Quantum transport properties in a quasi-2D- electron liquid

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work done together with

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13th spring theoretical physics conference
(May 3-5, 2006)

Summary

We have carried out a new systematic study of the quasi-particle effective mass, Renormalization constant, Lande' g factor and the spin susceptibility in a quasi-two dimensional electron liquid.

Our work is based on a recent extensive analysis of the electron self-energy and includes charge- and spin-density fluctuations beyond the "Random Phase Approximation" (RPA) through the use of static charge-charge and spin-spin many-body <u>local-field factors</u> (G□& G-) incorporating the quantum well thickness. These are very well known to be very important in quantitative calculations of properties of the electron liquid at strong-coupling (Q2D systems with large rs values where the experiments are done nowadays).

We find that the effective mass is substantially enhanced by spin fluctuations.

We will also discuss the relative merits of on-shell vs Dyson methods. In particular the divergence of the effective mass at very low densities (rs □1), <u>as found using the on-shell formula</u>, disappears within the Dyson scheme.

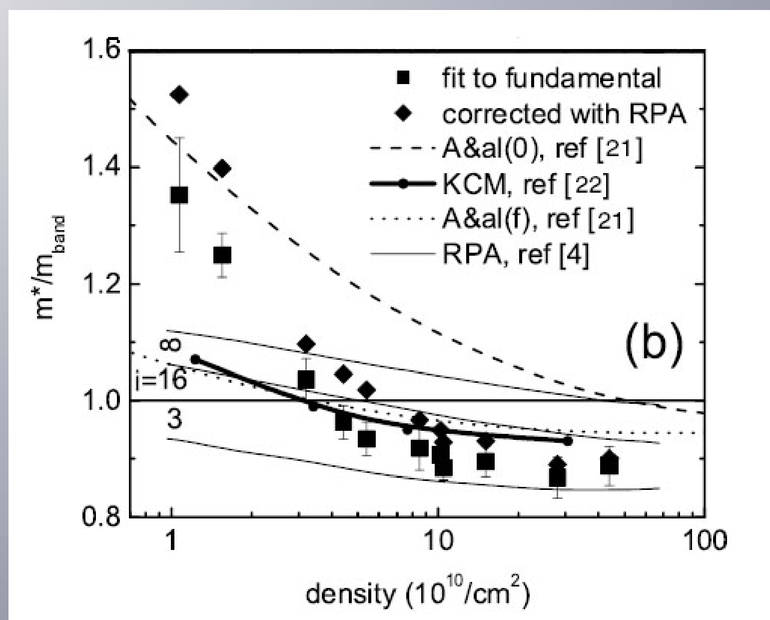
Finally we find the Lande' g factor and spin susceptibility and they are in good agreement with the recent experimental measurements.

Motivations

- ✓ **Lots of recent experimental works on Q2D electron liquids related to the issue of the apparent metal-insulator transition.**

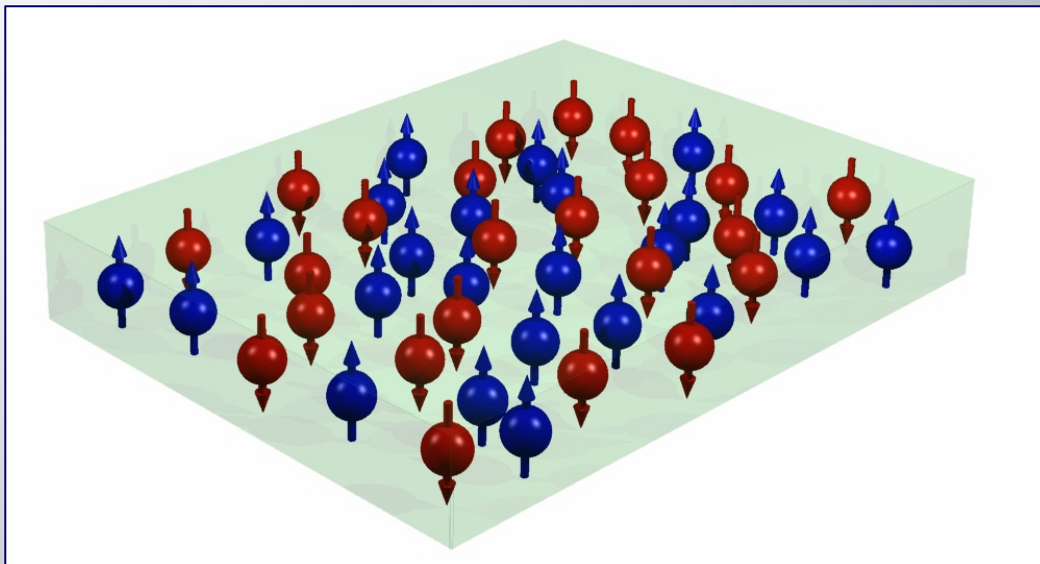
- ✓ **State-of-the-art Monte Carlo calculations (Moroni and Senatore) have not addressed the interplay between effective mass and modified Landè g-factor but have just provided us with the spin-susceptibility enhancement in strictly 2D EG**

♍$_S$/♍$_P$ $= (m^*/m_b)(g^*/g_b)$



Y. Tan *et al*., PRL**94**, 016405 (2005)

The quasi-2D electron liquid (jellium)



Coulomb
interaction
e^2/r+the effec
of thickness

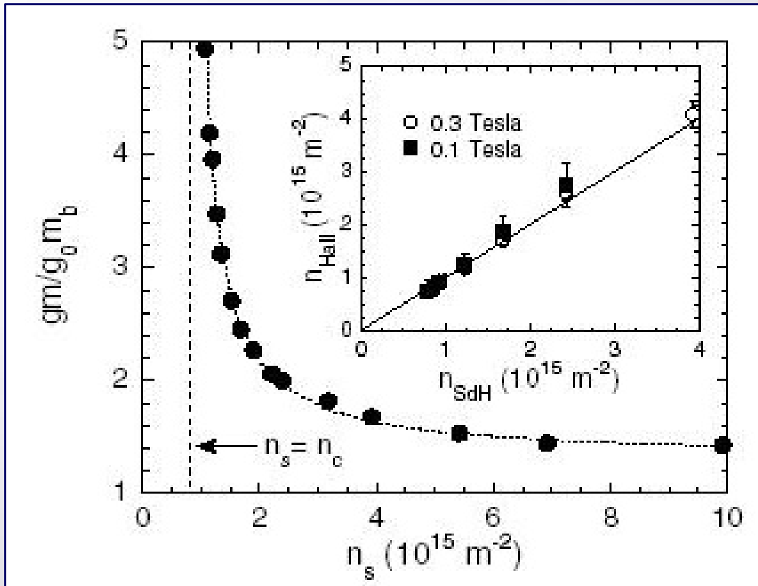
3 parameters @
zero magnetic field
and
spin-orbit coupling

