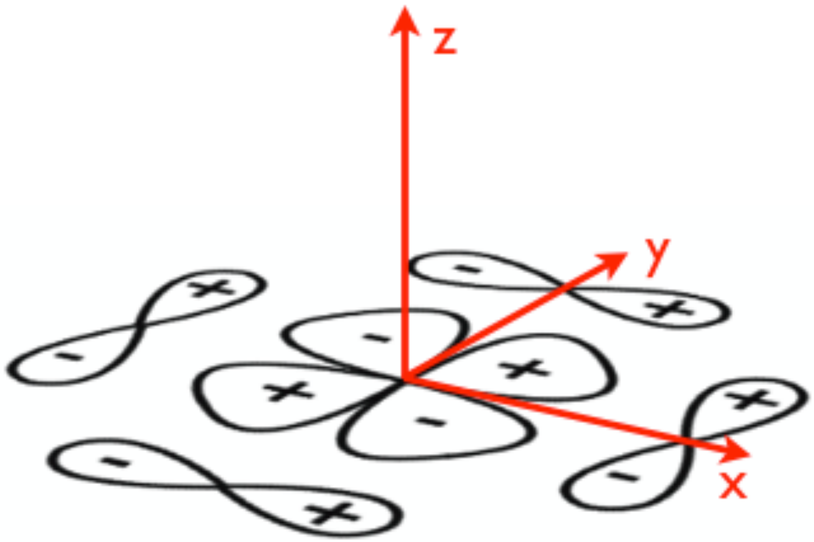
t_{2g} 2DEGs

John Tolsma, AHM - UT Austin
Marco Polini – SNS - Pisa

What is a t_{2g} 2DEG ?

