The spin susceptibility enhancement in wide AlAs quantum wells

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Outline

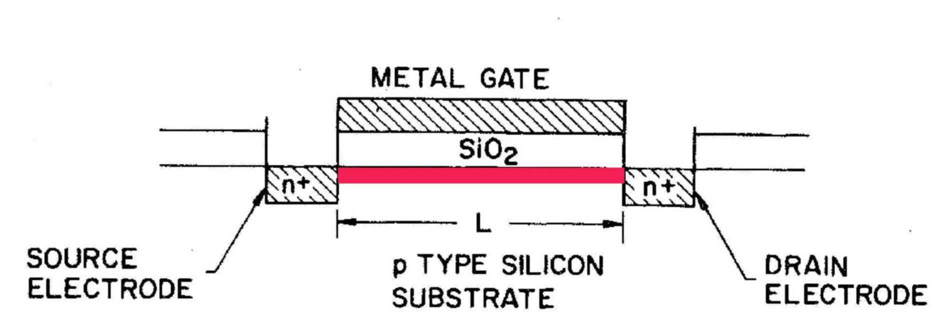
- Motivation
- Devices and 2D electron systems
- Spin susceptibility: experiments and previous QMC results
- Technique in brief and details of QMC simulations
- Predictions and comparison with experiments:
  - AlAs Quantum Wells (QWs)
- Conclusions

Motivation

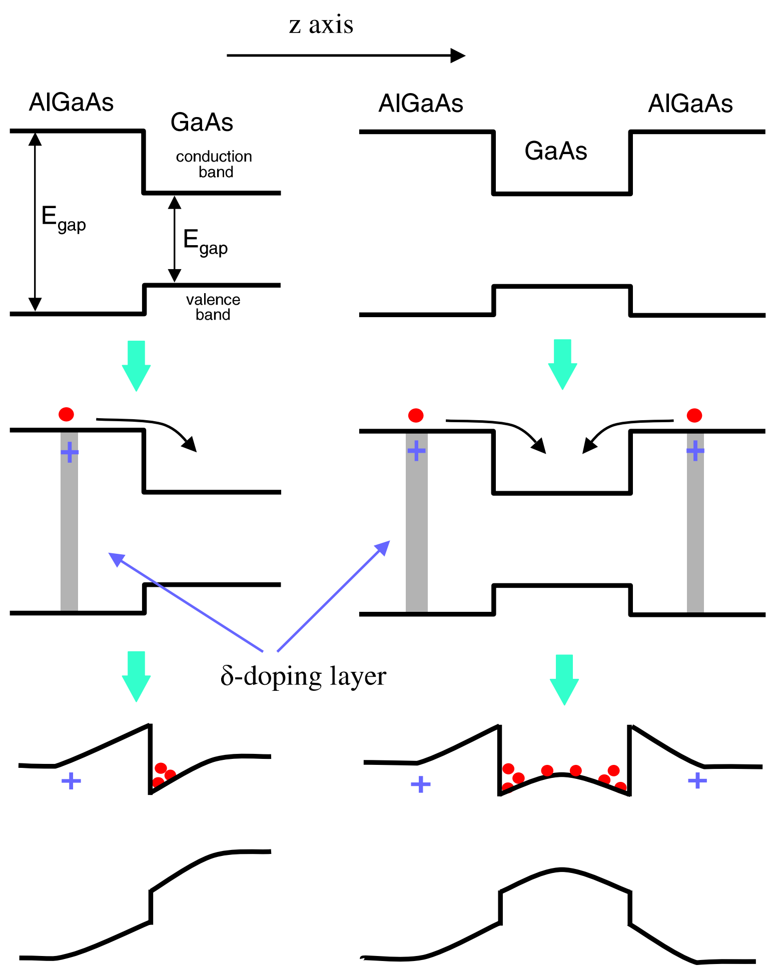
- 2DEG model system for 2D systems of electrons in solid-state devices.
- Improvements in fabrication techniques: cleaner and more dilute devices.
- Previously unexpected metal insulator transition.
- Measurements of the spin susceptibility enhancement: χ_s/χ_0 *increases as the density decreases*, but depends on *device details*.
- QMC capable of accounting for experimental evidence.

Definition of the system

- Two-dimensional electron gas (2DEG): system of electrons in two dimensions interacting via $1/r$ potential in a uniform neutralizing background of positive charges.
- 2DEG is a good approximation of 2D systems of electrons in solid state devices (*e.g.* in Si-MOSFETs, AlAs quantum wells, GaAs HIGFET, etc.).