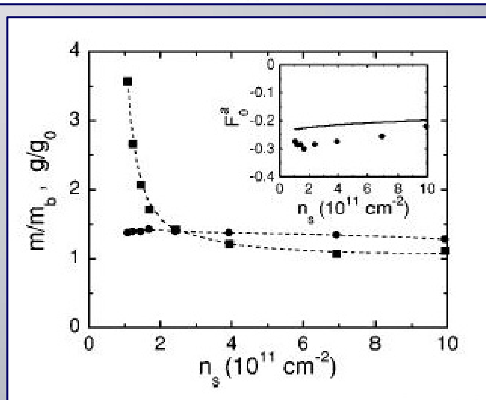
n_{2D}, ζ, T

Wigner-Seitz density parameter

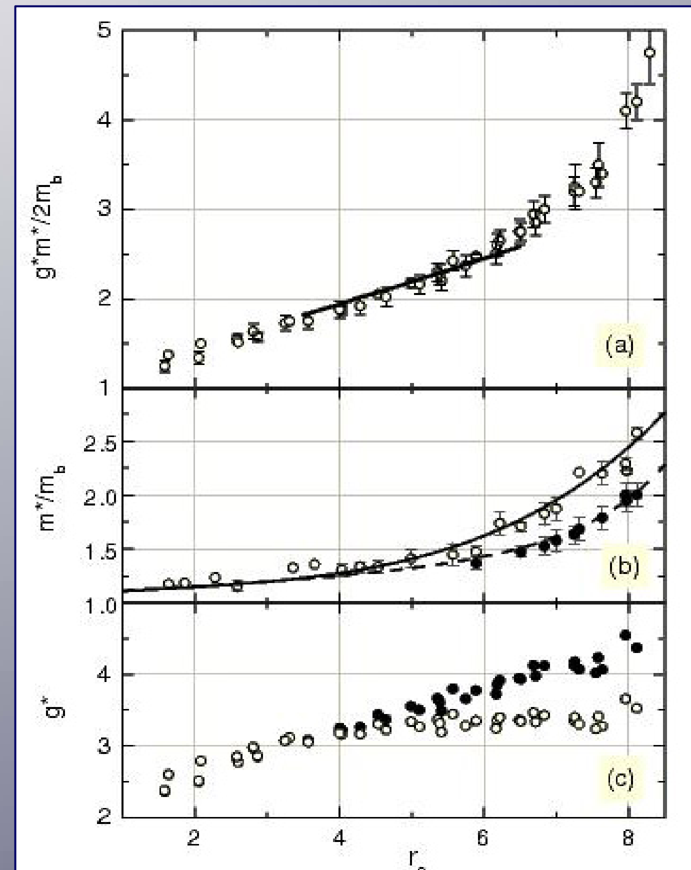
$$r_s = \left(\pi n_{2\mathrm{D}} a_B^2\right)^{-1/2}$$

Some of the recent experimental results in Silicon MOSFETs



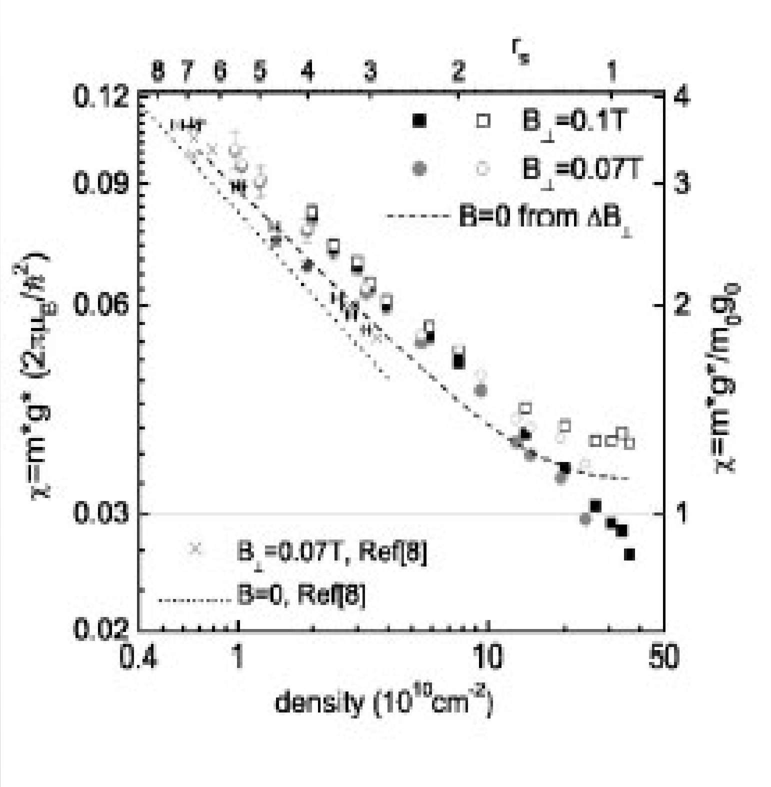


Shashkin *et al.*, PRL **87**, 086801 (2001)

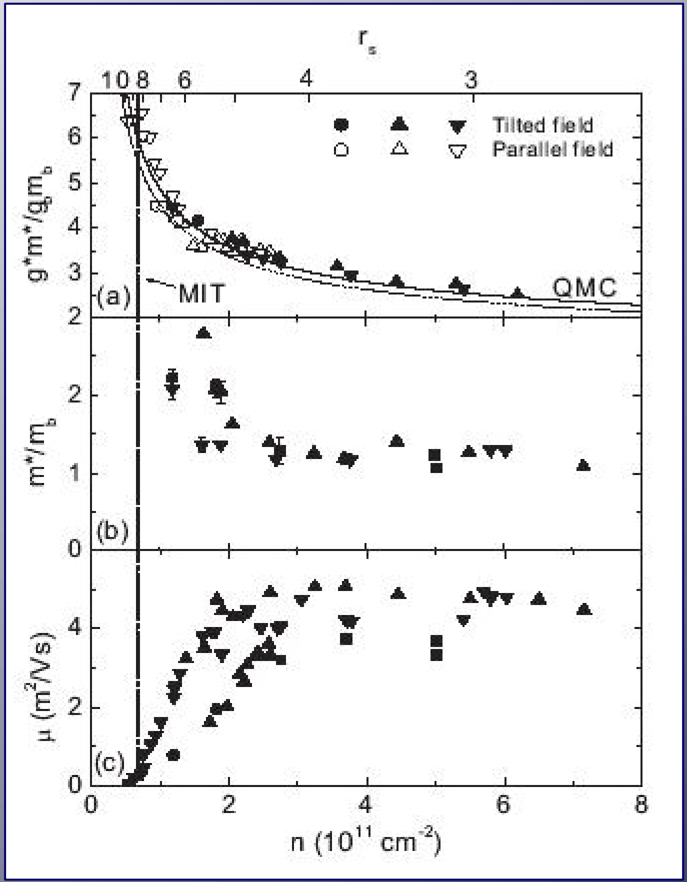


Pudalov *et al.*, PRL **88**, 196404 (2002)

