Orbital Ordering and Effective Mass Enhancement in t_{2g} Electron Gases

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Outline

- Why study Oxide 2DEGs?
- What is a t_{2g} electron gas?
  - Multiband 2DEG of d-orbitals with Coulomb interactions.
- Orbital and Spin ordering
  - t_{2g} 2DEGs can undergo interaction driven orbital and spin ordering transitions.
- Many-body mass enhancement
  - Band offset provides additional screening in anisotropic bands, and leads to larger mass enhancement.

Why Study Oxide 2DEGs?

Bulk Complex Oxides

- High Tc SC
- Mott Physics
- Strong interactions

2D Semiconductors

- Devices
- Electric Field Effect
- FQHE
- Growth techniques

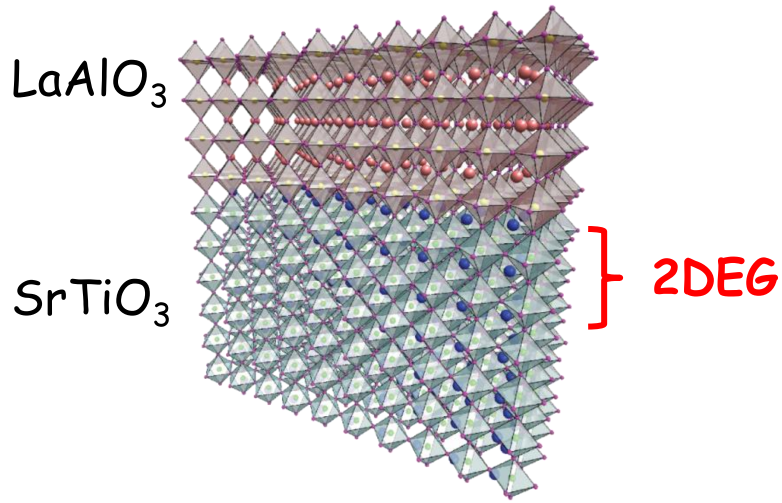
Oxide 2DEGs

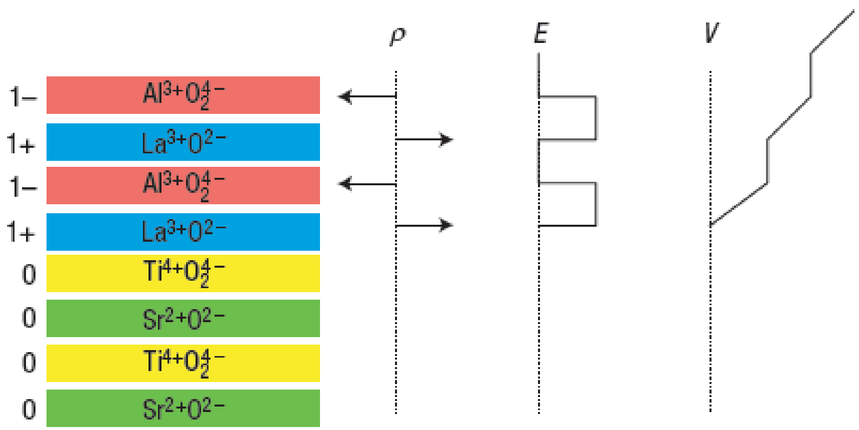
- Strongly correlated devices?
- Field effect tunable QPTs?
- ???

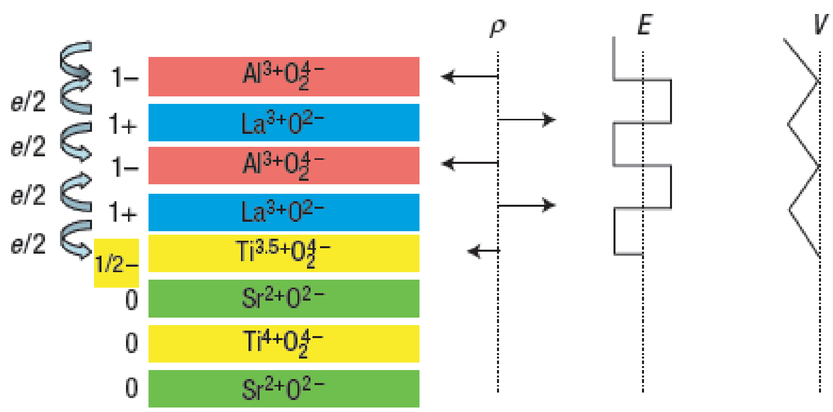
$LaAlO_3$ / $SrTiO_3$ Heterostructures

Ohtomo & Hwang Nature 2004

- Discover 2DEG at interface of two insulators.







t_{2g} 2DEGs

- LAO/STO heterostructures

  (J. Mannhart, Stuttgart, S. Ilani, Weizmann; J. Levy, Pittsburgh; Triscone, Geneva; R. Ashoori, MIT; H. Hwang, Stanford; & many more)

- δ-doped $SrTiO_3$, other d^0 systems

  (e.g. H. Hwang, Stanford)

- $SrTiO_3$ quantum wells (other d^0)

  (e.g. S. Stemmer, UCSB)

- $SrTiO_3$ surface states (other d^0)

  (e.g. Santander-Syro, Paris)

