_p\eta}$$

$$\Pi_0(q)=4\sum_{\mathbf{p}}\theta(p_F-|\mathbf{p}|)\frac{\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}}}{\omega_q^2+(\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}})^2}$$

◎ Need to calculate:

(1) $\Pi_{\mathrm{WI}}(q) \leftarrow \Pi_0(q)$ in GW

cf. F. Aryasetiawan and O. Gunnarsson, *Rep. Prog. Phys.* **61**, 237 (1998).

(2) $I(q) \leftarrow f_{xc}(\boldsymbol{q},\omega)$ in TDDFT

cf. L. Reining *et al. PRL* **94**, 186402(2005) ;*PRB* **72**, 125203 (2005).