Some of the recent experimental results in GaAs and AlAs heterostructures



W. – Tan *et al*. Phys. Rev. B **73**,045334 (2006)



K. Vakili *et al*., Phys. Rev. Lett **92**, 226401 (2004)

Microscopic calculation of the QP effective mass

PART I: **effective mass from self-energy**

(Other work: R. Asgari *et al*., In preparation (2006))

(R. Asgari et al., PRB **71,** 045323 (2005) **)**

(R. Asgari *et al*., Solid State Commun. **130**, 13(2004))

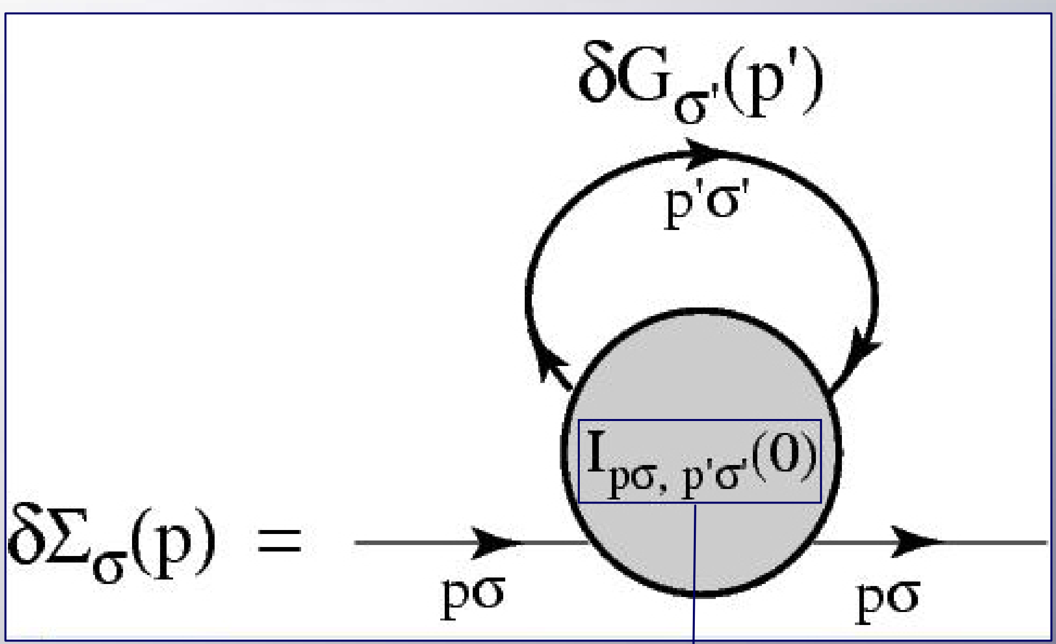
Ng & Singwi, PRB **34**, 7738 and 7743 (1986)

Yarlagadda & Giuliani, SSC **69**, 677 (1989)

Yarlagadda & Giuliani, PRB **49**, 7887 (1994) and **61**, 12556 (2000)

Yarlagadda & Giuliani, PRB **49**, 14188 (1994)

Self-energy



$$V^{\rm eff}_{\sigma\sigma'}(\mathbf{k}-\mathbf{k}', \omega-\omega')$$

Vignale & Singwi, PRB **32**, 2156 (1985)

Kukkonen-Overhauser effective interactions

$$V^{\rm eff}_{\uparrow\uparrow}(\mathrm{q},\Omega) = v_{\mathbf{q}} + \{v_{\mathbf{q}}[1-G_+(\mathrm{q})]\}^2\chi_C(\mathrm{q},\Omega) + [v_{\mathbf{q}}G_-(\mathrm{q})]^2\chi_S(\mathrm{q},\Omega)$$

$$V^{\rm eff}_{\uparrow\downarrow}(\mathrm{q},\Omega) = 2[v_{\mathbf{q}}G_-(\mathrm{q})]^2\chi_S(\mathrm{q},\Omega)\ .$$

Minimal (boring) details

$$\frac{1}{\varepsilon(\mathbf{q},\omega)} = 1 + v_{\mathbf{q}} \left[1 - G_+(\mathbf{q})\right]^2 \chi_{\rm C}(\mathbf{q},\omega) + 3\, v_{\mathbf{q}}\, G_-^2(\mathbf{q})\, \chi_{\rm S}(\mathbf{q},\omega)$$

Screened-exchange

$$\Sigma_{\rm SX}(\mathbf{k},\omega) = -\int \frac{d^2\mathbf{q}}{(2\pi)^2} \frac{v_{\mathbf{q}}}{\varepsilon(\mathbf{q},\omega - \xi_{\mathbf{k}+\mathbf{q}}/\hbar)} \Theta(-\xi_{\mathbf{k}+\mathbf{q}}/\hbar)$$

Coulomb hole

$$\Sigma_{\rm CH}(\mathbf{k},\omega) = -\int \frac{d^2\mathbf{q}}{(2\pi)^2} v_{\mathbf{q}} \int_0^{+\infty} \frac{d\Omega}{\pi} \frac{\Im m[\varepsilon^{-1}(\mathbf{q},\Omega)]}{\omega - \xi_{\mathbf{k}+\mathbf{q}}/\hbar - \Omega + i\delta}$$