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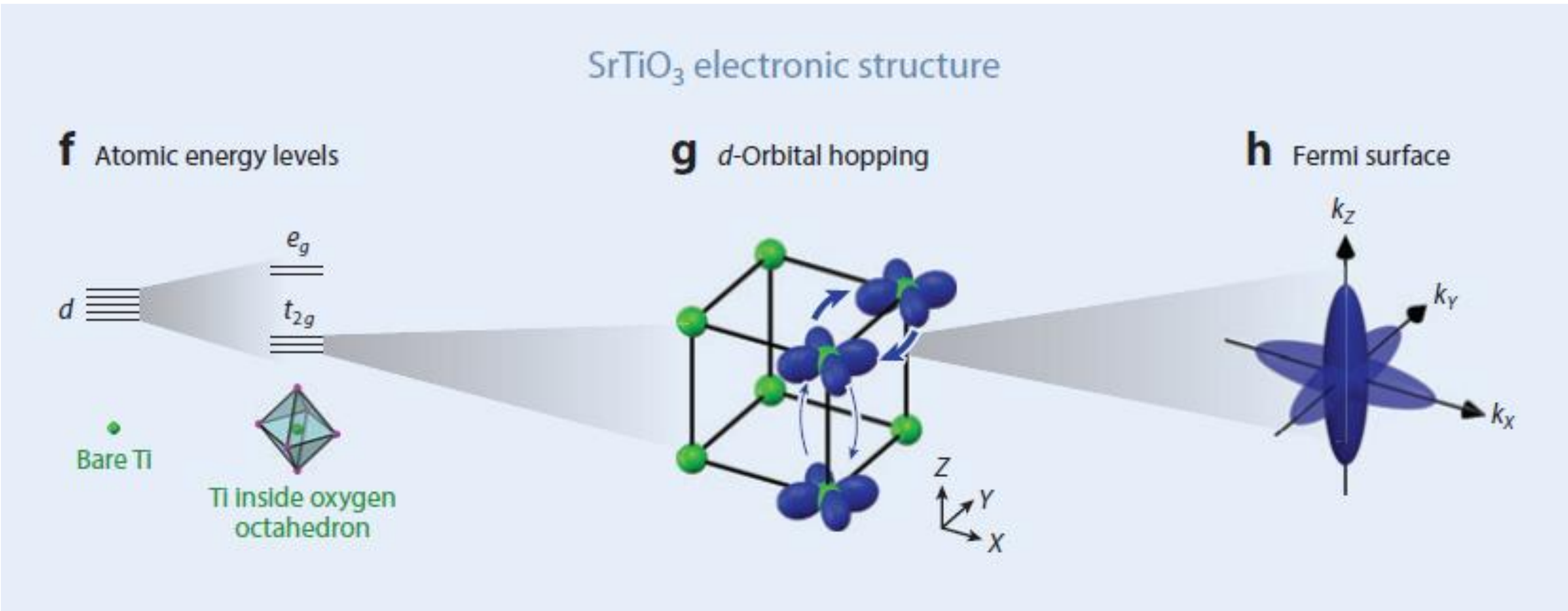
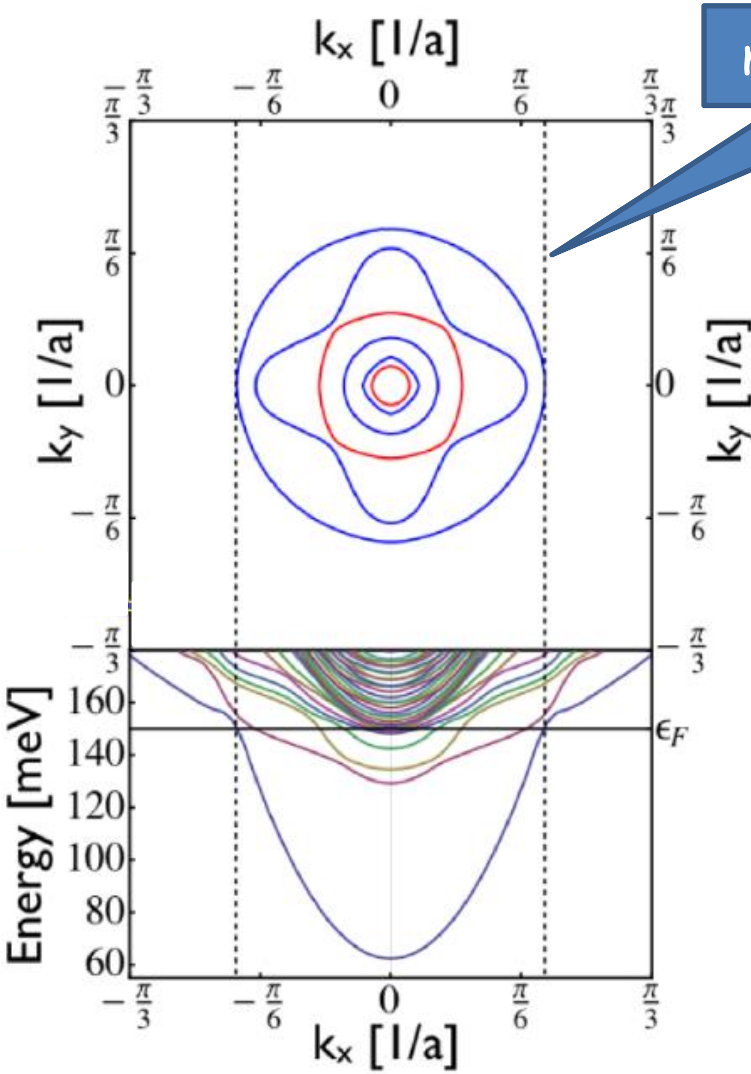
What is a t_{2g} 2DEG?