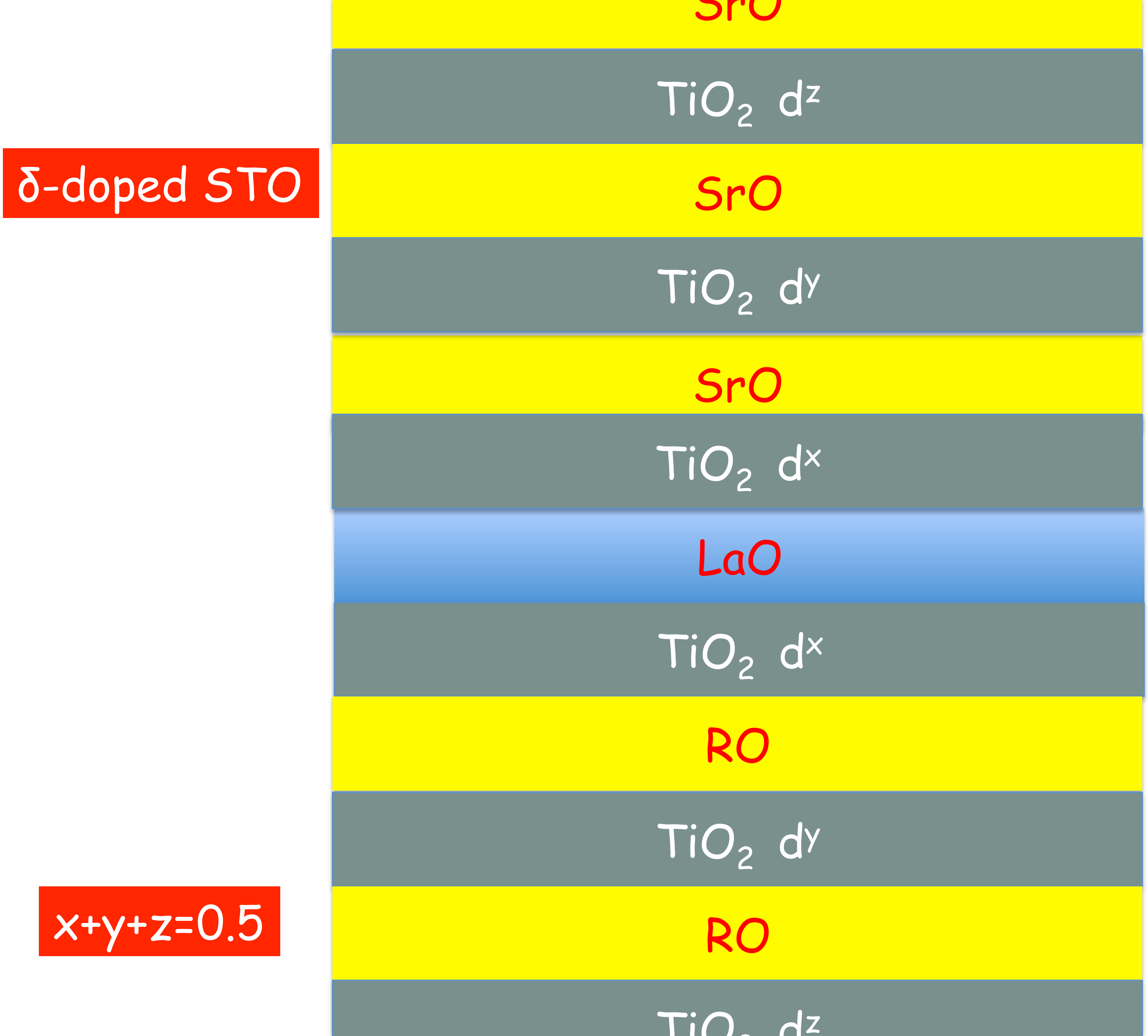
t_{2g} k.p



$$h_\alpha = \begin{pmatrix} \mathcal{L}_5 k_x^2 + \mathcal{M}_5^{\parallel} k_y^2 + \mathcal{M}_5^{\perp} k_z^2 & \mathcal{N}_5 k_x k_y & \mathcal{N}_{45}^{\star} k_x k_z \\ \mathcal{N}_5 k_x k_y & \mathcal{L}_5 k_y^2 + \mathcal{M}_5^{\parallel} k_x^2 + \mathcal{M}_5^{\perp} k_z^2 & \mathcal{N}_{45}^{\star} k_y k_z \\ \mathcal{N}_{45} k_x k_z & \mathcal{N}_{45} k_y k_z & \mathcal{M}_4 (k_x^2 + k_y^2) + \mathcal{L}_4 k_z^2 \end{pmatrix}$$

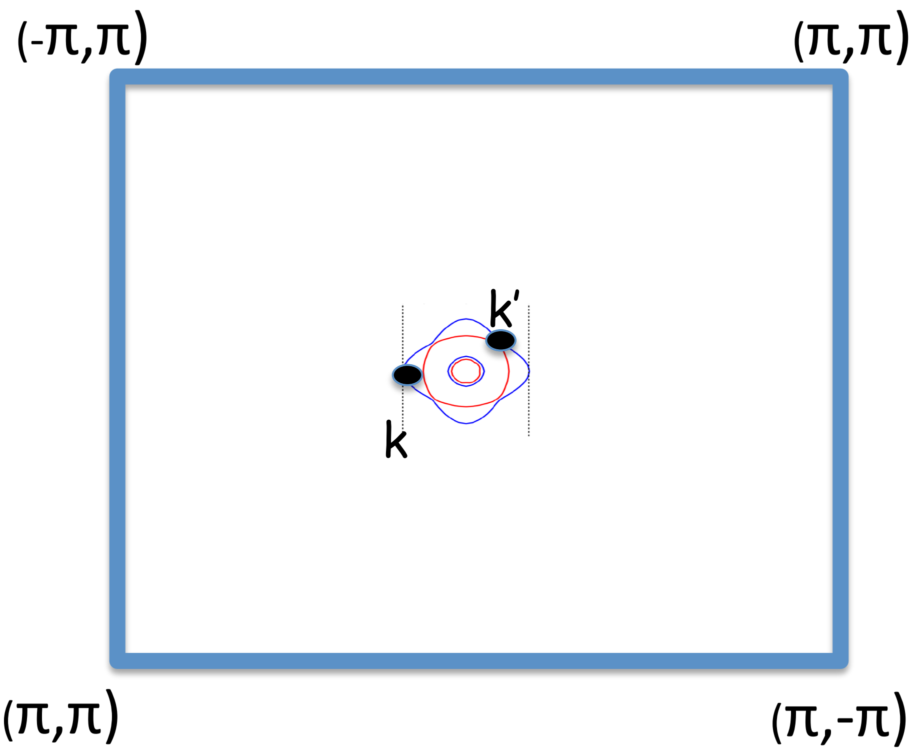
STO

M ≈ 1.2 L ≈ 0.08 N ≈ 0


SrO
TiO2 dz
δ-doped STO
SrO
TiO2 dy
SrO
TiO2 dx
LaO
TiO2 dx
RO
TiO2 dy
x+y+z=0.5
RO