Bosonic-like Schrödinger equations for the spin-resolved pair functions

(❖) $$\left[-\frac{\hbar^2}{2\mu}\nabla^2_{\mathbf{r}} + v(r) + W_{\rm B}^{\sigma\sigma'}(r) + W_{\rm e}^{\sigma\sigma'}(r) + v_{\rm P}^{\sigma\sigma'}(r)\right][g_{\sigma\sigma'}(r)]^{1/2} = 0$$

these approximate the excess potential

Purely bosonic HNC/0 two-component induced interaction:

$$W_{\rm B}^{\sigma\sigma}(q) = -\frac{\varepsilon_q}{2n_\sigma}\left\{2S_{\sigma\sigma}(q) - 3 + [S^2_{\bar\sigma\bar\sigma}(q) + S^2_{\sigma\bar\sigma}(q)]/\Delta^2\right\}$$

$$W_{\rm B}^{\sigma\bar\sigma}(q) = -\frac{\varepsilon_q}{2\sqrt{n_\sigma n_{\bar\sigma}}}\left\{2S_{\sigma\bar\sigma}(q) - S_{\sigma\bar\sigma}(q)[S_{\bar\sigma\bar\sigma}(q) + S_{\sigma\sigma}(q)]/\Delta^2\right\}$$

Chosen to cancel the spin-parallel part of the W_B interaction in the low r_s limit

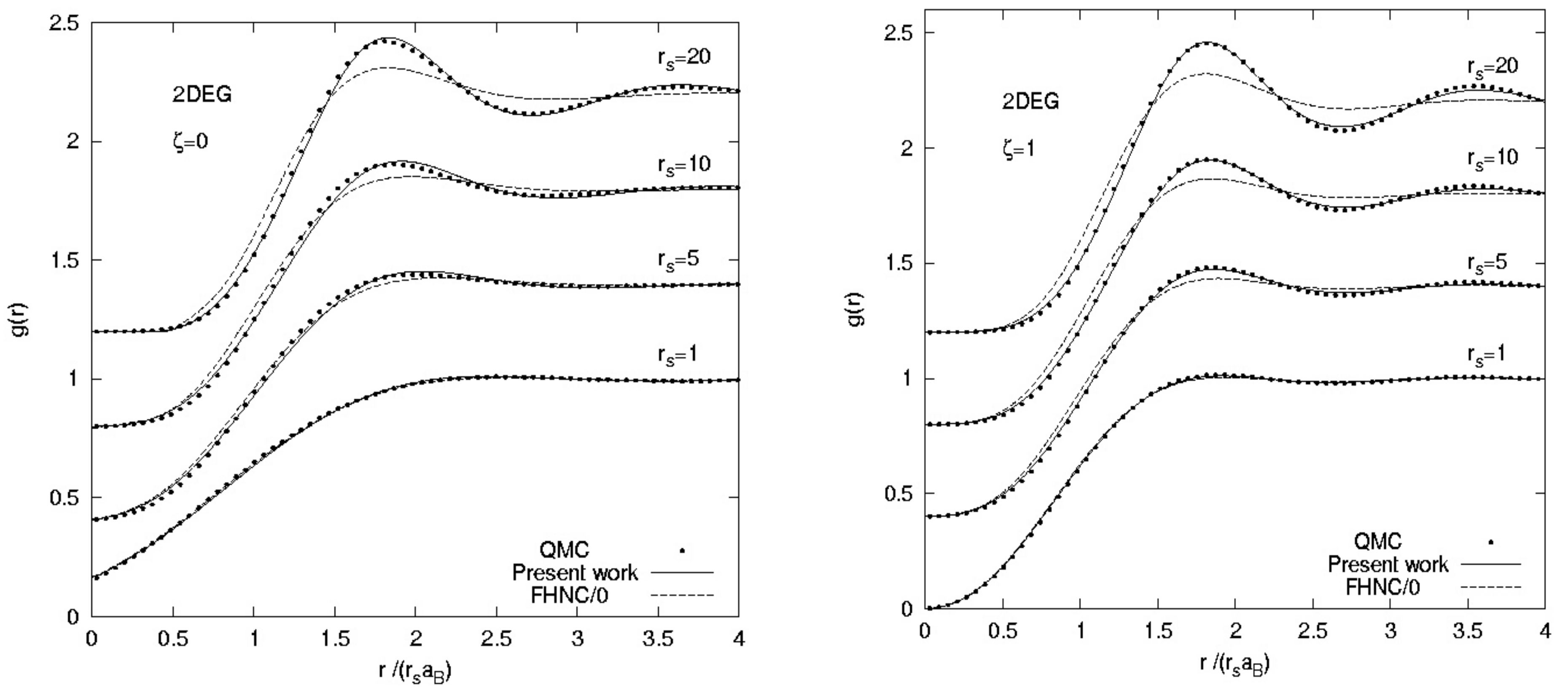
$$W_{\rm e}^{\sigma\sigma}(q) = \frac{\varepsilon_q}{2n_\sigma}\left[\frac{S^{\rm HF}_{\sigma\sigma}(q) - 1}{S^{\rm HF}_{\sigma\sigma}(q)}\right]^2[2\,S^{\rm HF}_{\sigma\sigma}(q) + 1]$$

$$\lim_{r_s\to 0} v_{\rm P}^{\sigma\sigma'}(r) = \frac{\hbar^2}{2\mu}\frac{\nabla^2\sqrt{g^{\rm HF}_{\sigma\sigma'}(r)}}{\sqrt{g^{\rm HF}_{\sigma\sigma'}(r)}}.$$

This choice for the Kohn-Sham potential satisfies all the list of know sum-rules

Kallio *and* Piilo, PRL **77**, 4237 (1996)
B. Davoudi, R. Asgari, M. Polini and M. Tosi, PRB **68**,155112 (2003)