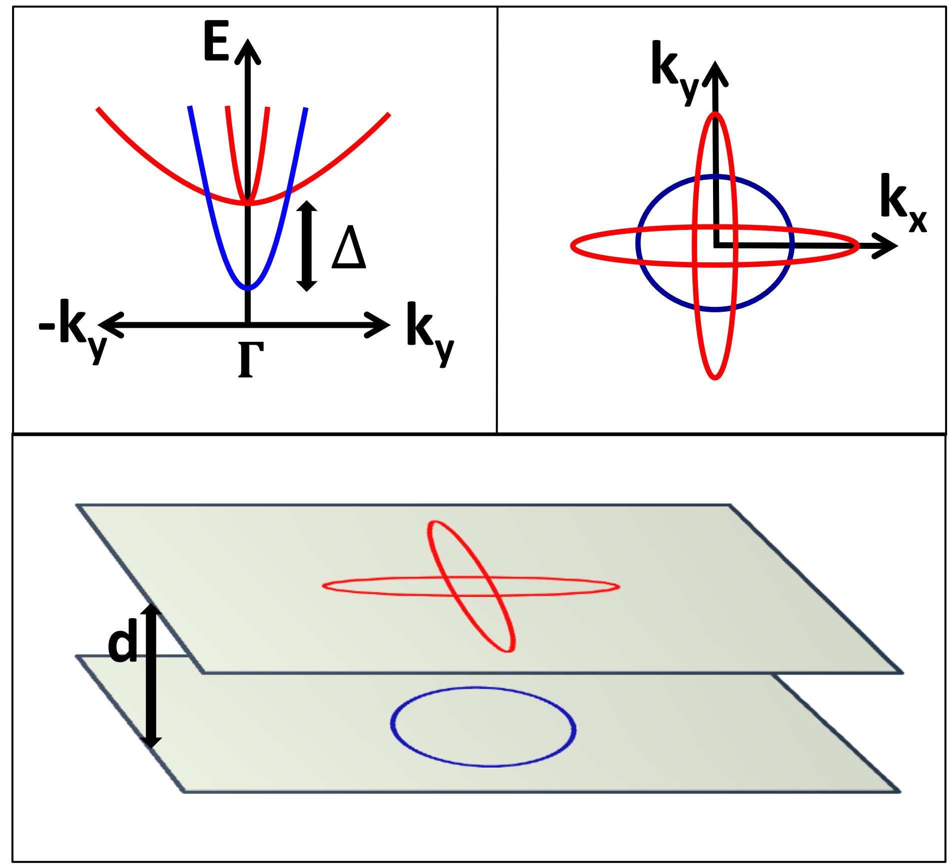


Sulpizio et al, Ann. Rev. Mat. Res. 2014

t_{2g} band structure

$n = 7 \times 10^{13}\ cm^{-2}$





Stengel PRL 2011

G. Khalsa and A. H. MacDonald PRB 2012

t_{2g} 2DEG model

$$\mathcal{H}_{t2g} = \sum_{i=1,N_{xy}} \frac{p_{ix}^2}{2m_L} + \frac{p_{iy}^2}{2m_L} + \sum_{i=1,N_{xz}} \left[\frac{p_{ix}^2}{2m_L} + \frac{p_{iy}^2}{2m_H} + \Delta\right] + \sum_{i=1,N_{yz}} \left[\frac{p_{ix}^2}{2m_H} + \frac{p_{iy}^2}{2m_L} + \Delta\right]$$

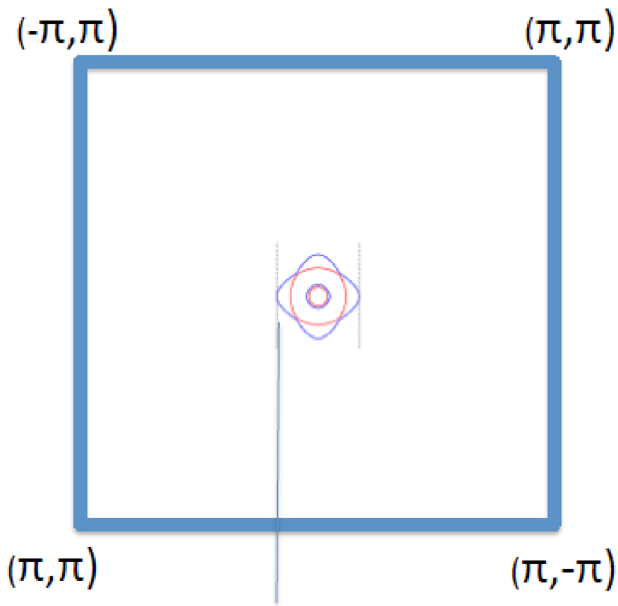
The model captures…

- Carrier distribution
- Band Offset
- Anisotropy

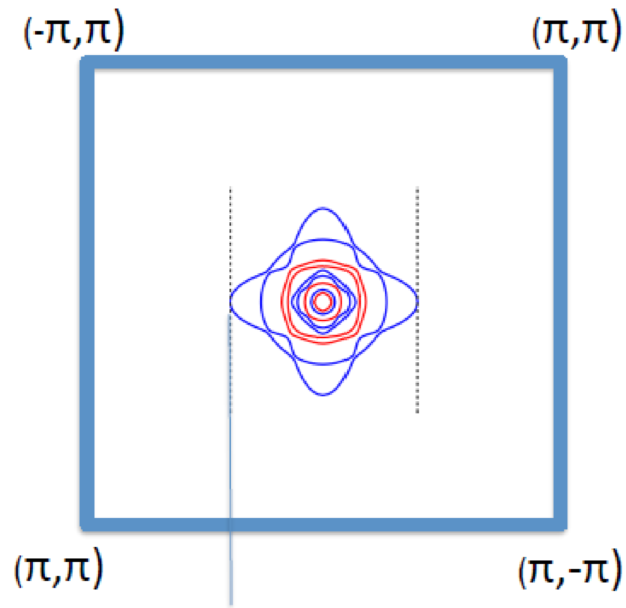
The model misses…

- Spin-Orbit coupling
- Non-180° M-O-M bonds

Small Fermi Surfaces



π/10
$n = 8 \times 10^{12}$



π/3
$n = 2 \times 10^{14}$

$$\langle k' | V_{ee} | k \rangle \sim \sum_{|R| < k_F^{-1}} \frac{e^2}{R} e^{i(k-k')\cdot R}$$