TiO_2 d^1
RO
TiO_2 d^x
SrO
TiO_2 d^{1-2x}
SrO
TiO_2 d^x
RO
TiO_2 d^1
RO

Small Fermi Surfaces

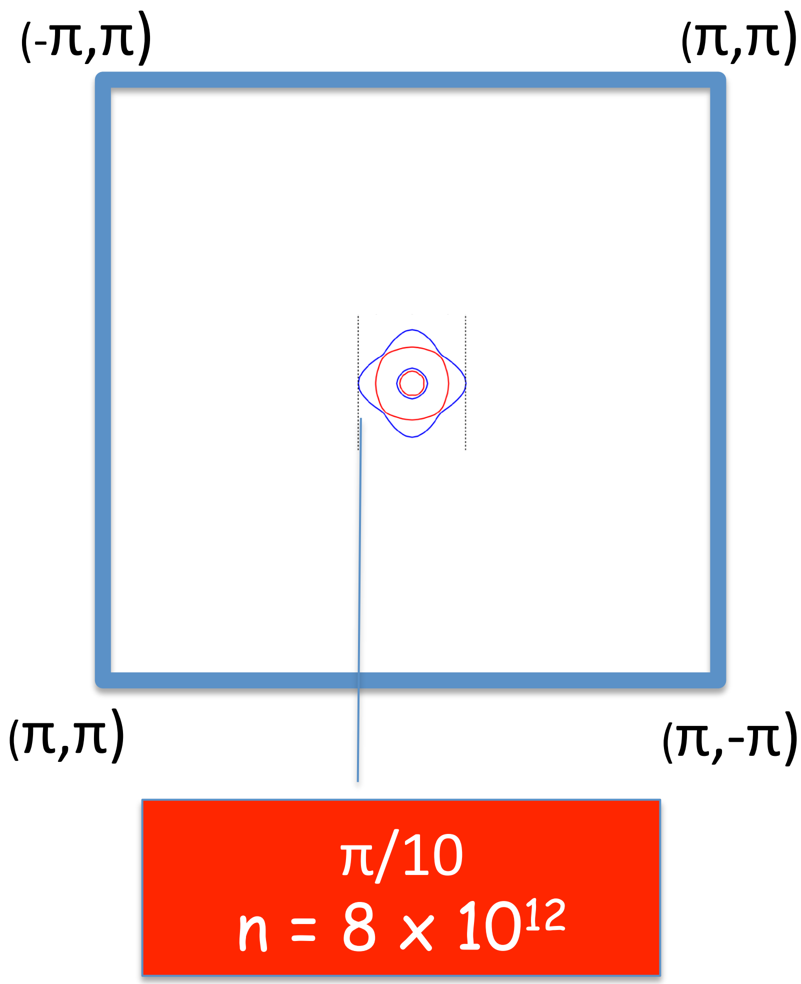


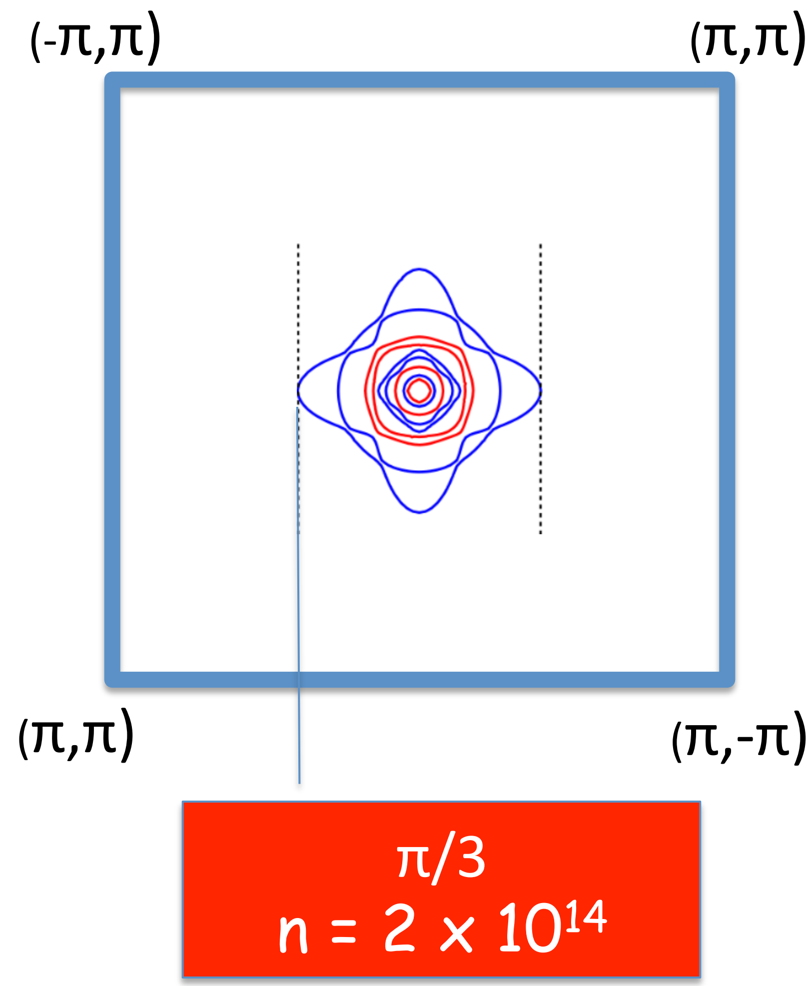
$$\langle k'|V_{ee}|k\rangle \sim \sum_{|R|<k_F^{-1}} \frac{e^2}{R}\, e^{i(k-k')\cdot R}$$