Paramagnetic and fully spin-polarized results in 2D EG

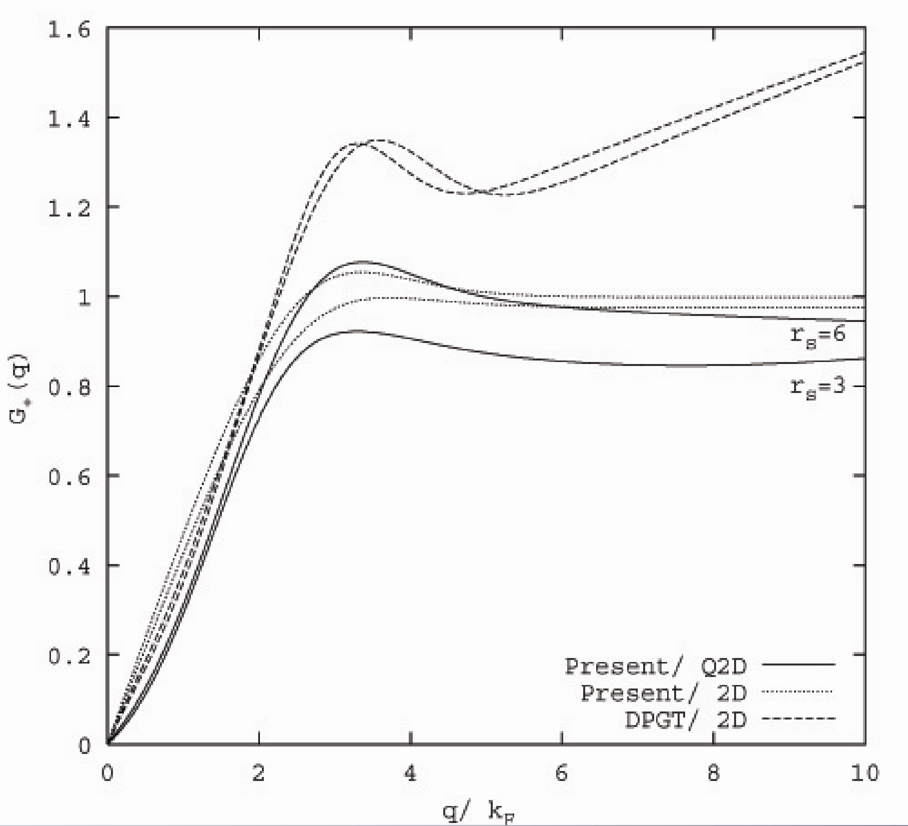


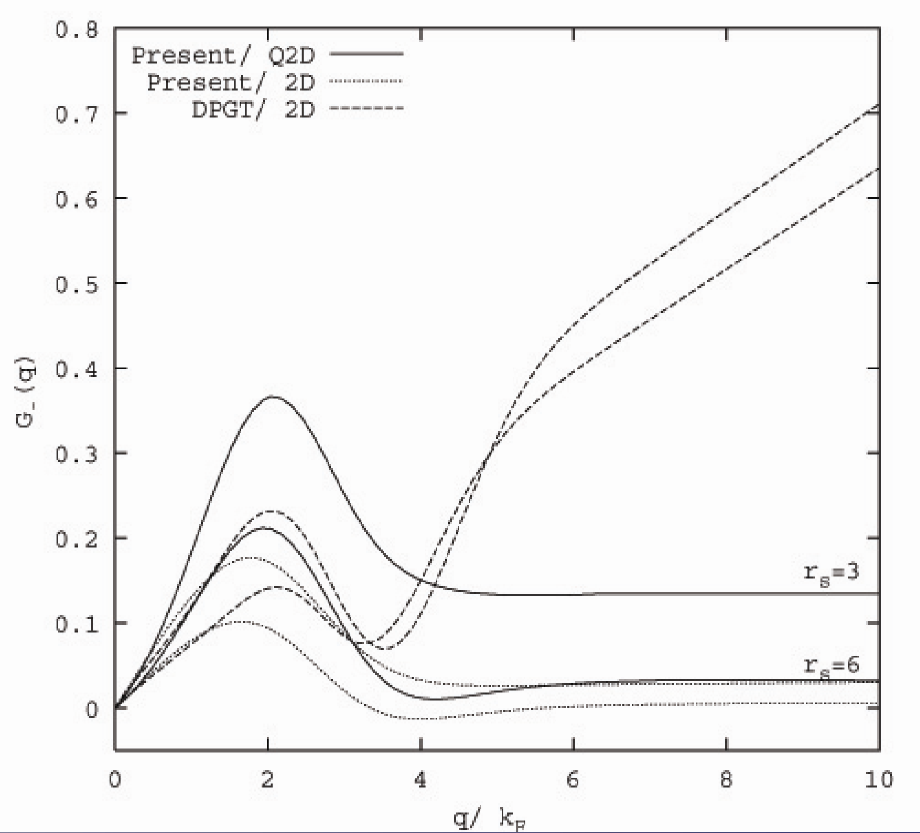
QMC: P. Gori-Giorgi, S. Moroni and G. B. Bachelet, Phys. Rev. B **70**, 115102 (2004)

R. Asgari , B. Davoudi and M. P. Tosi, Solid State Commun. **130**, 13 (2004)

$$G_+(q) = 1 - \frac{\sqrt{2}}{4r_s}\left(\frac{q}{k_F}\right)^3 \frac{1}{F(qd)}\left[\frac{1}{S_+(q)^2} - \frac{1}{S_{HF}(q)^2}\right]$$

$$G_-(q) = -\frac{\sqrt{2}}{4r_s}\left(\frac{q}{k_F}\right)^3 \frac{1}{F(qd)}\left[\frac{1}{S_-(q)^2} - \frac{1}{S_{HF}(q)^2}\right]$$





Asgari, Subasi, Sabouri, Tanatar, Accepted Phy. Rev. B (2006)

Effective mass from QP excitation energy

Dyson equation for the QP excitation energy

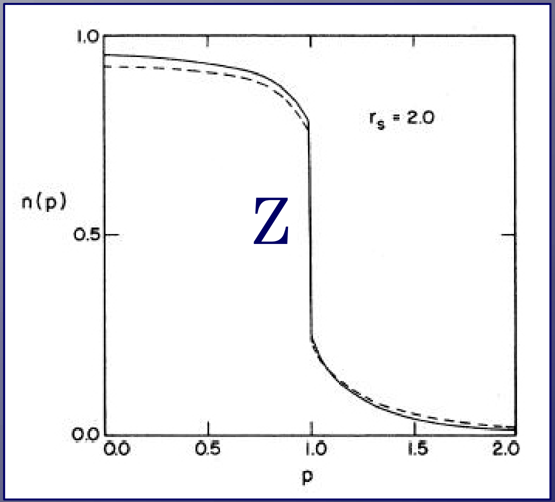
$$\delta\mathcal{E}_{\mathrm{QP}}(\mathbf{k}) = \frac{\hbar^2}{2m}(\mathbf{k}^2 - k_F^2) + \Re e\Sigma^{\mathrm{R}}_{\mathrm{ret}}(\mathbf{k},\omega)\Big|_{\omega=\delta\mathcal{E}_{\mathrm{QP}}(\mathbf{k})/\hbar}$$