t_{2g} model Hamiltonian

$$\mathcal{H}_{t2g} = \sum_{i=1,N_{xy}} \frac{p_{ix}^2}{2m_L} + \frac{p_{iy}^2}{2m_L}$$
$$+ \sum_{i=1,N_{xz}} \left[\frac{p_{ix}^2}{2m_L} + \frac{p_{iy}^2}{2m_H} + \Delta\right]$$
$$+ \sum_{i=1,N_{yz}} \left[\frac{p_{ix}^2}{2m_H} + \frac{p_{iy}^2}{2m_L} + \Delta\right]$$
$$+ \sum_{i<j} \frac{e^2}{\epsilon|r_i - r_j|}$$

The model captures…

- Carrier distribution
- Band Offset
- Anisotropy
- Small F.S. (Coulomb)
- Interface Confinement

The model misses…

- Spin-Orbit coupling
- Non-180° M-O-M bonds

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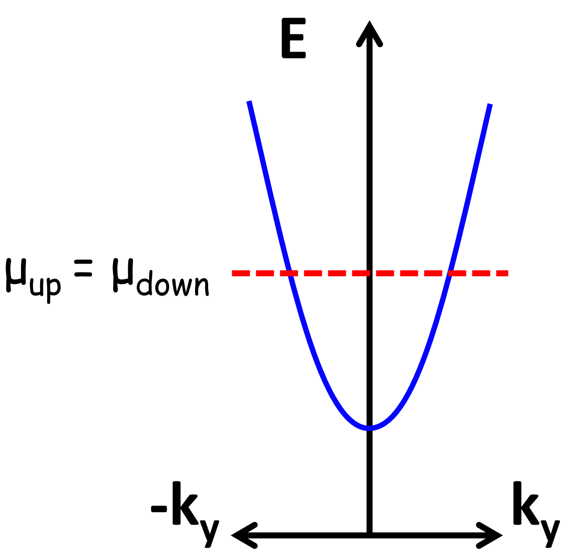
Bloch Ferromagnetism?