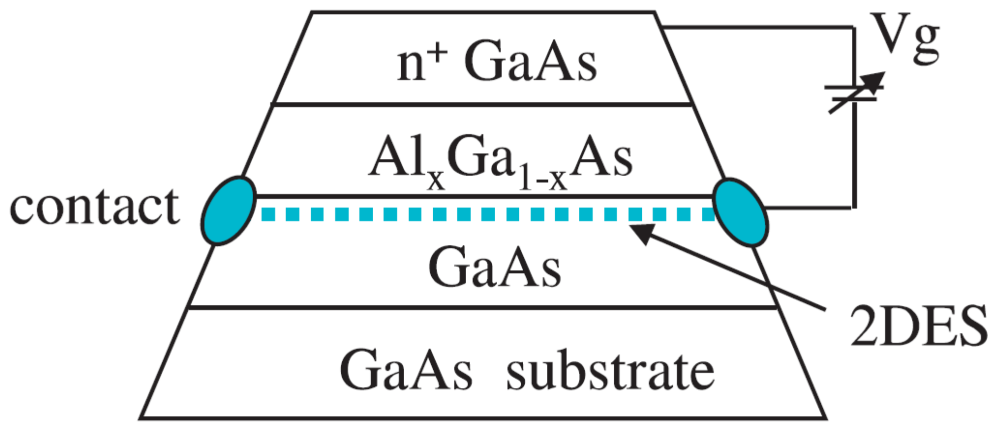


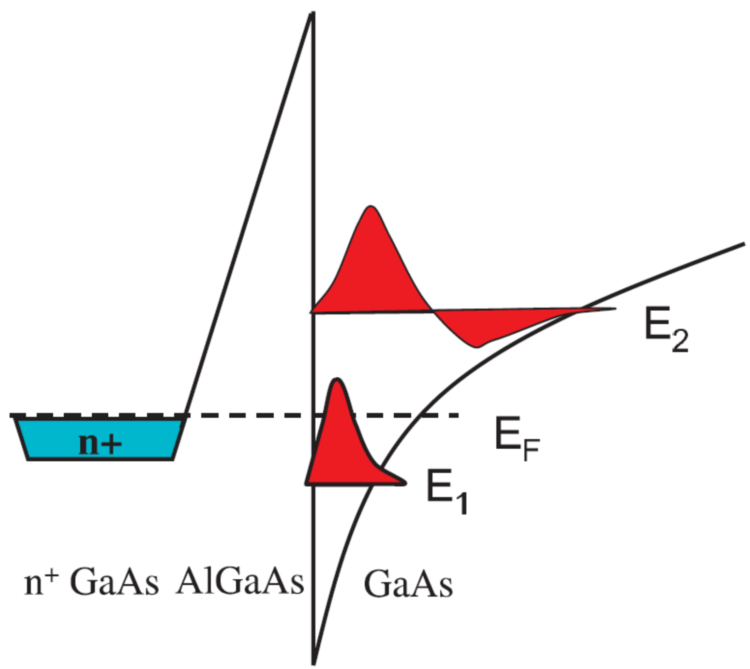
Heterojunctions and quantum wells



(a) heterojunction (b) quantum well

2D confinement in the HIGFET

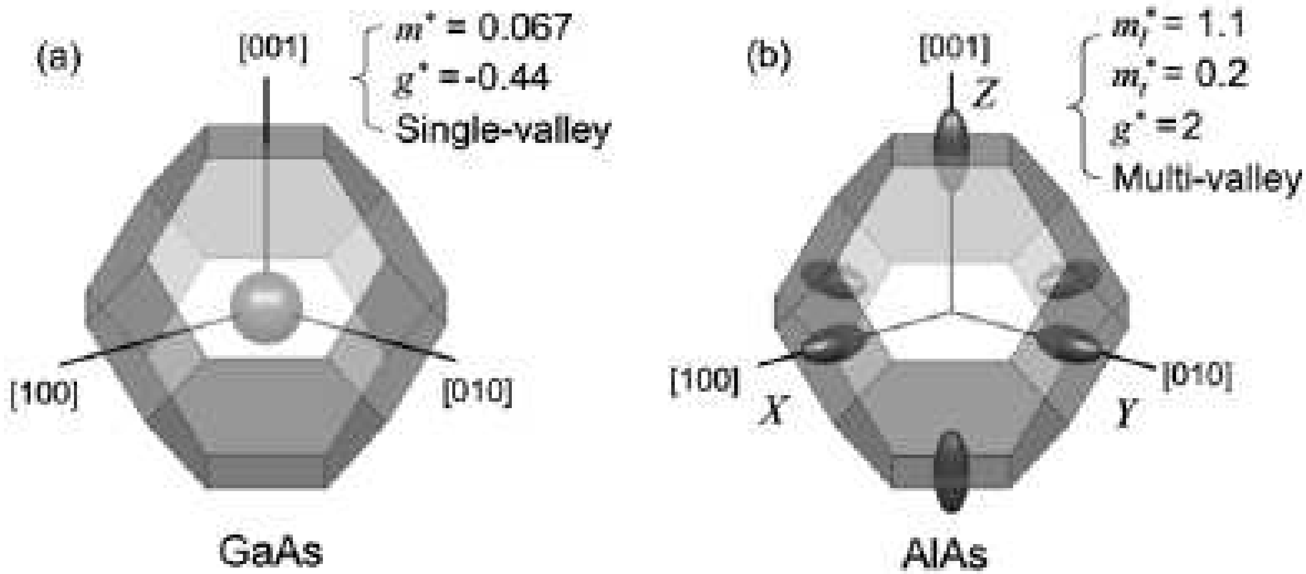




Important features of the devices:

- Valley degeneracy:
  - 1-valley systems: $\vec{k}$, $\sigma = \uparrow, \downarrow$;
  - 2-valley systems: $\vec{k}$, $\sigma = \uparrow, \downarrow$, $v = 1, 2$.
- Finite transverse thickness.
- Disorder: scattering of carriers from different impurity sources.
- Mass anisotropy.

Valley degeneracy and mass anisotropy



Schematic drawing of the Brillouin zone and constant energy surfaces of the lowest energy bands for bulk GaAs (a) and bulk AlAs (b)

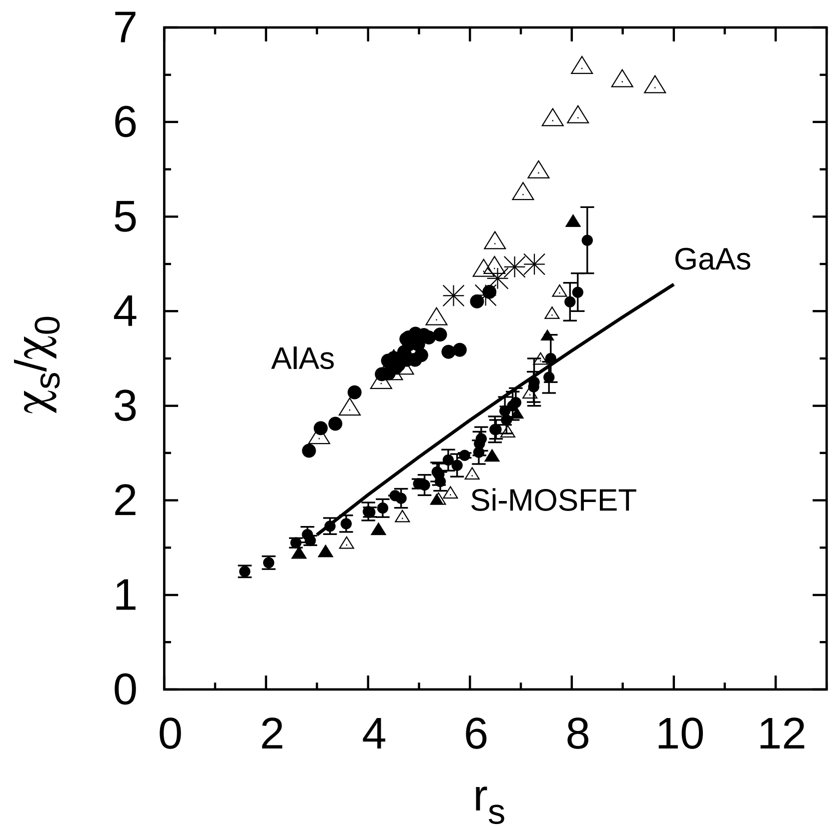
Measurements of χ_s

Spin susceptibility enhancement χ_s/χ_0 *increases with the coupling* r_s ($r_s \propto n^{-1/2}$), but depends on device details (number of occupied valleys, thickness, disorder, mass anisotropy).

- AlAs: Vakili et al,PRL '04
- GaAs: Zhu et al, PRL '03
- Si-MOSFET:

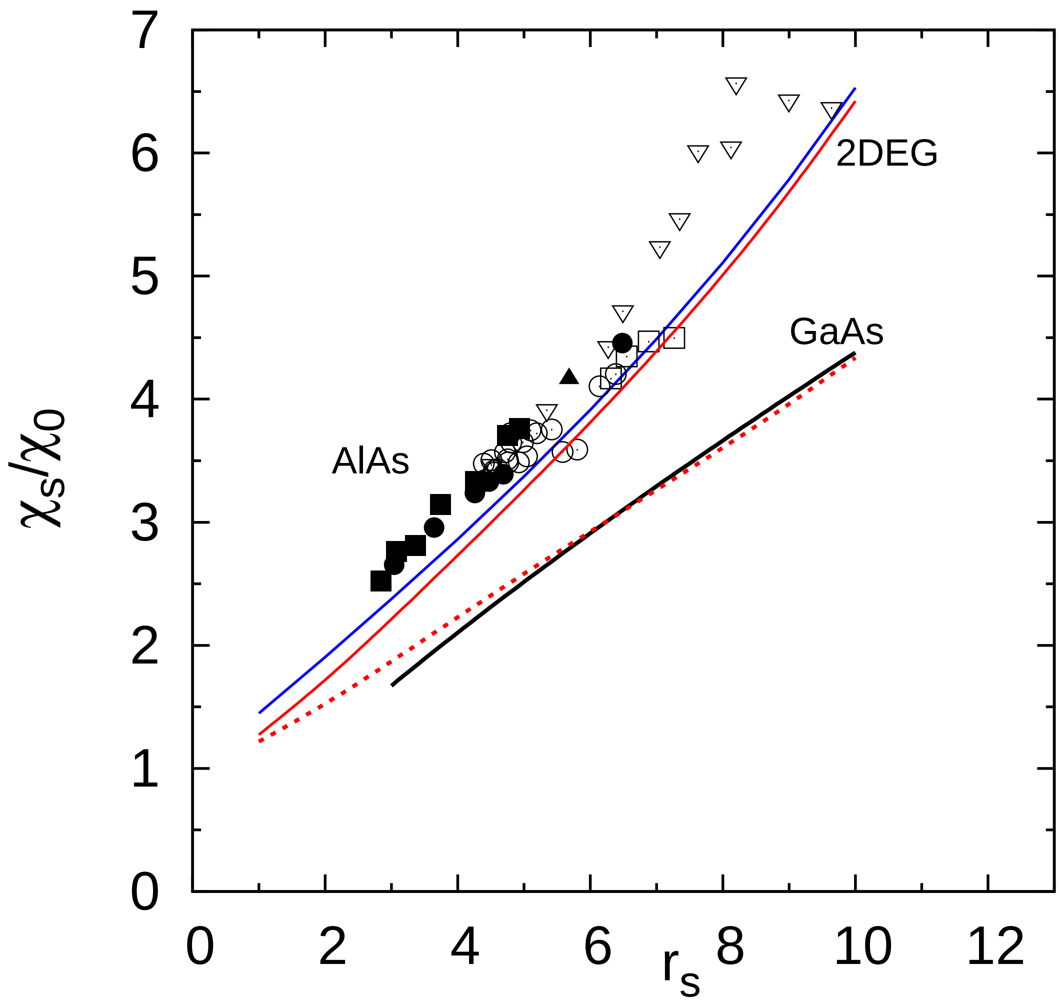
  Pudalov et al, PRL '02

  Shashkin et al, PRL '01



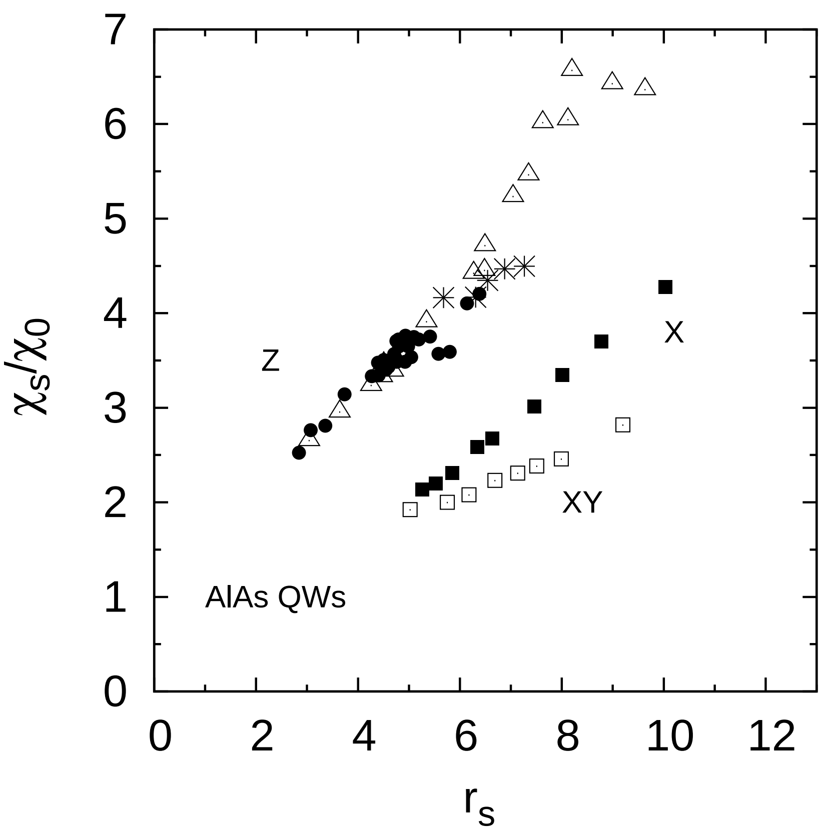
Theory and experiments: one valley

De Palo et al, PRL. 2005: Effect of thickness

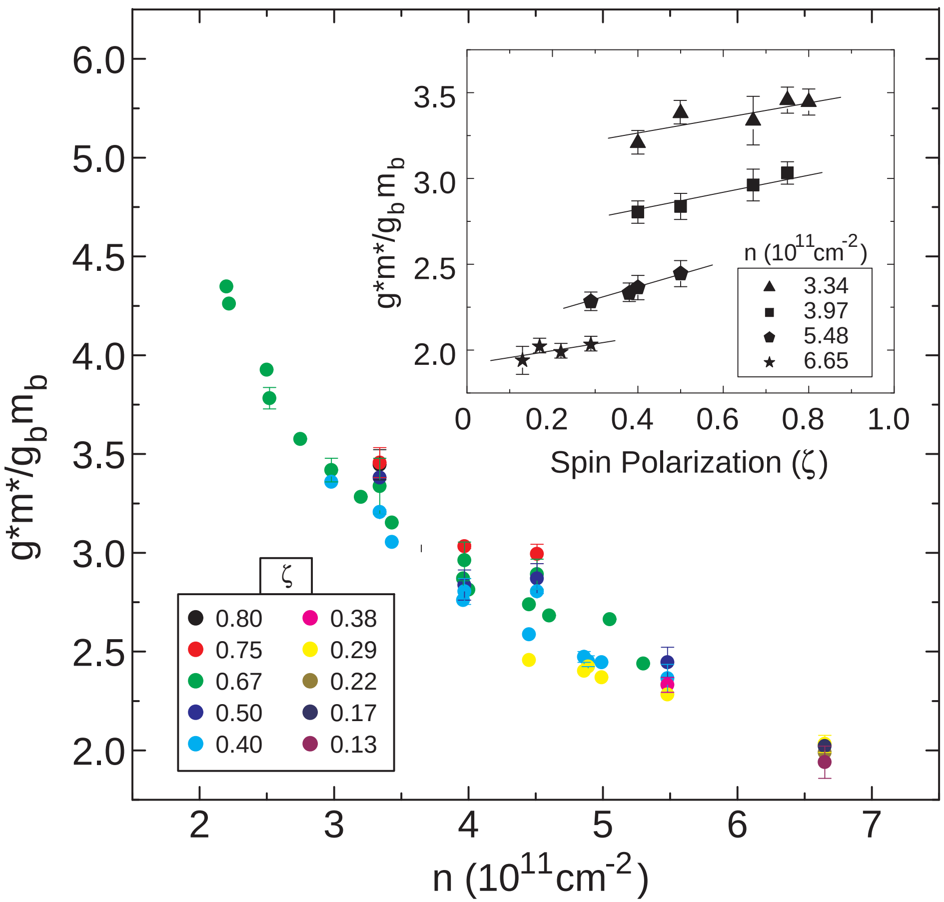


Effects on χ_s/χ_0

- Z: Vakili et al, PRL ’04 (1v isotropic masses)
- X,XY: Gunawan et al., PRL ’06 (1v,2v anisotropic masses)



Experiments in 15nm 1v AlAs QW



T. Gokmen *et al.*, PRB ’07

Description of the theoretical model I

2DEG at $T = 0$ and $B = 0$ with valley degeneracy and mass anisotropy:

$$H = -\frac{\hbar^2}{2}\sum_{i=1}^{N/2}\left[\frac{\nabla_{i,x}{}^2}{m_x} + \frac{\nabla_{i,y}{}^2}{m_y}\right] + \sum_{i=1}^{N/2}\left[\frac{\nabla_{i,x}{}^2}{m_y} + \frac{\nabla_{i,y}{}^2}{m_x}\right]$$
$$+\frac{1}{2A}\sum_{\mathbf{q}\neq\mathbf{0}} v(q)[\rho_{\mathbf{q}}\rho_{-\mathbf{q}} - N], \qquad \rho_{\mathbf{q}} = \sum_{\nu,i_\nu} e^{i\mathbf{q}\cdot\mathbf{r}_{\mathbf{i}_\nu}}.$$

- $m_x = m_t = 0.205 m_0$, $m_y = m_l = 1.05 m_0$ (T. Gokmen *et al.*, PRB 2007);
- $v(q) = (2\pi e^2/\epsilon q)F(q)$.
- $F(q) = 1$ for a *strictly 2D* egas.

Description of the theoretical model II

Important parameters of the system:

- r_s parameter: $1/n = A/N = \pi(r_s a_B^*)^2$, $a_B^* = \hbar^2\epsilon/(m_b e^2)$.
- Spin polarization $\zeta = (N_\uparrow - N_\downarrow)/N$ (*symmetric valleys*).
- Effective mass $m_b = \sqrt{m_x m_y} \simeq 0.46 m_0$ or anisotropy factor $\alpha = (m_y/m_x)^{1/4} \simeq 5^{1/4}$

$$
\begin{aligned}
H &= -\frac{1}{r_s^2}\sum_{i=1}^{N/2}\left[\alpha^2\nabla_{i,x}^2 + \frac{\nabla_{i,y}^2}{\alpha^2}\right] + \sum_{i=1}^{N/2}\left[\frac{\nabla_{i,x}^2}{\alpha^2} + \alpha^2\nabla_{i,y}^2\right] \\
&+ \frac{1}{r_s}\frac{1}{A}\sum_{\mathbf{q}\neq\mathbf{0}}\frac{2\pi}{q}F(q)[\rho_{\mathbf{q}}\rho_{-\mathbf{q}} - N]
\end{aligned}
$$

(energy in Rydberg* and lengths in units of $r_s a_B^*$).