t_{2g} Electron Gas Model

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

Small Fermi Surfaces





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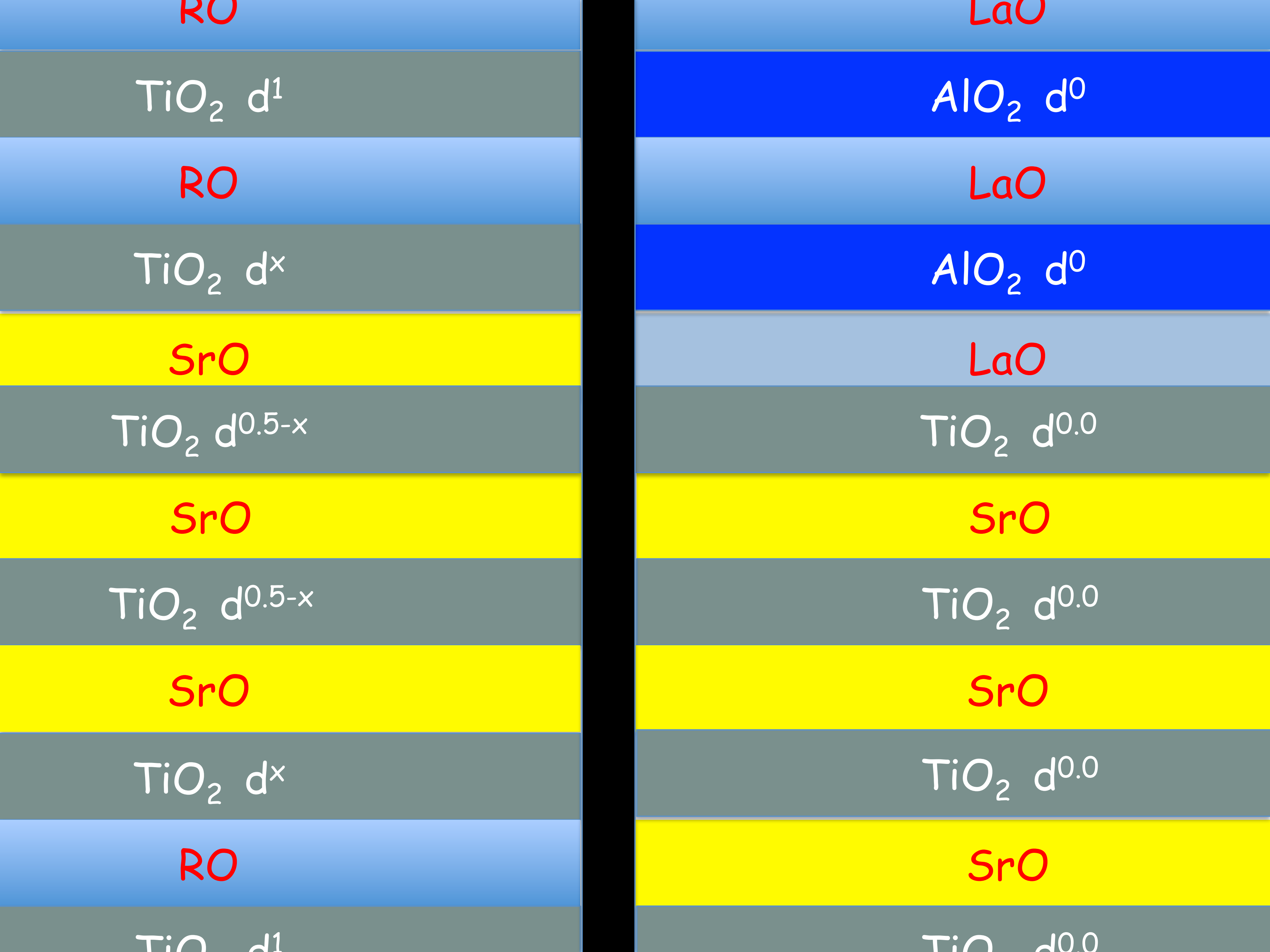
Applications

- δ-doped STO, other d^0s
- STO (other d^0) quantum wells
- surface STO (other d^0) 2DEGS
- LAO/STO ?


RO
TiO2 d1
RO
TiO2 dx
SrO
TiO2 d0.5-x
SrO
TiO2 d0.5-x
SrO
TiO2 dx
RO
LaO
AlO2 d0
LaO
AlO2 d0
LaO
TiO2 d0.0
SrO
TiO2 d0.0
SrO
TiO2 d0.0
SrO

t_{2g} Electron Gas Model

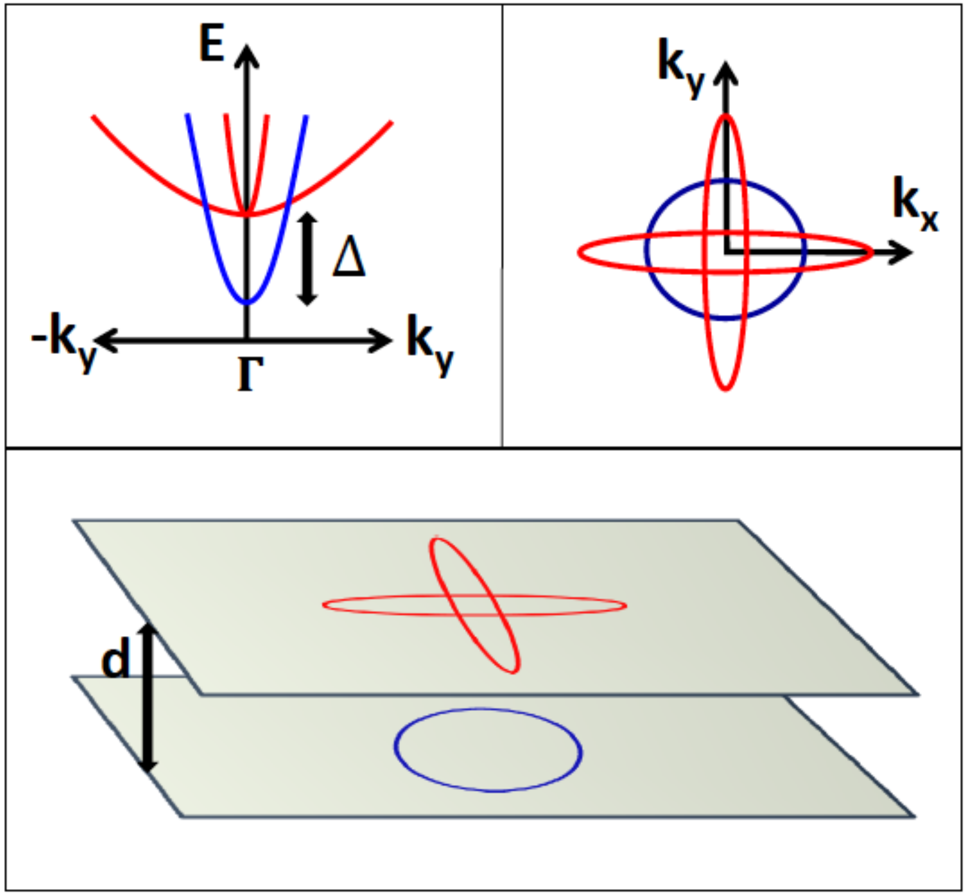
$$\mathcal{H}_{t2g} = \sum_{i=1,N_{xy}} \frac{p_{ix}^2}{2m_L} + \frac{p_{iy}^2}{2m_L} + \sum_{i=1,N_{xz}} \left[\frac{p_{ix}^2}{2m_L} + \frac{p_{iy}^2}{2m_H} + \Delta\right] + \sum_{i=1,N_{yz}} \left[\frac{p_{ix}^2}{2m_H} + \frac{p_{iy}^2}{2m_L} + \Delta\right] + \sum_{i<j} \frac{e^2}{\epsilon|r_i -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