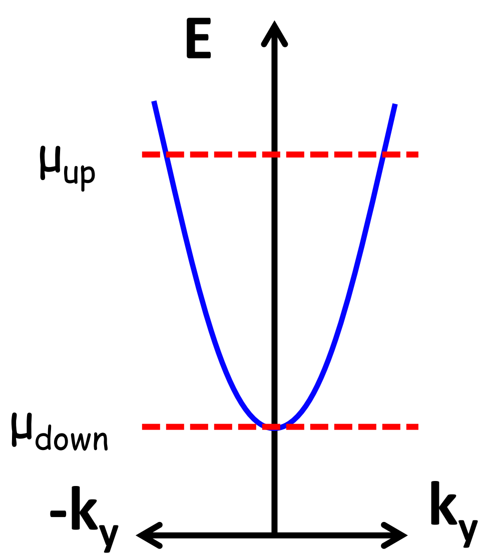
$n = 1/\pi(a_B r_S)^2$

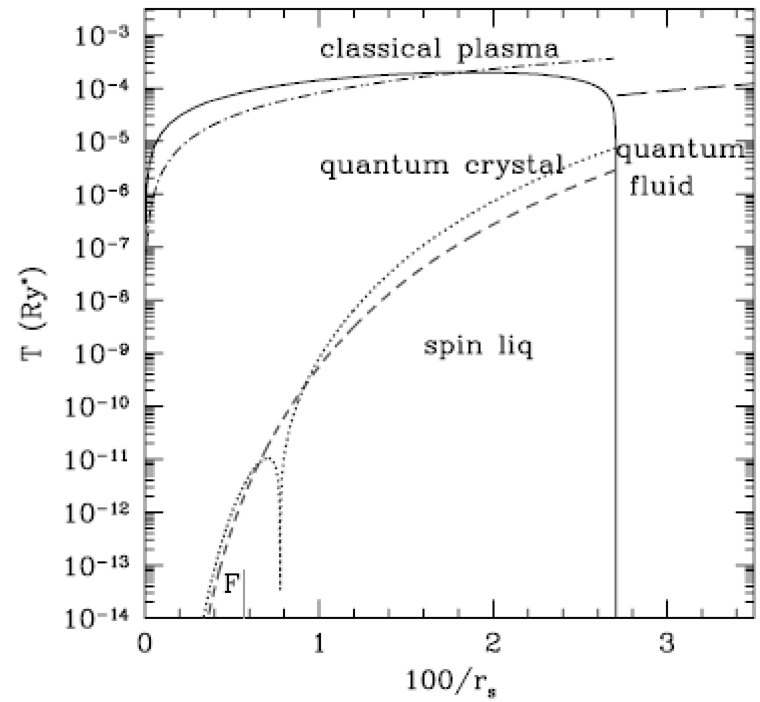
$E_{Coulomb}/E_{Kinetic} \sim r_S$

Normal



Bloch FM





B. Bernu, L. Candido, and D. M. Ceperley, PRL, 2001

t_{2g} Ground State Energy in RPA

Ground state energy
via
Coupling constant integration

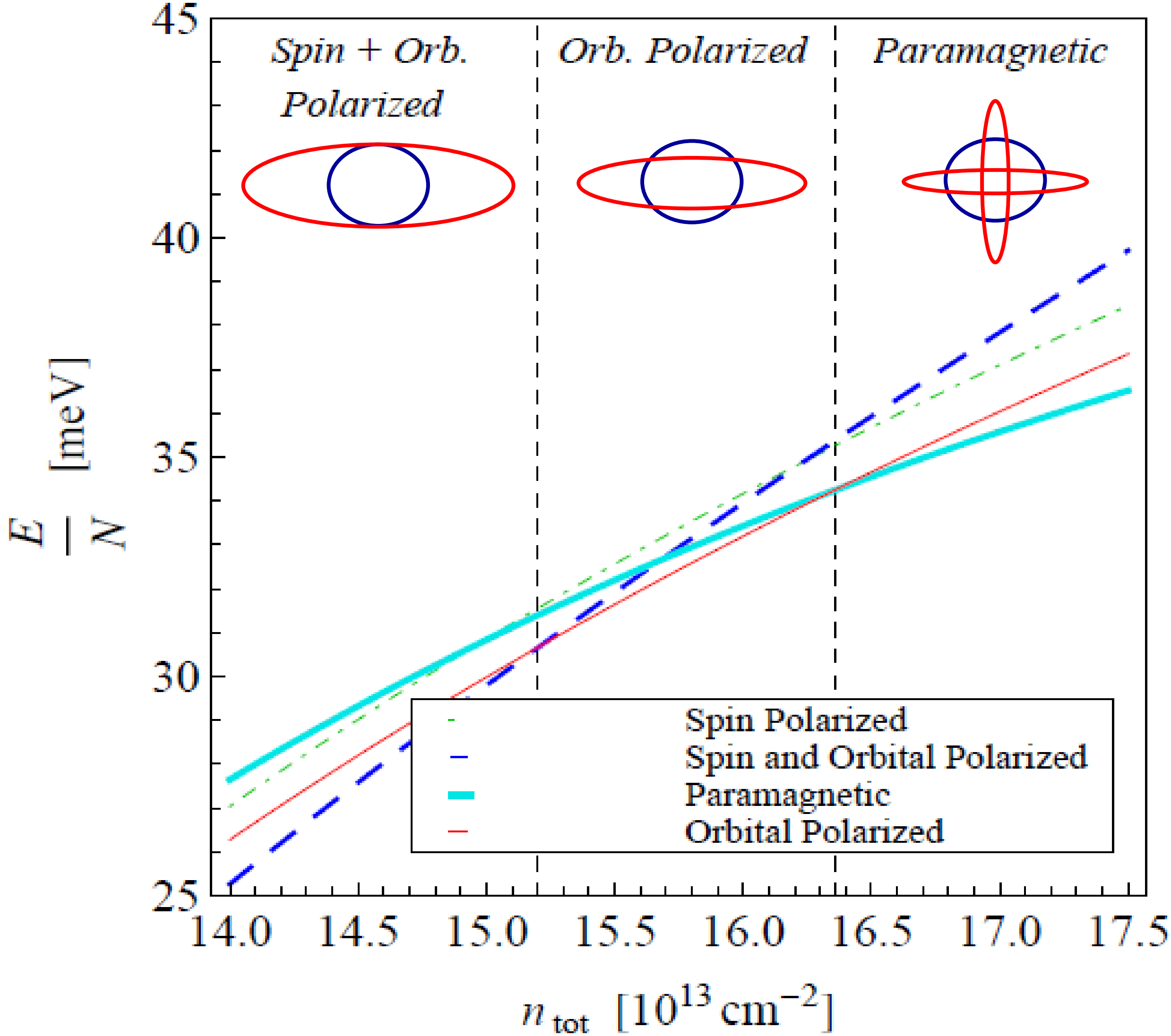
$$\langle \hat{T} \rangle + \frac{1}{2L^2}\int_0^1 \frac{d\lambda}{\lambda} \sum_q v_q \, \underbrace{\left(\langle n_{-q} n_q \rangle_\lambda - N\right)}_{S(q)}$$