The thickness for AlAs QWs

- $F(q) = \frac{1}{4\pi^2+a^2q^2}\left(3aq + \frac{8\pi^2}{aq} - \frac{32\pi^4}{a^2q^2}\frac{1-e^{-aq}}{4\pi^2+a^2q^2}\right)$ (Gold, PRB 1987).
- $\epsilon = 10$;
- a the QW width; in the considered experiments: $a = 11nm,\ 15nm$.

Before going on...

By considering suitable coordinate transformations it is possible to transfer the anisotropy into the potential energy term. In the 1v case, e.g.

$x \to \alpha x,\ y \to y/\alpha$ and

$$H = -\frac{1}{r_s^2}\sum_{i=1}^{N}\nabla_i{}^2 + \frac{1}{r_s}\frac{1}{A}\sum_{\mathbf{q}\neq\mathbf{0}}\frac{2\pi}{q}F(q)[\tilde{\rho}_{\mathbf{q}}\tilde{\rho}_{-\mathbf{q}} - N],$$

where $\tilde{\rho} = \sum_i \exp i[\alpha\, q_x\, x + q_y\, y/\alpha]$.

- In the non-interacting limit this transformation exactly maps the anisotropic system onto the isotropic one.
- For non-zero coupling, we have an effective Hamiltonian with anisotropic interaction.

The Spin Susceptibility

- A 2D electron gas with $N_\uparrow$ and $N_\downarrow$ up and down spin electrons, $\zeta = (N_\uparrow - N_\downarrow)/N$, has an energy per particle $\varepsilon(\zeta)$ (... from QMC). In an in-plane magnetic field $\mathbf{B} = B\hat{z}$,

$$\varepsilon(\zeta, B) = \varepsilon(\zeta) + \gamma\zeta B, \qquad \gamma = \frac{g\mu_B}{2}$$

- Equilibrium polarization $\zeta(B)$

$$\frac{\partial\varepsilon(\zeta, B)}{\partial\zeta} = 0 \quad \longrightarrow \quad \varepsilon'(\zeta) = -\gamma B \quad \longrightarrow \quad \zeta(B)$$

- The spin susceptibility is defined as

$$\chi_s = \left.\frac{dM}{dB}\right|_{B=0} = -n\gamma \left.\frac{d\zeta}{dB}\right|_{B=0} = n\gamma^2 \left.\frac{1}{\varepsilon''(\zeta)}\right|_{\zeta=0}$$

- Knowledge of $\varepsilon(\zeta)$ ($\leftarrow$ QMC) allows for χ_s estimates!!!

Technique

- QMC (and DMC) simulations provide very accurate results:
  - ground state energies;
  - pair distribution functions;
  - static responses.
- Fermion wave functions have nodes!
- Fixed-node (or fixed-phase) approximation: we assume the nodal (phase) structure of Φ_0 is the same as for Ψ_T.
- FN-DMC (or FP-DMC) satisfies a variational principle.

Simulation “details”

- Choice of trial wave function:

$$\Psi_T = J(R) \prod_{\sigma,\nu} D^{\sigma\nu}(R_{\sigma\nu}), \quad D^{\sigma\nu}(R_{\sigma\nu}) = \det[\exp(i\mathbf{k}_{i_{\sigma\nu}} \cdot \mathbf{s}_{j_{\sigma\nu}})].$$

  We have considered:

  - Plane-wave (PW) nodes: $\mathbf{s}_{j_{\sigma\nu}} = \mathbf{r}_{j_{\sigma\nu}}$
  - J(R): $u(\tilde{r}) = \frac{a\,\tilde{r}+b\,\tilde{r}^2}{1+c\,\tilde{r}+d\,\tilde{r}^2}$, with $\tilde{r}^2_{\alpha\beta} = p^{(x)}_{\alpha\beta}\, x^2_{\alpha\beta} + p^{(y)}_{\alpha\beta}\, y^2_{\alpha\beta}$.

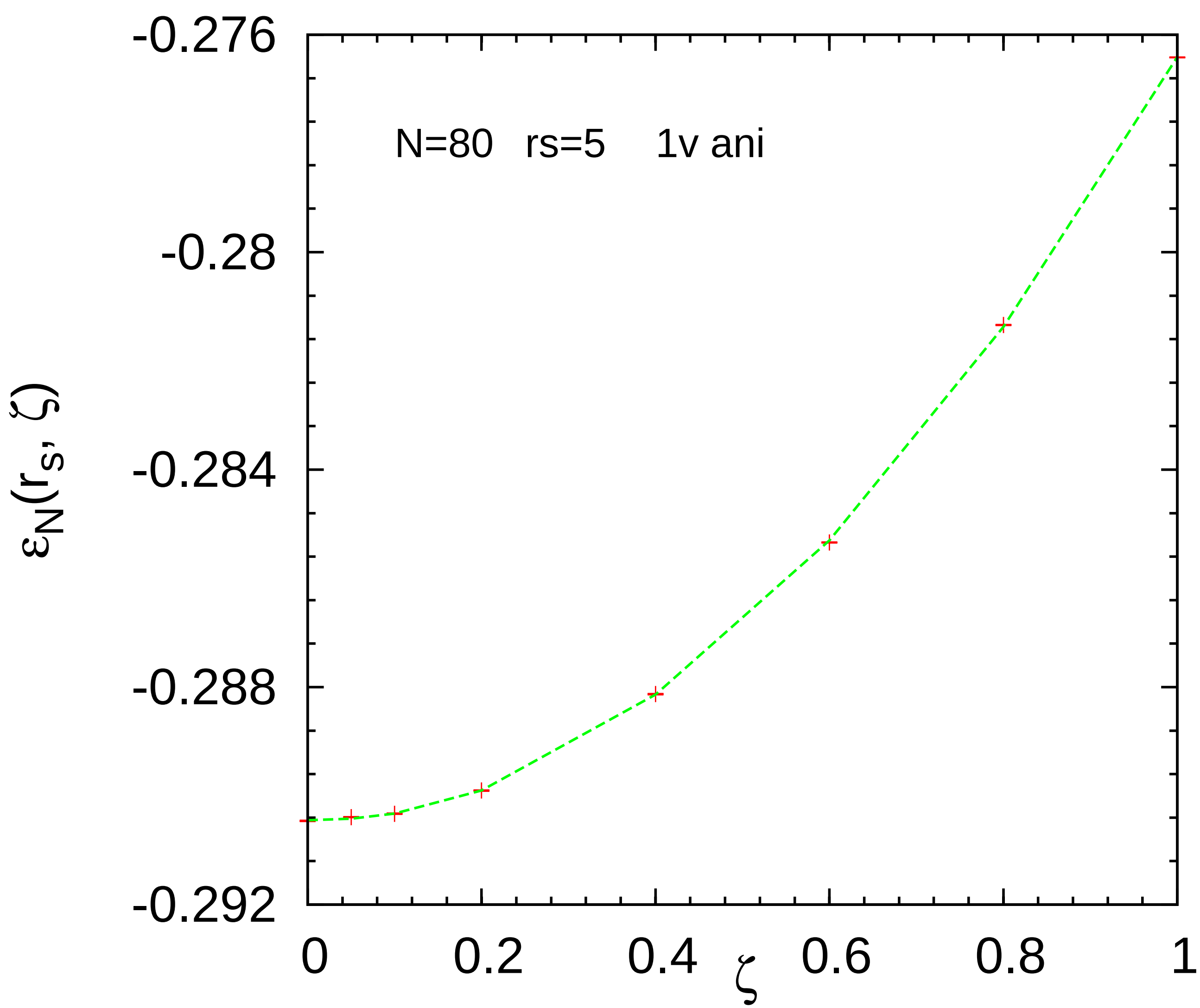
- Size extrapolation to get results in the thermodynamic limit.

- Use of twist-averaged boundary conditions (TABC) to reduce size effects on the kinetic energy at finite N and to get $\epsilon(\zeta)$ at *fixed* N.

- We have performed DMC simulations at 8 different values of ζ for various r_s, for 1v and 2v, strictly-2D or system with finite thickness.