- ❑ δ-doped STO, other d^0s
- ❑ STO (other d^0) quantum wells
- ❑ surface STO (other d^0) 2DEGS
- ❑ LAO/STO ?

t_{2g} Electron Gas Model

Missing

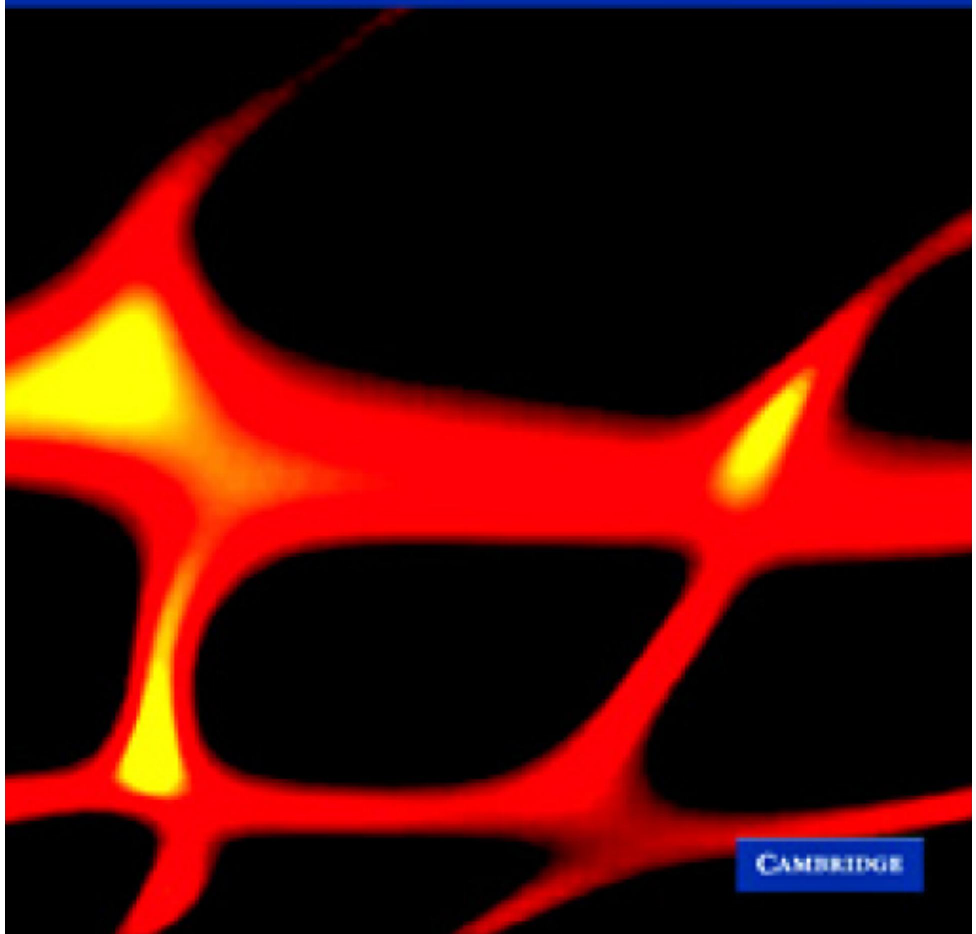
- ❑ Spin-Orbit
- ❑ non-180 M-O-M bonds



Ordinary 2DEG Properties

Gabriele F. Giuliani and Giovanni Vignale

Quantum Theory of the Electron Liquid



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PHYSICAL REVIEW VOLUME 112, NUMBER 3 NOVEMBER 1, 1958