Landau theory

$$\frac{1}{m^*} = \frac{1}{\hbar^2 k_F}\,\frac{d\delta\mathcal{E}_{\mathrm{QP}}(k)}{dk}\Big|_{k=k_F}$$

$$\frac{m^*_{\mathrm{D}}}{m} = \frac{Z^{-1}}{1 + (m/\hbar^2 k_F)\,\partial_k \Re e\Sigma^{\mathrm{R}}_{\mathrm{ret}}(k,\omega)\big|_{k=k_F,\omega=0}}$$

$$Z = \frac{1}{1 - \hbar^{-1}\,\partial_\omega \Re e\Sigma^{\mathrm{R}}_{\mathrm{ret}}(k,\omega)\big|_{k=k_F,\omega=0}}$$

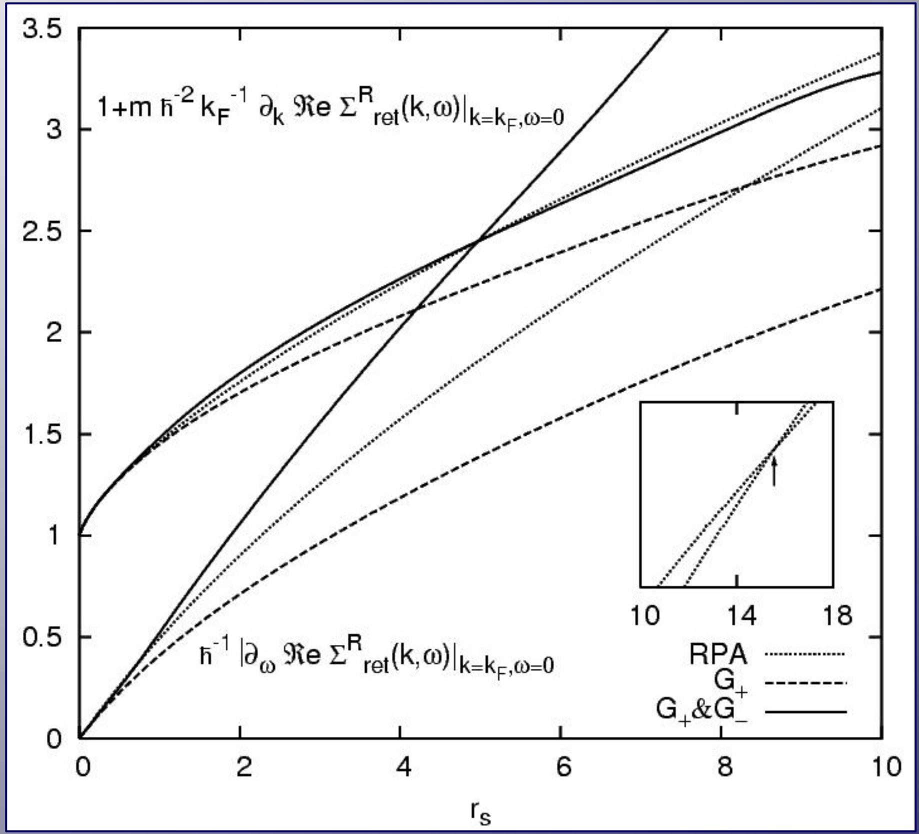


Santoro & Giuliani, PRB **39**, 12818 (1989)

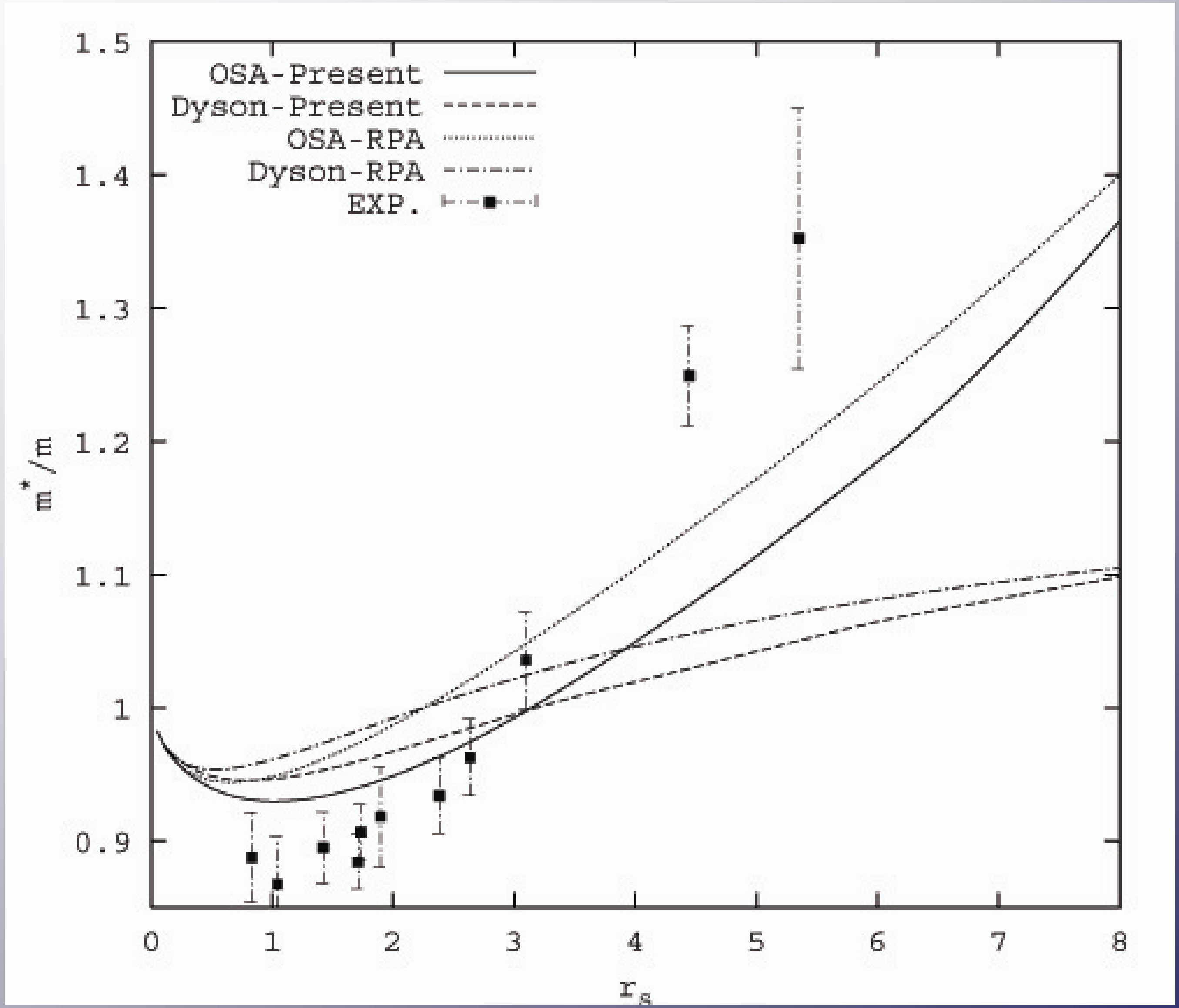
On-shell approximation (OSA): weak-coupling theory