$(e^2 \rightarrow \lambda e^2)$

Density structure factor
via
Fluctuation - Dissipation Theorem

$$S(q) = -\frac{\hbar}{\pi n}\int_0^\infty Im\, \chi(q,\omega)\, d\omega$$

Orbital and Spin Ordering



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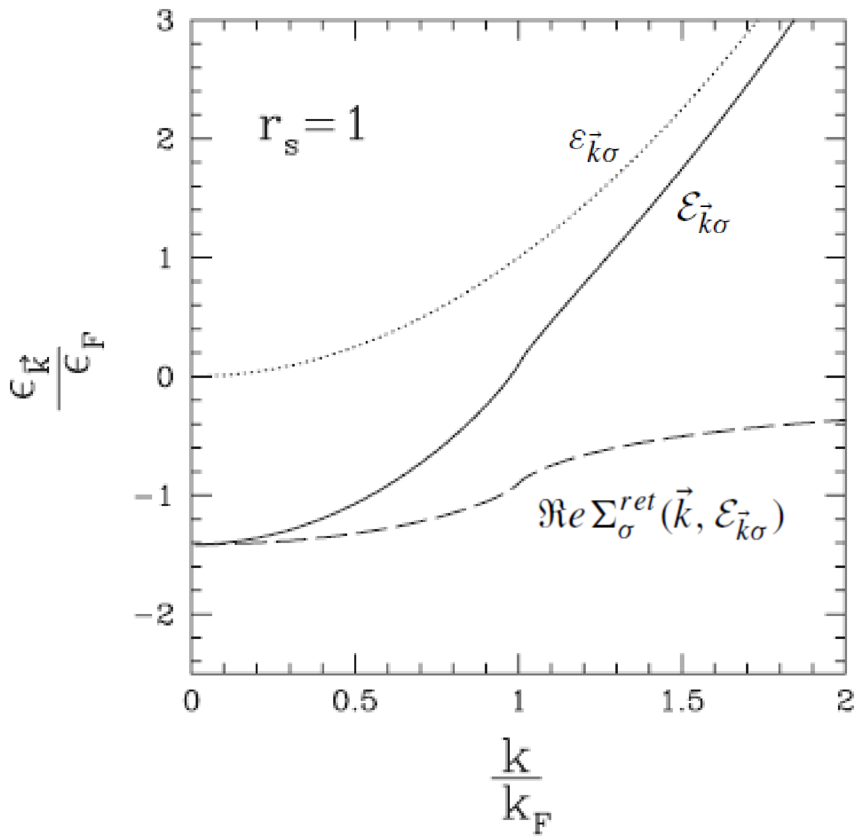
Many-body mass enhancement



Landau quasiparticle energy

$$\mathcal{E}_{\vec{k}\sigma} = \varepsilon_{\vec{k}\sigma} + \Re e\,\Sigma_\sigma^{ret}(\vec{k}, \mathcal{E}_{\vec{k}\sigma})$$

Quasiparticle effective mass

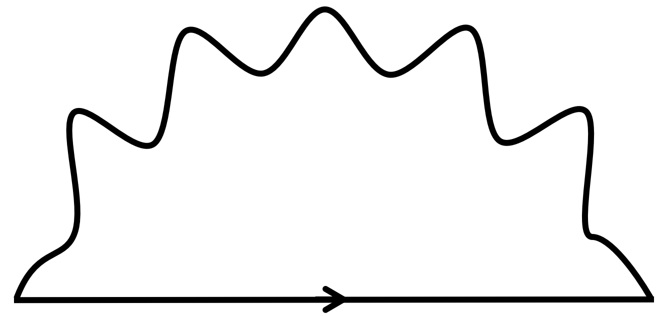
$$\mathcal{E}_{k\sigma} \simeq \mu + \frac{\hbar^2 k_F (k - k_F)}{m^*}$$

$$\boxed{\frac{\hbar^2 k_F}{m^*} = \left.\frac{d\mathcal{E}_{k\sigma}}{dk}\right|_{k=k_F}}$$

G. F. Giuliani and G. Vignale, “Quantum theory of the electron liquid”

G^0W self energy

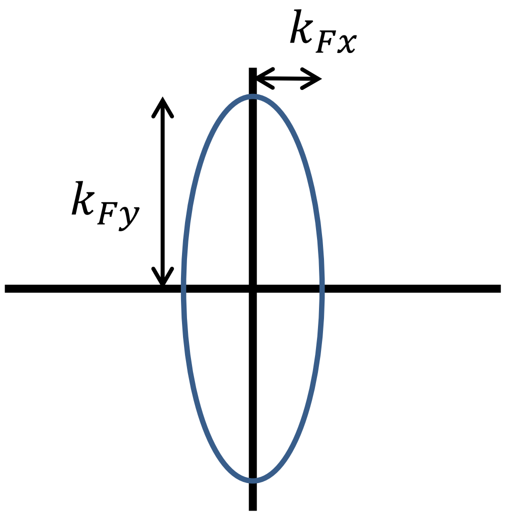
- GW is dynamically screened exchange.