Electron Self-Energy Approach to Correlation in a Degenerate Electron Gas*†

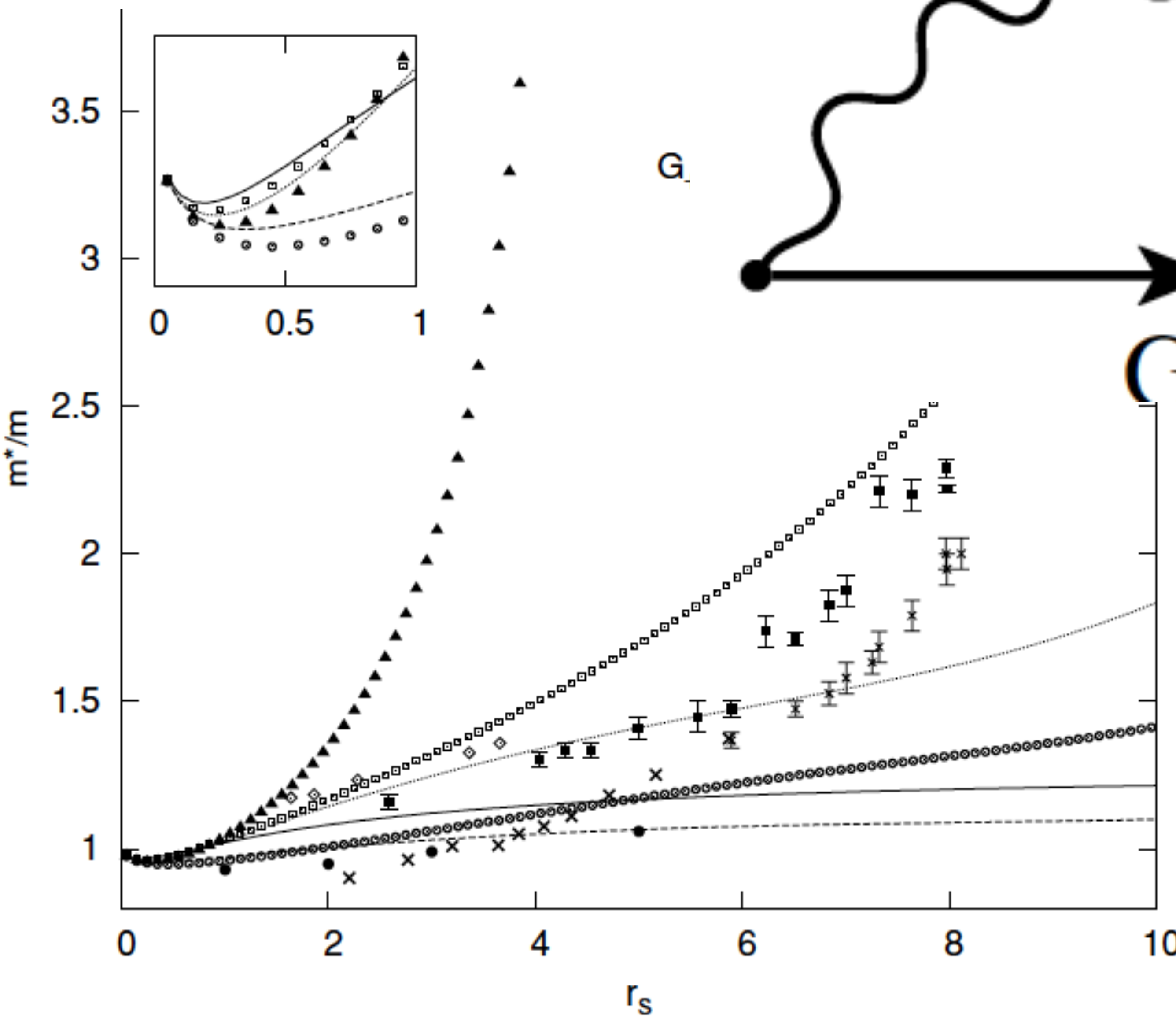
JOHN J. QUINN AND RICHARD A. FERRELL
University of Maryland, College Park, Maryland

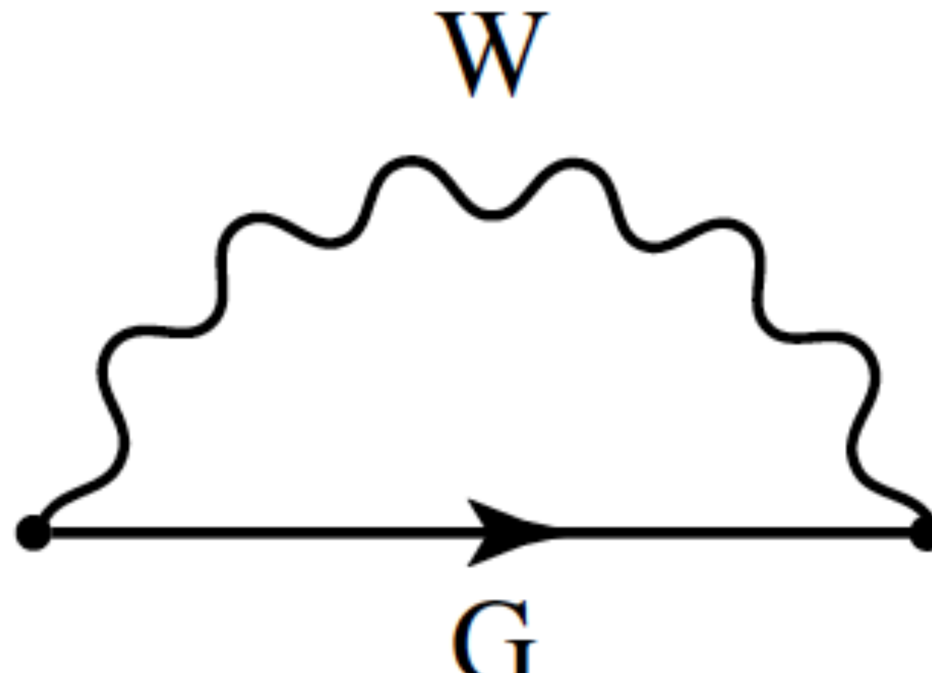
(Received June 9, 1958)