$$\delta\mathcal{E}_{\mathrm{QP}}(\mathbf{k}) \simeq \frac{\hbar^2}{2m}(\mathbf{k}^2 - k_F^2) + \Re e\Sigma^{\mathrm{R}}_{\mathrm{ret}}(\mathbf{k},\omega)\Big|_{\omega=\hbar(\mathbf{k}^2-k_F^2)/2m}$$

$$\frac{m^*_{\mathrm{OSA}}}{m} = \frac{1}{1 + (m/\hbar^2 k_F)\,\partial_k \Re e\Sigma^{\mathrm{R}}_{\mathrm{ret}}(k,\omega)\Big|_{k=k_F,\omega=0} + \hbar^{-1}\,\partial_\omega \Re e\Sigma^{\mathrm{R}}_{\mathrm{ret}}(k,\omega)\Big|_{k=k_F,\omega=0}}$$



Numerical results: Theory vs Experimental



Microscopic calculation of the QP spin- susceptibility

$$\frac{\chi_P}{\chi_S} = \frac{m_b}{m^*} + \frac{m_b}{\pi\hbar^2}\int_0^{2\pi}\frac{d\theta}{2\pi} f_a(\cos\theta)\ ,$$

$f_a(\cos\theta) \equiv S(f^{\uparrow\uparrow}_{\mathbf{k},\mathbf{k}'} - f^{\uparrow\downarrow}_{\mathbf{k},\mathbf{k}'})/2$

$$f^{\sigma\sigma'}_{\mathbf{k},\mathbf{k}'} = \left.\frac{\delta^2 E[\{\mathcal{N}_{\mathbf{k},\sigma}\}]}{\delta\mathcal{N}_{\mathbf{k},\sigma}\delta\mathcal{N}_{\mathbf{k}',\sigma'}}\right|_{\mathcal{N}_{\mathbf{k},\sigma}=\mathcal{N}^{(0)}_{\mathbf{k},\sigma}}\ ,$$

(recall that $f^{\sigma\sigma'}_{\mathbf{k},\mathbf{k}'}$ scales like $1/S$), $\cos\theta = \mathbf{k}\cdot\mathbf{k}'/k_F^2$ with $\mathbf{k},\mathbf{k}' \in \mathcal{S}_F$.

$$\frac{\chi_S}{\chi_P} = \frac{\dfrac{m^*}{m_b}}{1 - \dfrac{m^*}{m_b}(f_{SX} - f_{CH})}\ .$$

$$f_{SX} = \frac{m_b}{\hbar^2}\int_0^{2\pi}\frac{d\theta}{(2\pi)^2}\mathcal{V}_q\left\{1 + \mathcal{V}_q[1-G_+(q)]^2\chi_C(q,0) - \mathcal{V}_q G_-^2(q)\chi_S(q,0)\right\}_{q=|\mathbf{k}-\mathbf{k}'|}\ .$$

$$\chi_C(q,\omega) = \frac{\chi_0(q,\omega)}{1 - \mathcal{V}_q[1-G_+(q)]\chi_0(q,\omega)}$$

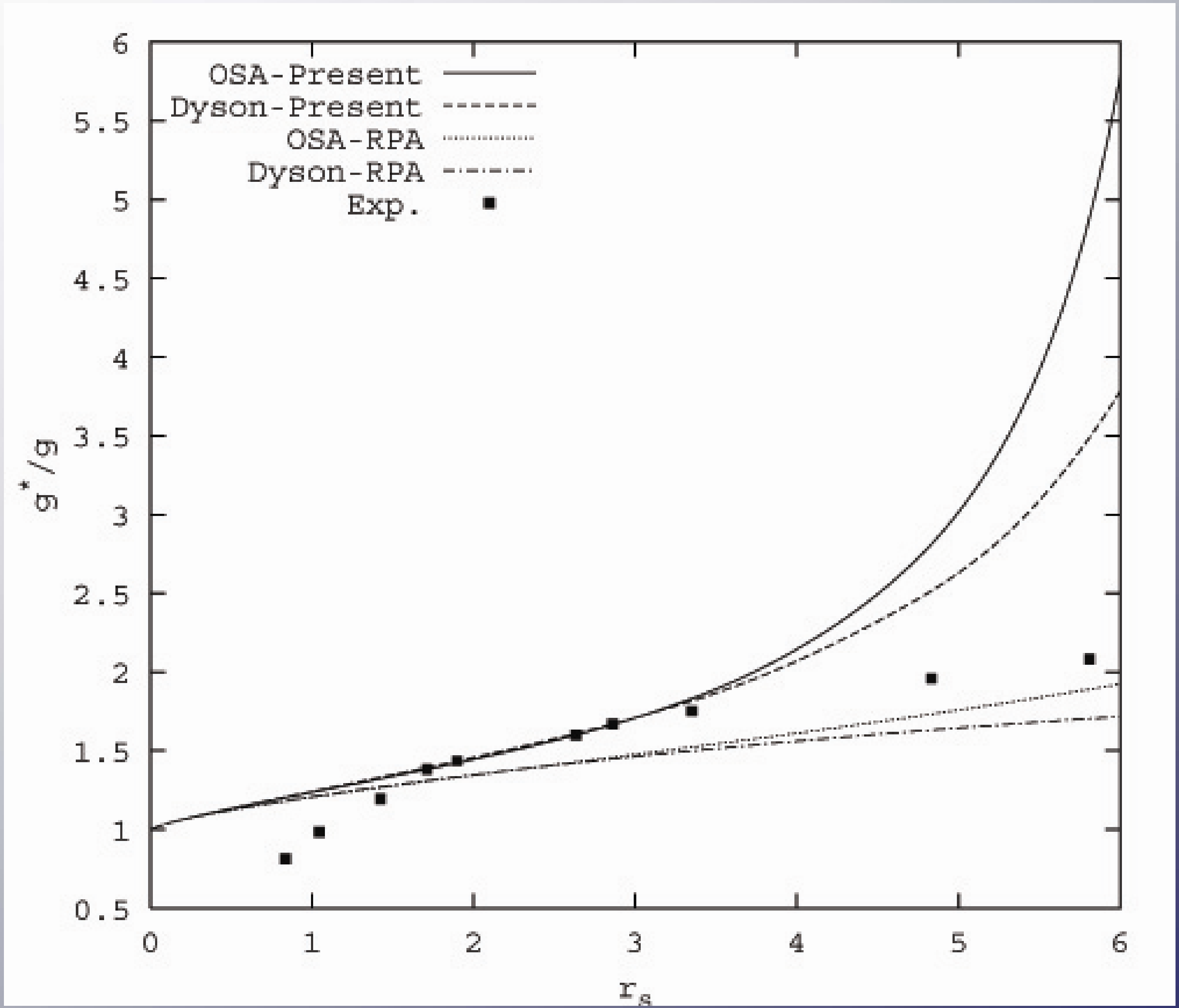
$$\chi_S(q,\omega) = \frac{\chi_0(q,\omega)}{1 + \mathcal{V}_q G_-(q)\chi_0(q,\omega)}\ ,$$