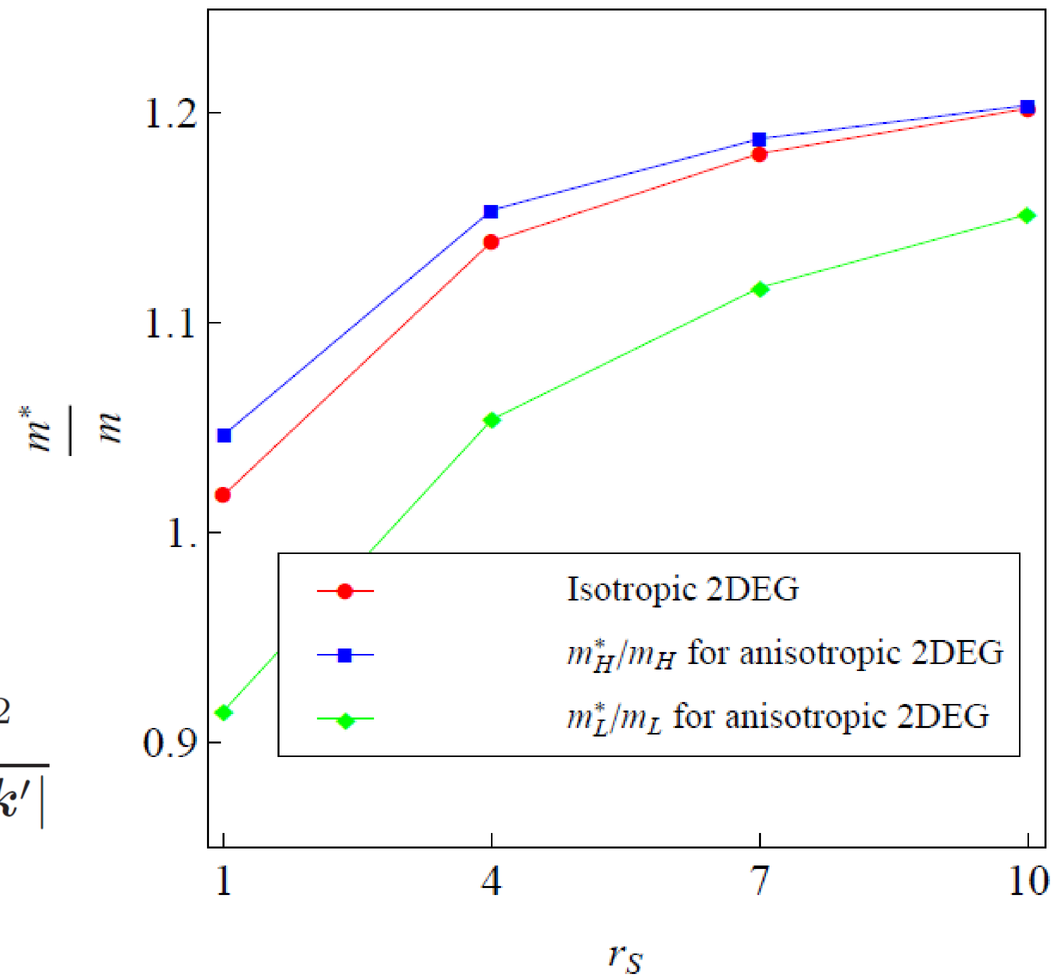
$$\Sigma^{\star, G0W}_{b\sigma}(\boldsymbol{k}, i\omega_n) = \frac{-1}{\beta\hbar L^2} \sum_{\boldsymbol{q}, i\Omega_m} W^{RPA}_{b\sigma, b\sigma}(\boldsymbol{q}, i\Omega_m) \mathcal{G}^0_{b\sigma}(\boldsymbol{k} - \boldsymbol{q}, i\omega_n - i\Omega_m)$$

a) J. J. Quinn & R. A. Ferrell Phys. Rev. 1958
b) T. M. Rice, Ann. Phys., 1965
c) G. E. Santoro & G. F Giuliani, Phys. Rev., 1979