John Quinn

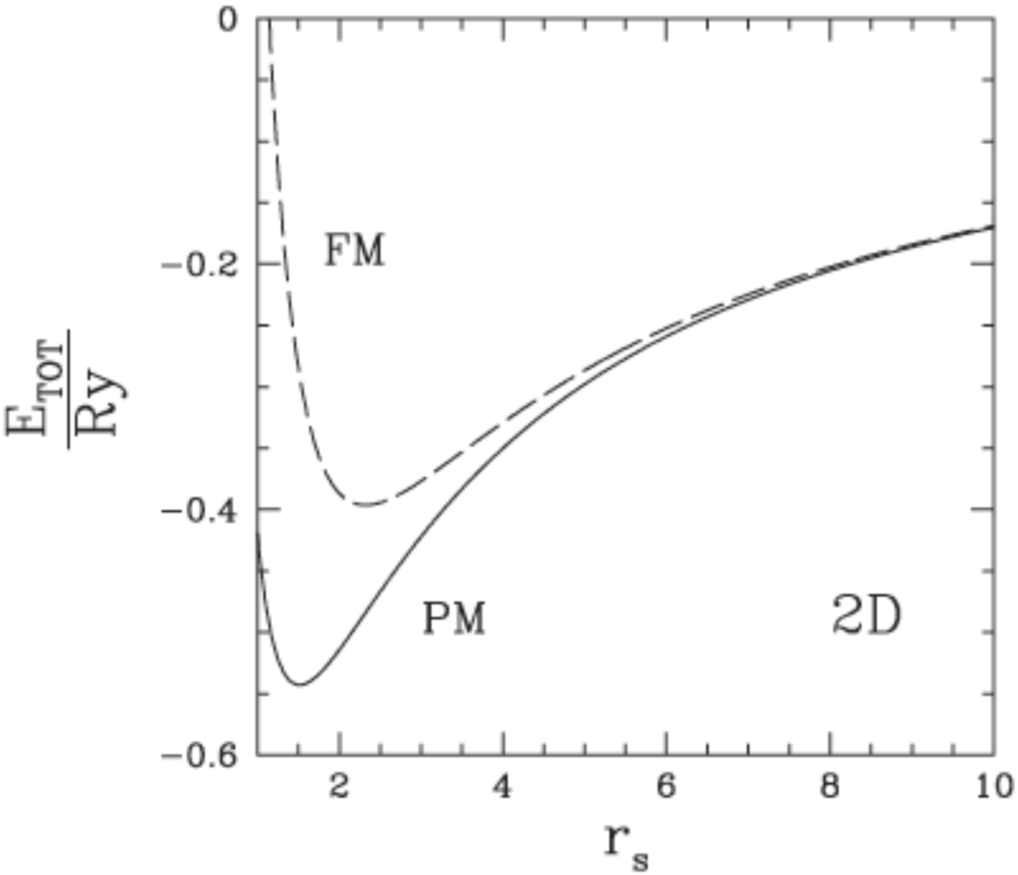
Capri 2014

Effective Mass Enhancement





2DEG Ferromagnetism ?