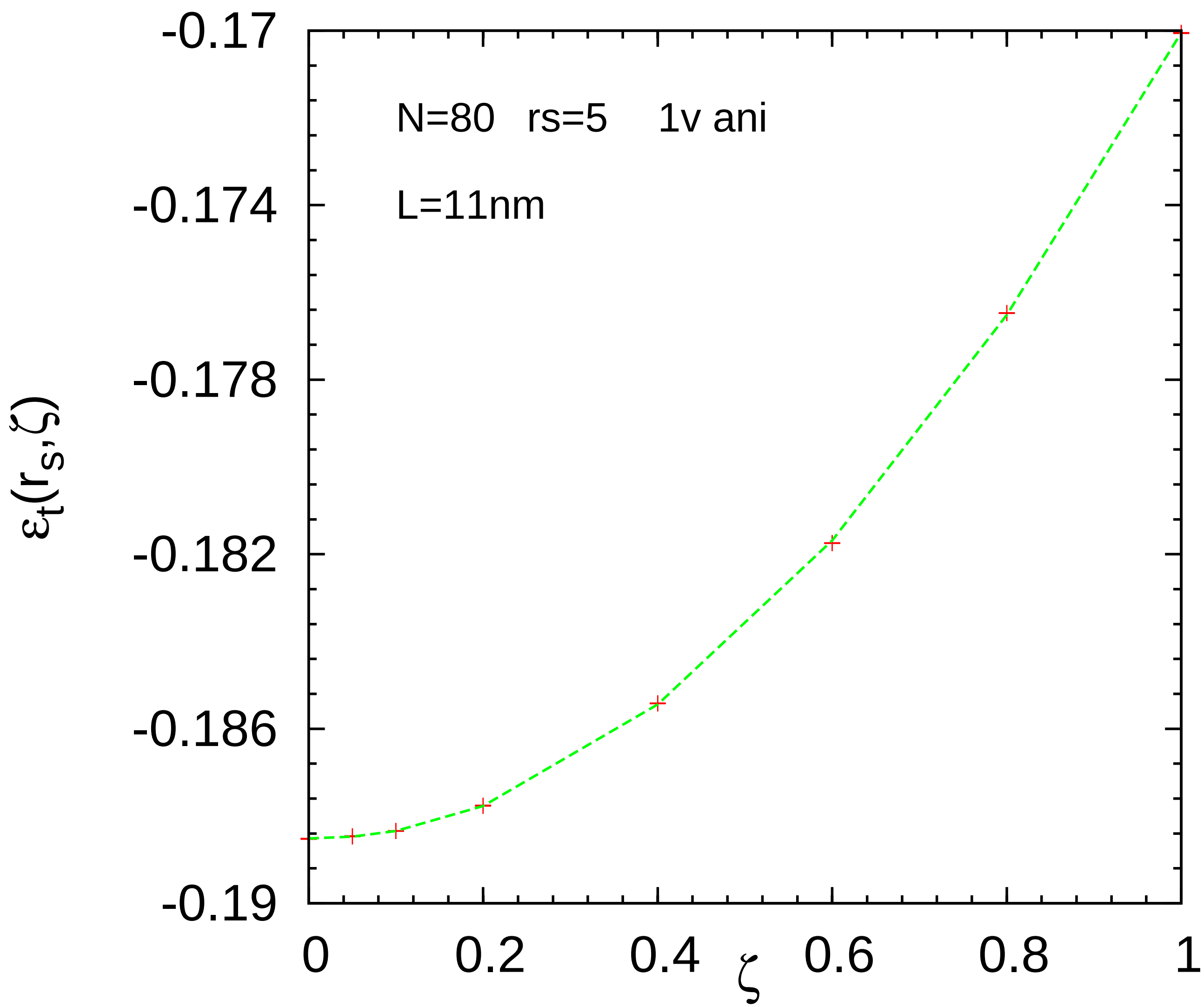
Energy per particle: Example I

TABC-DMC energy for 1v strictly-2D anisotropic system



Energy per particle: Example II

TABC-DMC energy for 1v quasi-2D anisotropic system



“Rough” ζ-fit of the energies (given r_s!)

At given r_s we fit

$$\varepsilon(r_s,\zeta) = \sum_{i=0}^{2} a_i \zeta^{2i} \equiv \varepsilon_N(r_s,\zeta) - k(r_s)\,\Delta T_N(r_s,\zeta),$$

$$\Delta T_N(r_s,\zeta) = \varepsilon_{0N}(r_s,\zeta) - \varepsilon_0(r_s,\zeta), \quad \varepsilon_0(r_s,\zeta) = \frac{1+\zeta^2}{g_v r_s^2}.$$

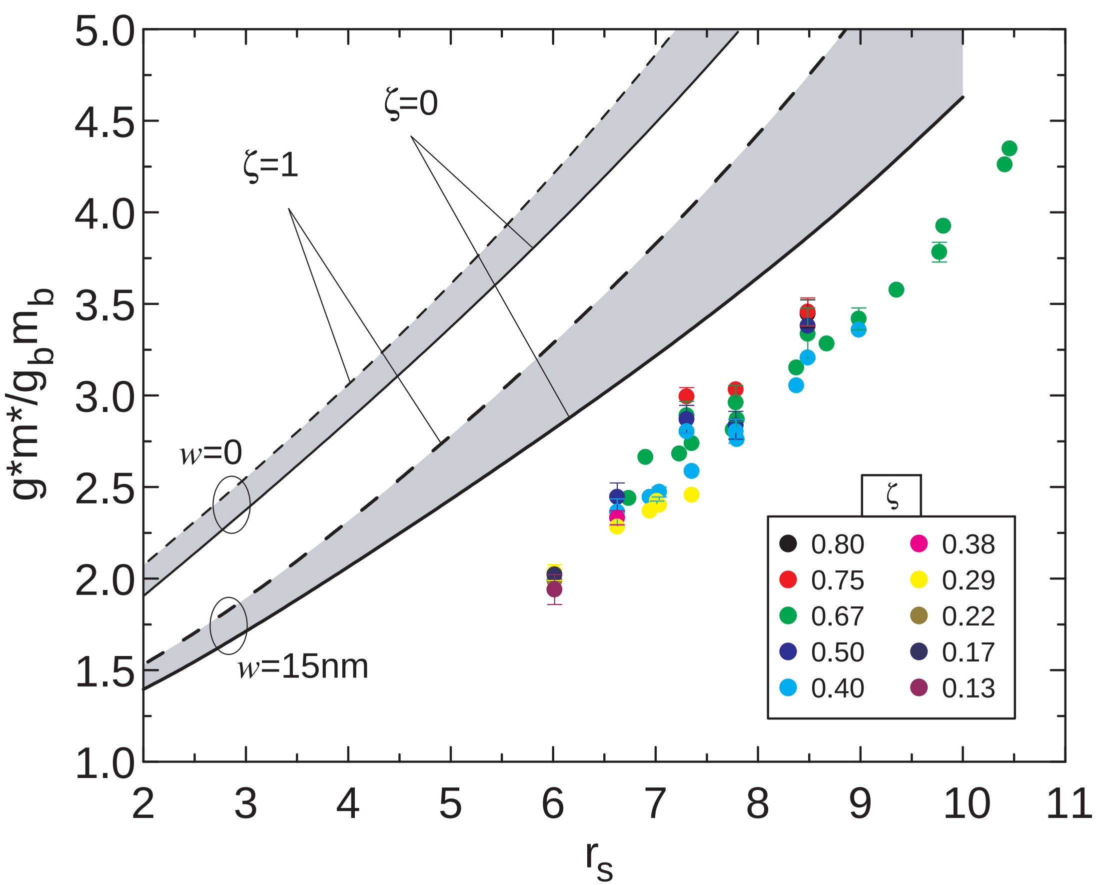
Enhancement ratio:

$$\frac{\chi_s}{\chi_0} = \frac{\varepsilon_0''(0)}{\varepsilon''(0)} = \frac{1}{g_v\, a_1\, r_s^2}.$$