$$f_{CH} = \frac{2m_b^2}{\pi^3\hbar^4}\int_0^\infty dz\int_0^\infty du\ \mathcal{V}_q^2\left\{\frac{[1-G_+(q)]G_-(q)}{Q_-(q,i\omega)Q_+(q,i\omega)}\mathcal{P}_+(z,u) + \frac{G_-^2(q)}{Q_-^2(q,i\omega)}\mathcal{P}_-(z,u)\right\}\ ,$$

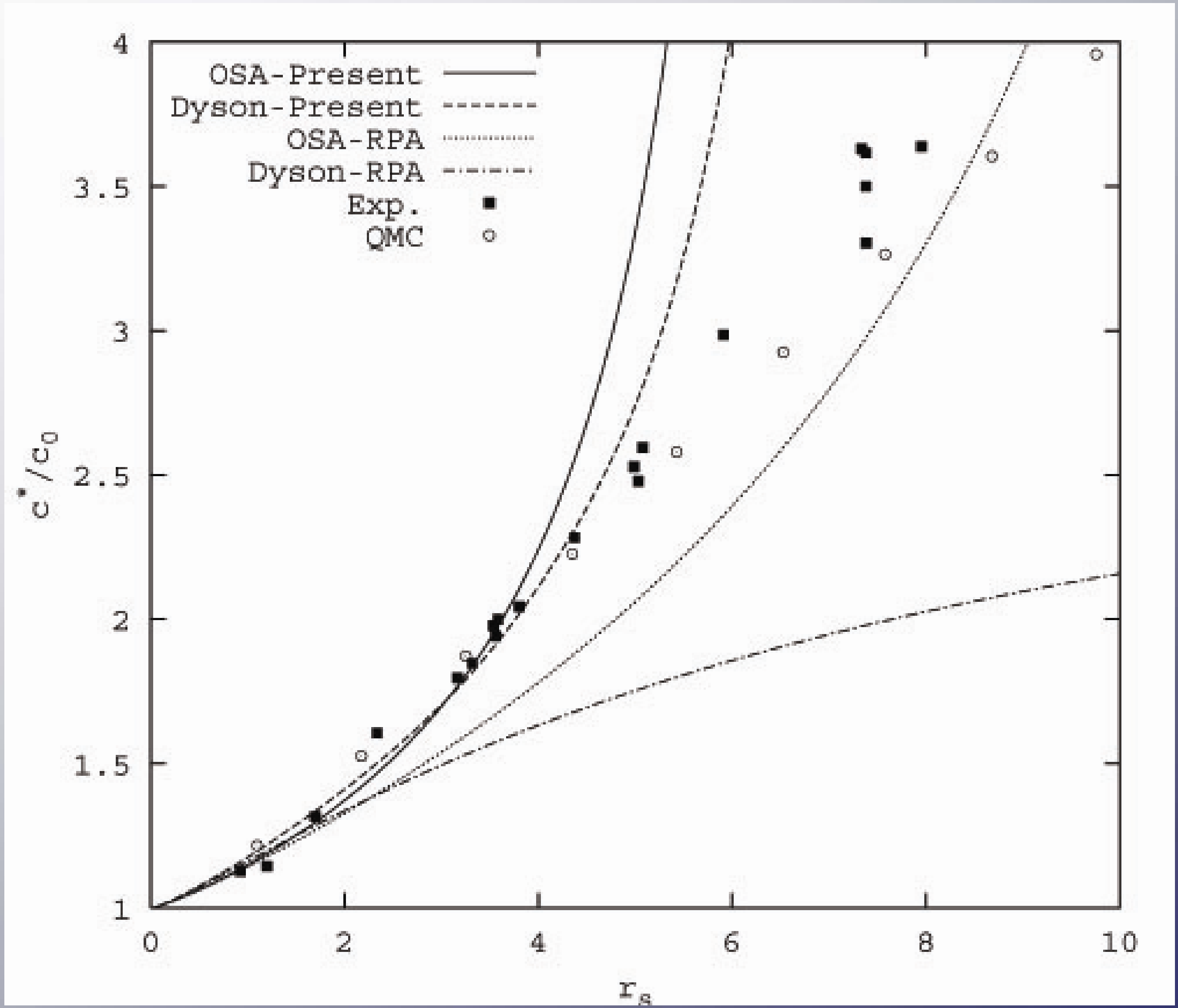
$z = q/(2k_F)$, $u = m_b\omega/(\hbar k_F q)$, $Q_\pm(q,i\omega) \equiv \chi_0(q,i\omega)/\chi_{C,S}(q,i\omega)$,

$$\mathcal{P}_\pm(z,u) \equiv \frac{[(z^2-u^2-1)^2+(2zu)^2]^{1/2} \pm (z^2-u^2-1)}{(z^2-u^2-1)^2+(2zu)^2}\ .$$

Numerical results: lande' g-factor vs Experimental



Numerical results: Spin Susceptibility vs Experimental



Low-T specific heat of an electron liquid

Quasiparticle-quasiparticle interactions **do not enter** the low-temperature specific heat

$$\mathcal{C}_V(T) = \frac{\pi^2}{3}\frac{m^*}{m}\frac{k_B^2 T}{\varepsilon_F}$$

basic thermodynamics

$$\mathcal{C}_V(T) = \left.\frac{\partial \mathcal{U}(T)}{\partial T}\right|_V$$