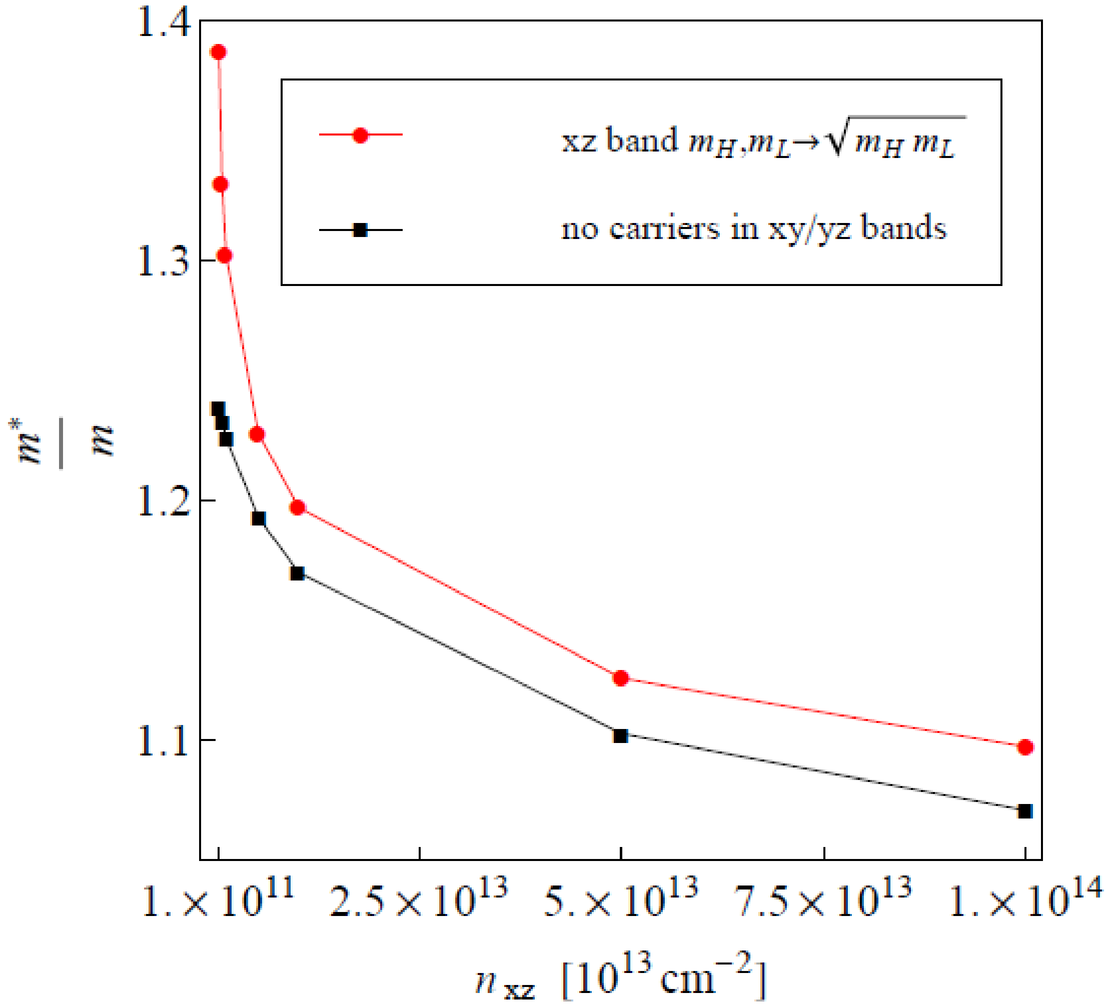
Anisotropic mass enhancement

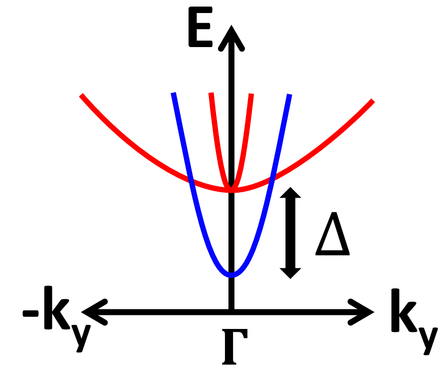


$$\Sigma_{\sigma}^{HF}(\boldsymbol{k}) = \frac{-1}{L^2}\sum_{\boldsymbol{k}'} n_{\mathrm{F}}(\boldsymbol{k}')\frac{2\pi e^2}{|\boldsymbol{k}-\boldsymbol{k}'|}$$

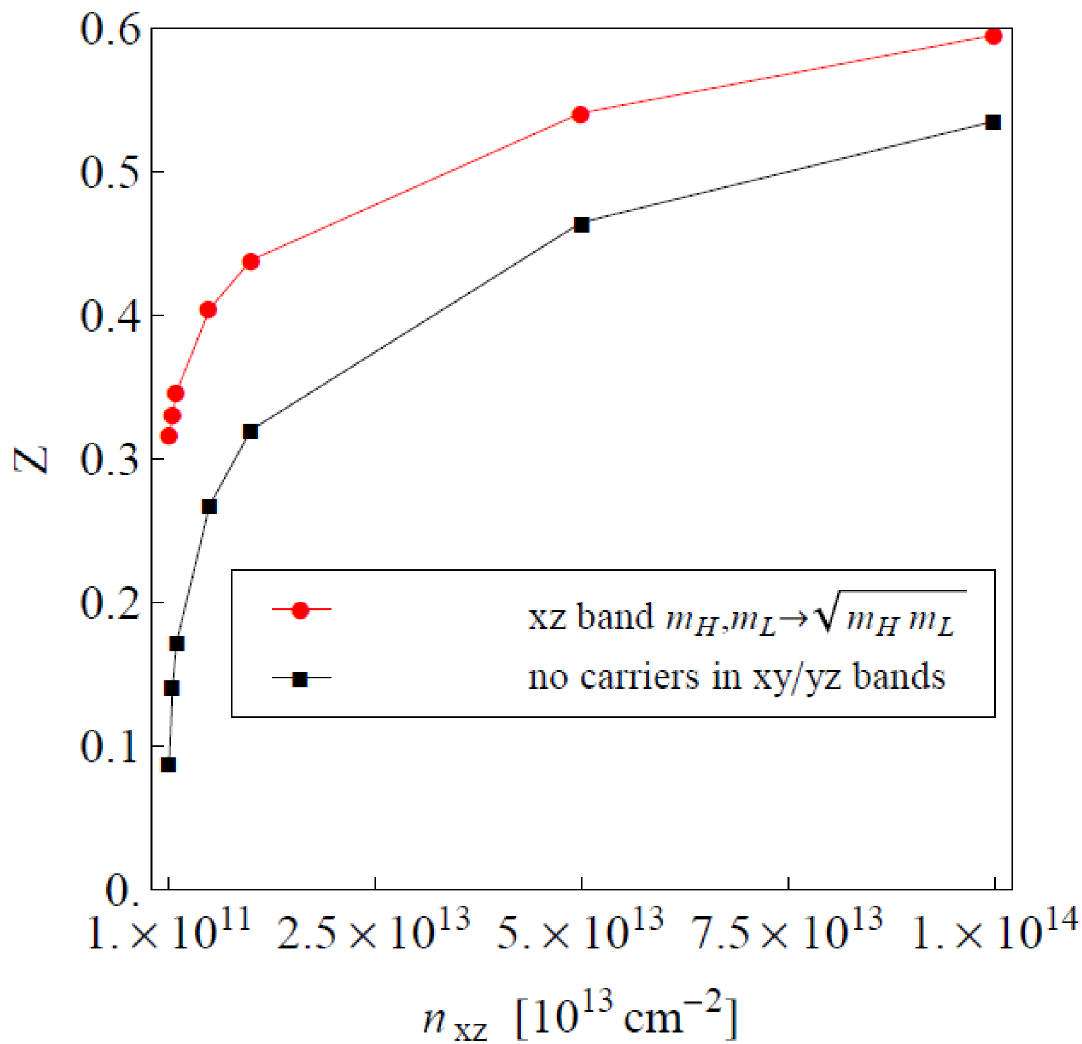


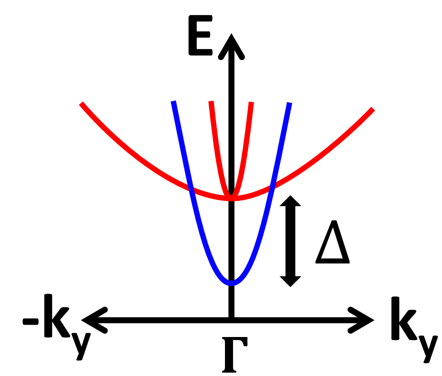
Many-body mass enhancement





Renormalization Constant Z





Conclusion

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