Approximate treatment of mass anisotropy

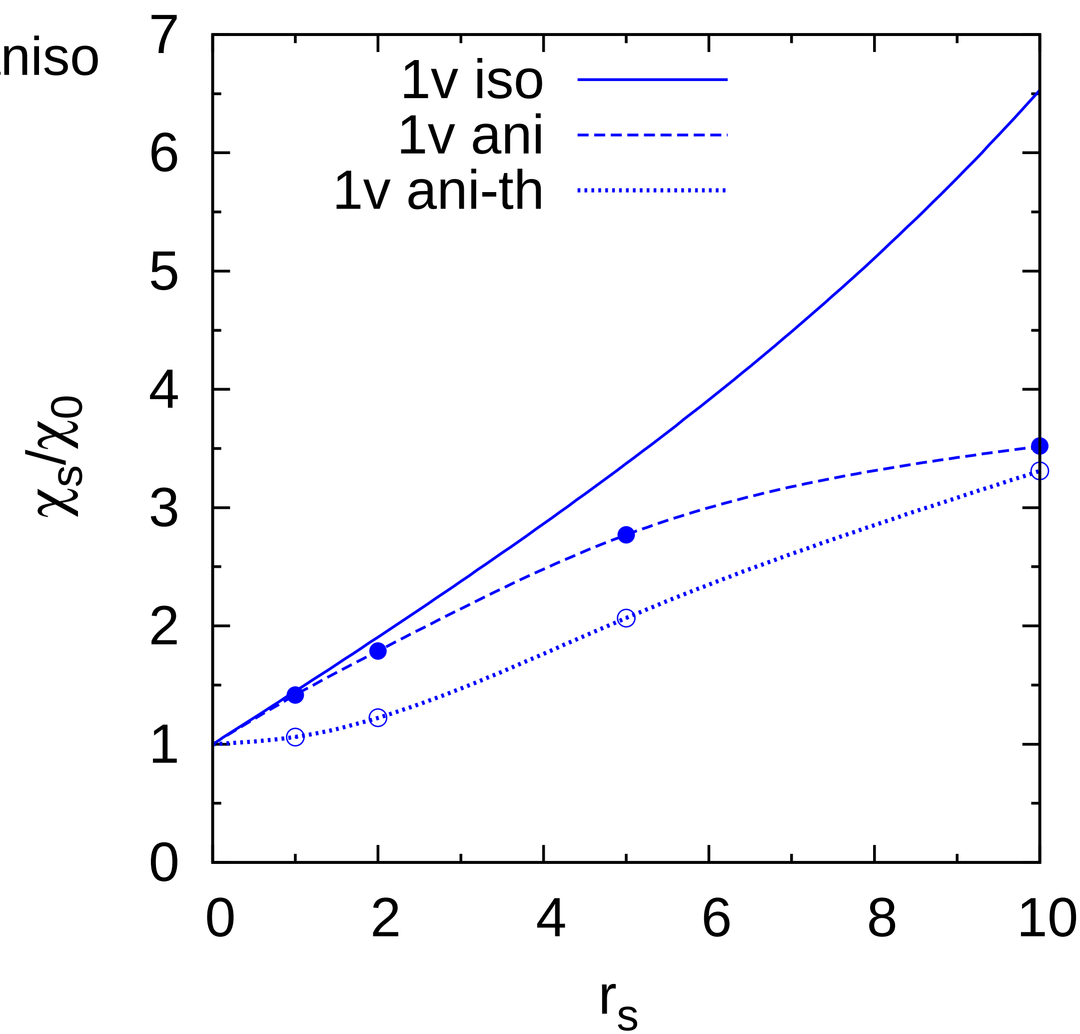
T. Gokmen *et al.*, PRB 2007

- Neglected intrinsic dependence on anisotropy
- Thickness within perturbation theory



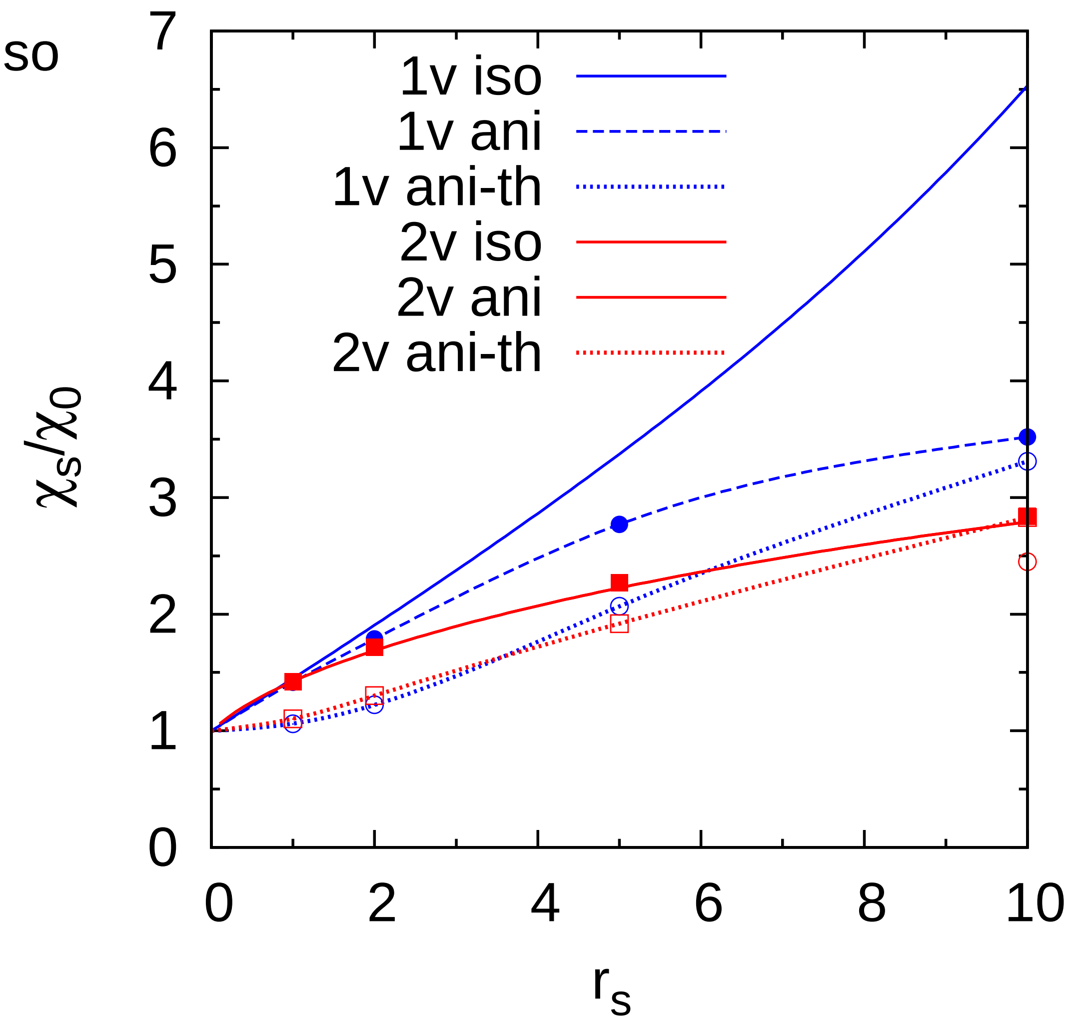
QMC full simulation results I

- Strictly-2DEG iso and aniso
- 11nm 2DEG iso and aniso
- 1v



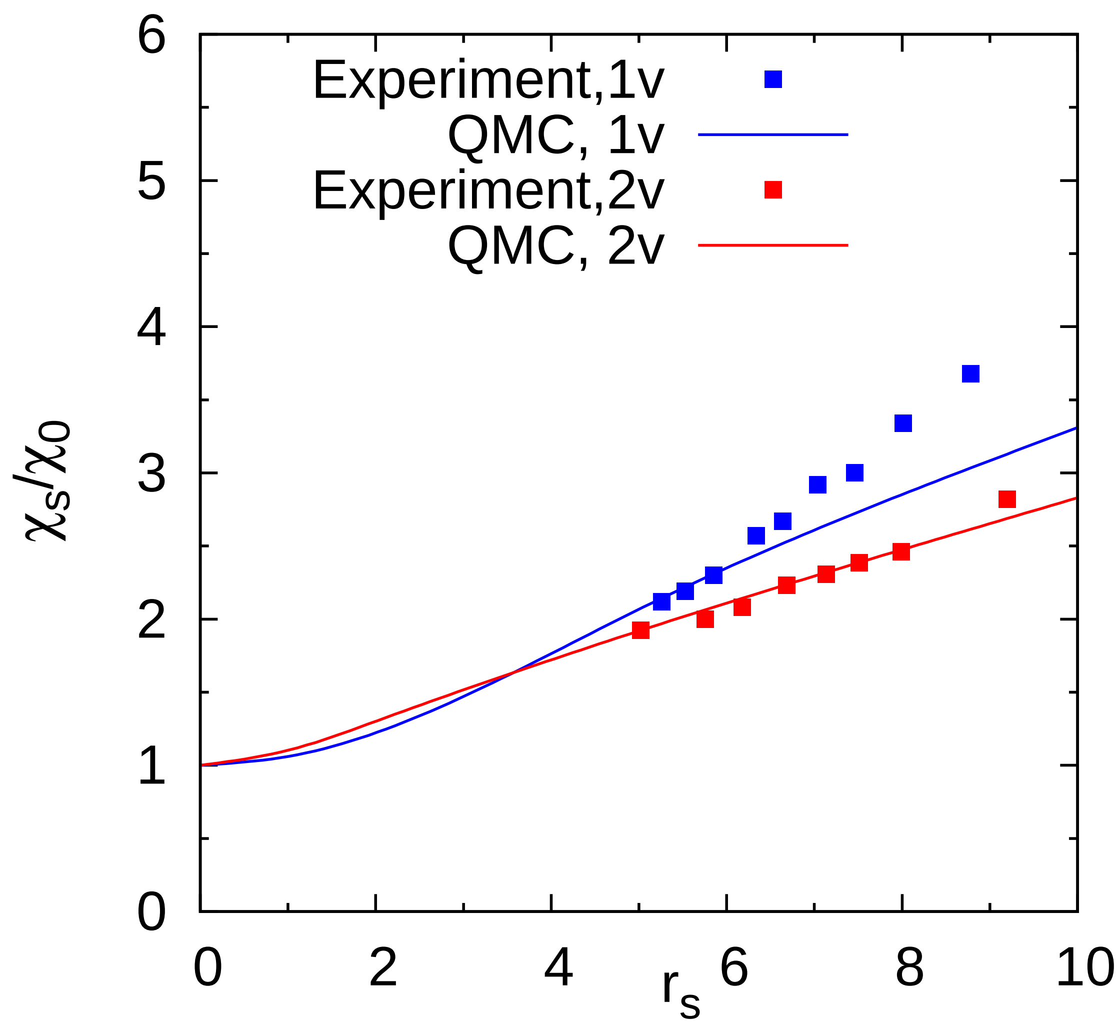
QMC full simulation results II

- Strictly-2DEG iso and aniso
- 11nm 2DEG iso and aniso
- 1v and 2v



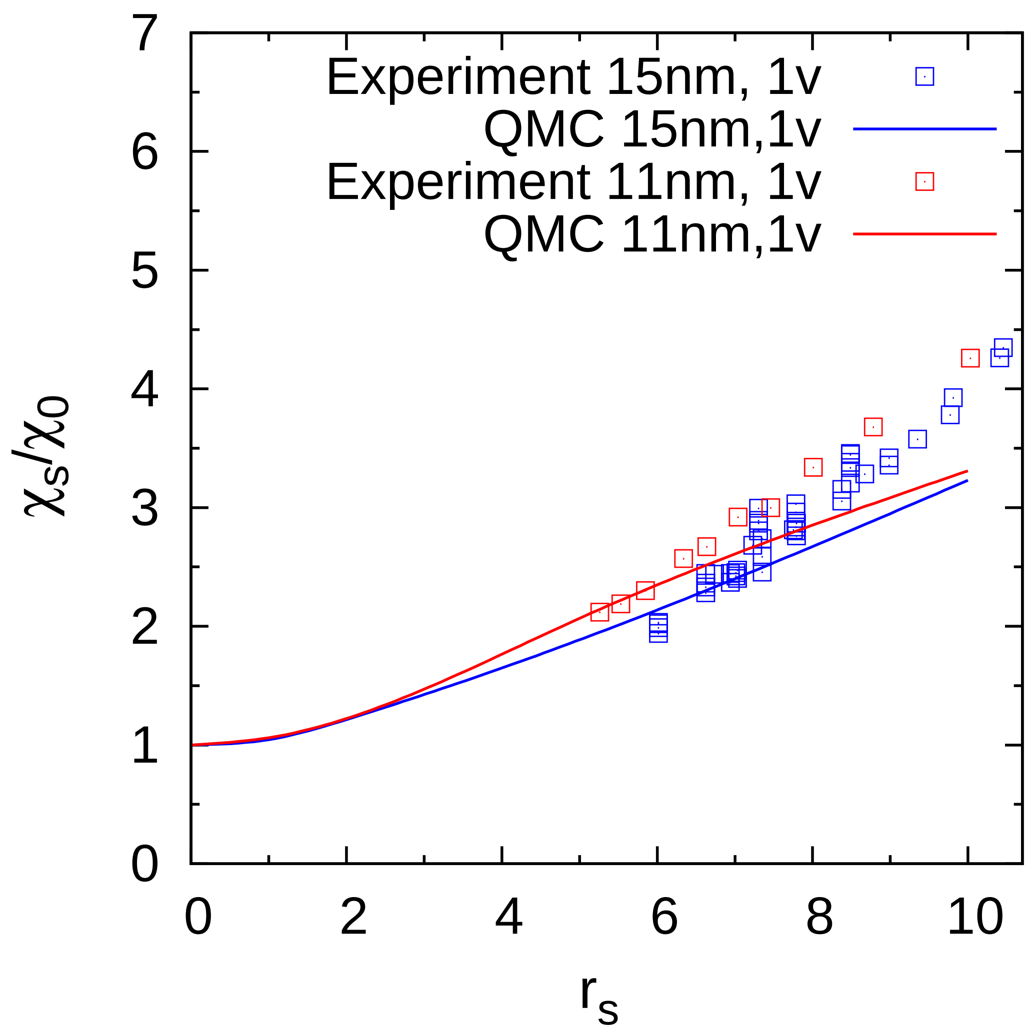
DMC and anisotropic 11nm-AlAs Qws

- 1v and 2v



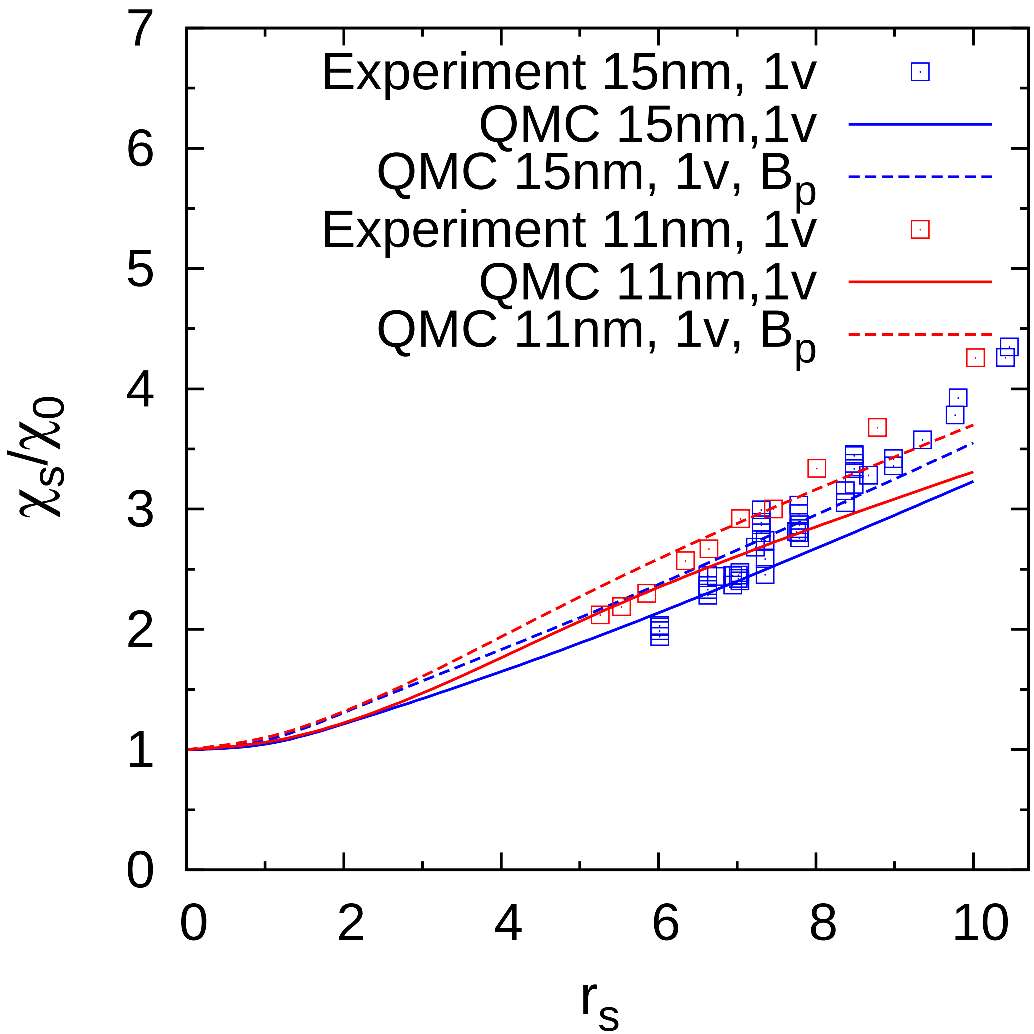
DMC vs 11nm– and 15nm–AlAs Qw I

- 1v 2DEG
- 15nm and 11nm

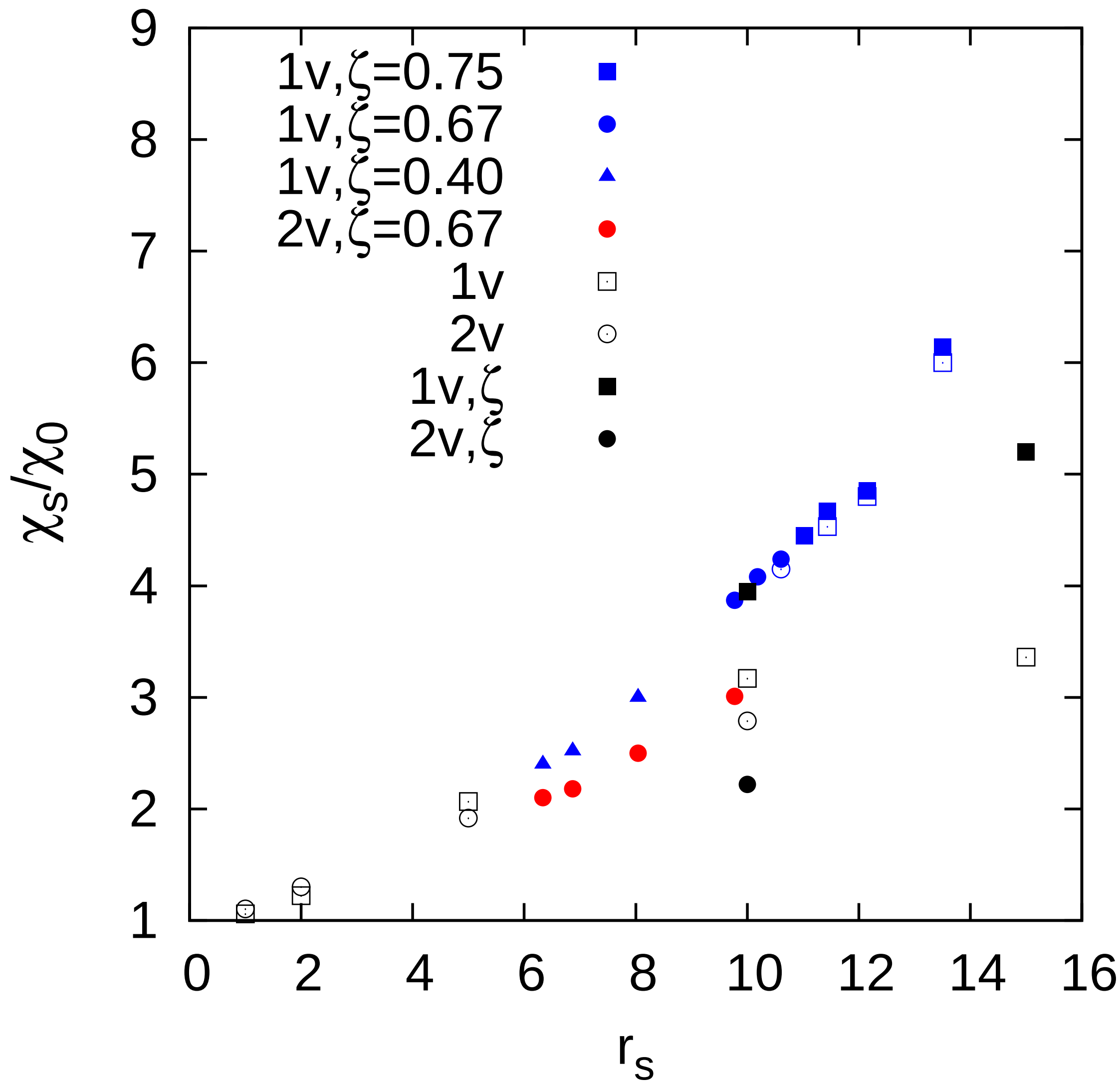


DMC vs 11nm– and 15nm–AlAs Qw II

- 1v 2DEG
- 15nm and 11nm



L=11nm, finite ζ



Conclusions

- Valley degeneracy and thickness reduces spin-susceptibility enhancement.
- Mass anisotropy suppresses the spin-susceptibility enhancement in 1v systems.
- For 2v mass anisotropy is counterbalanced by the different orientation of the Fermi surfaces.
- Finite ζ enhances χ_s/χ_0 (2v?).

Measuring the spin susceptibility

- Transport measurements. Tilted field technique (Fang & Stiles, 1968): exploits Shubnikov-de Haas oscillations and gives access to quasiparticle parameters (g^*, m^*).
- Magnetoresistance saturation (Okamoto, 1989; Shashkin, 2001). Changes in the behavior of magnetoresistance with the parallel component of B allows the determination of the polarization field B_p, from which g^*m^* can be extracted (with *ad-hoc* assumptions).
- Thermodynamic measurements (Prus, 2003; Shashkin, 2006). Measurement of $\partial\mu/\partial B$ (μ= chemical potential here) allows for the determination of $M(B)$.

Boundary conditions

- N particles in a box of side L.
- PBC: $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_i + L\hat{\mathbf{x}}, \ldots) = \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots)$.
- TABC: ($[H, T_{L\mathbf{n}}] = 0$)

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_i + L\hat{\mathbf{x}}_\alpha, \ldots) = e^{i\theta_{x\alpha}}\, \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots),\ (\alpha = 1, \ldots, d).$$

  - How to do the twist average

$$\langle O \rangle_{\boldsymbol{\theta}} = \frac{1}{(2\pi)^d} \int d\boldsymbol{\theta}\, \langle \Psi(\mathbf{R}, \boldsymbol{\theta}) | O | \Psi(\mathbf{R}, \boldsymbol{\theta}) \rangle ?$$

  - Calculation of $\sum_i \omega_i O_i$ using a grid defined by points $\boldsymbol{\theta}_i$ with weights ω_i (such that $\sum_i \omega_i = 1$) in the region in which one averages.

Fixed Phase (FP) approximation

- Consider *e.g. real* H and *complex* $\Psi(R) = |\Psi(R)| \cdot \exp[i\varphi(R)]$.
- Real and imaginary parts of Schrödinger equation yield

$$\left[-\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \tilde{V}(R) \right] |\Psi(R)| = E|\Psi(R)|,$$

$$\sum_{i=1}^{N} \nabla_i \cdot \left[|\Psi^2(R)| \nabla_i \varphi(R) \right] = 0,$$

with *effective potential* $\tilde{V}(R) = V + \frac{\hbar^2}{2m} \sum_{i=1}^{N} \left[\nabla_i \varphi(R) \right]^2.$

- FP approximation: make a choice for the phase φ and solve bosonic problem for $|\Psi|$.

2DEG energies: iso vs aniso, 1v-2v