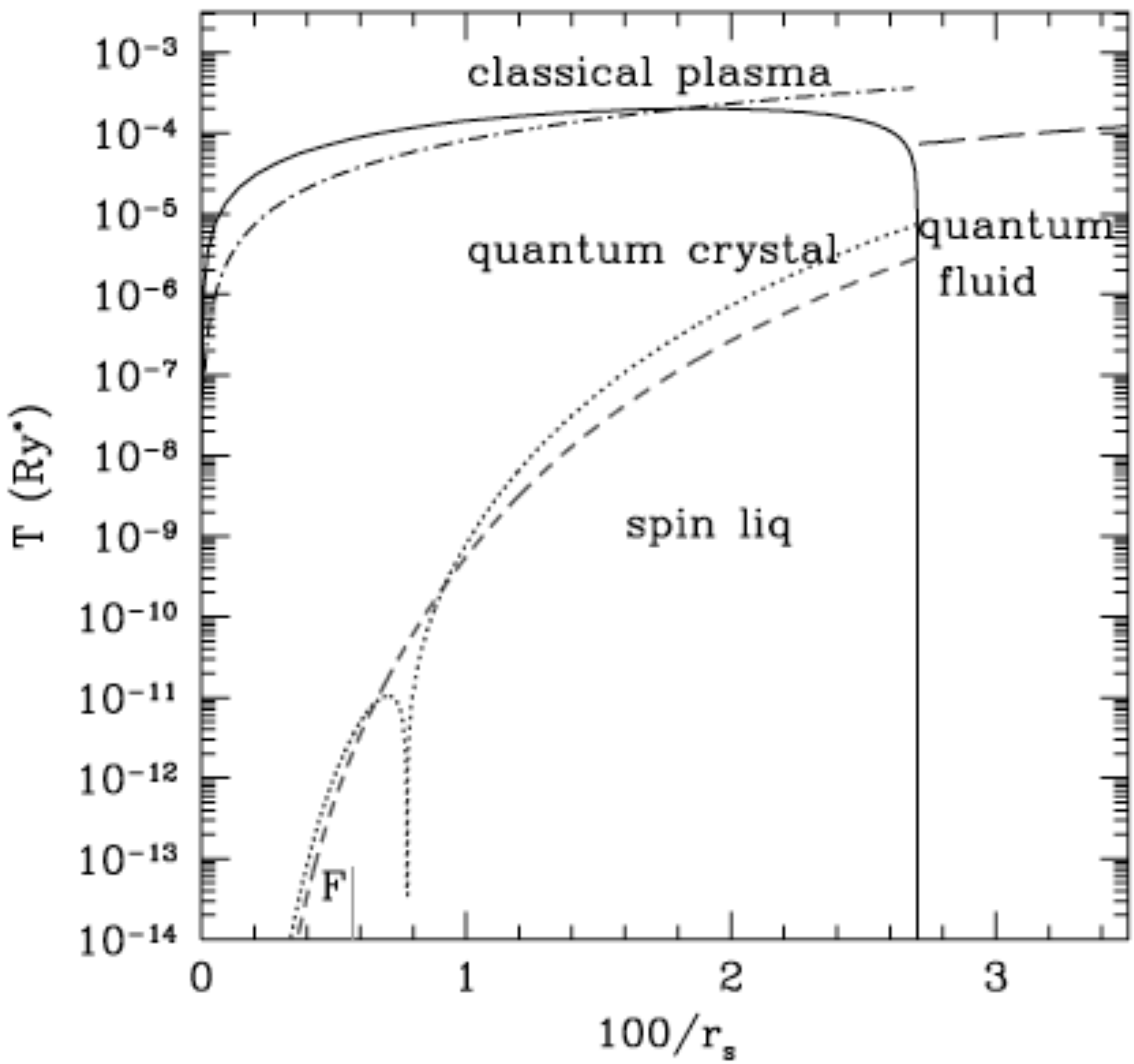


$n \approx 1/(\pi r_s^2 a_0^2)$

$T \approx h^2/m a_0^2 r_s^2$

$U \approx e^2 / r_s$

2DEG phase diagram



Ceperley

Senatore

QMC

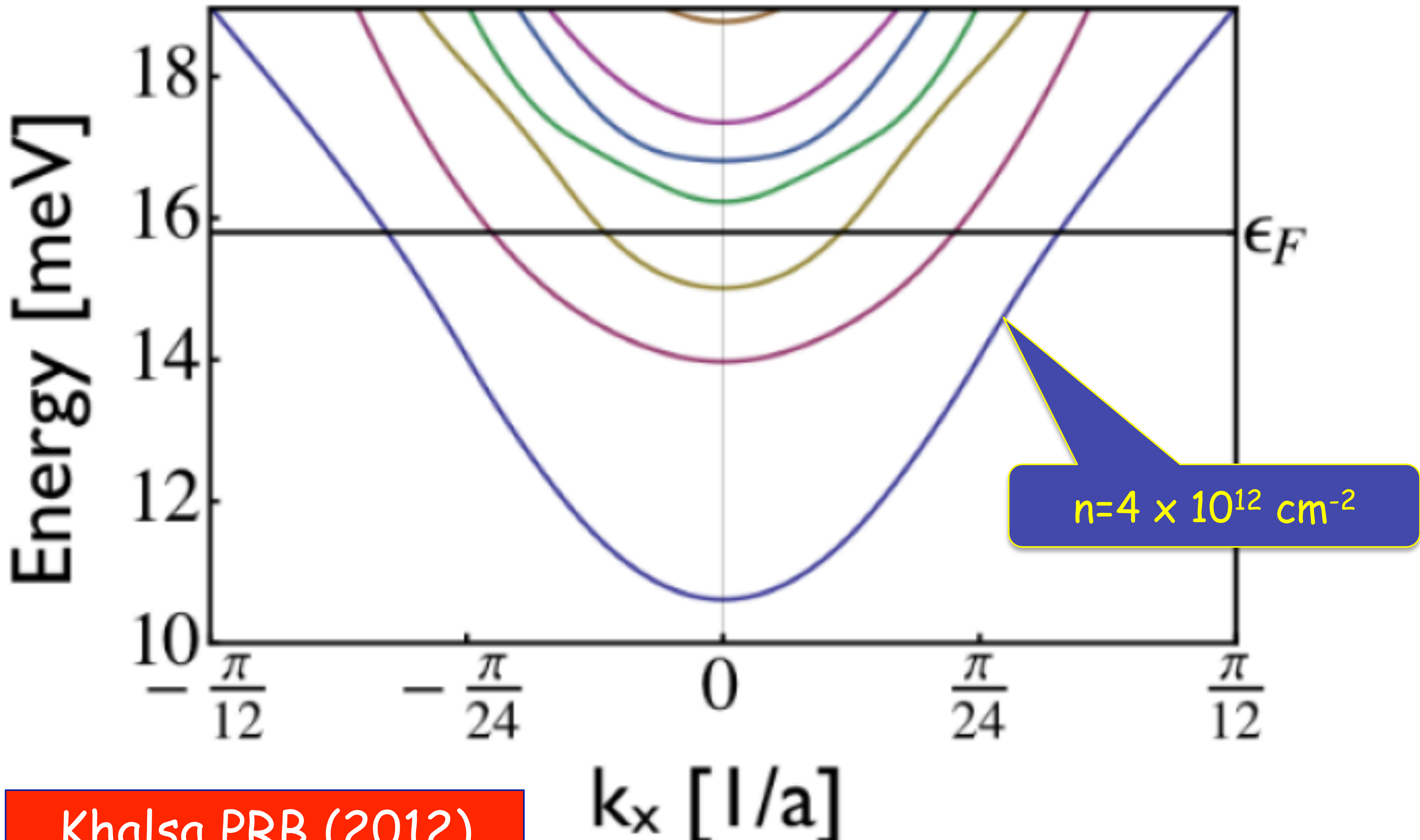
t_{2g} 2DEG Properties

Size Quantization and Dielectric Screening

$$\boxed{\frac{\hbar^2}{mw^2} \sim \frac{eE_0 w}{\epsilon} \sim \frac{4\pi e^2 n_T w}{\epsilon}}$$

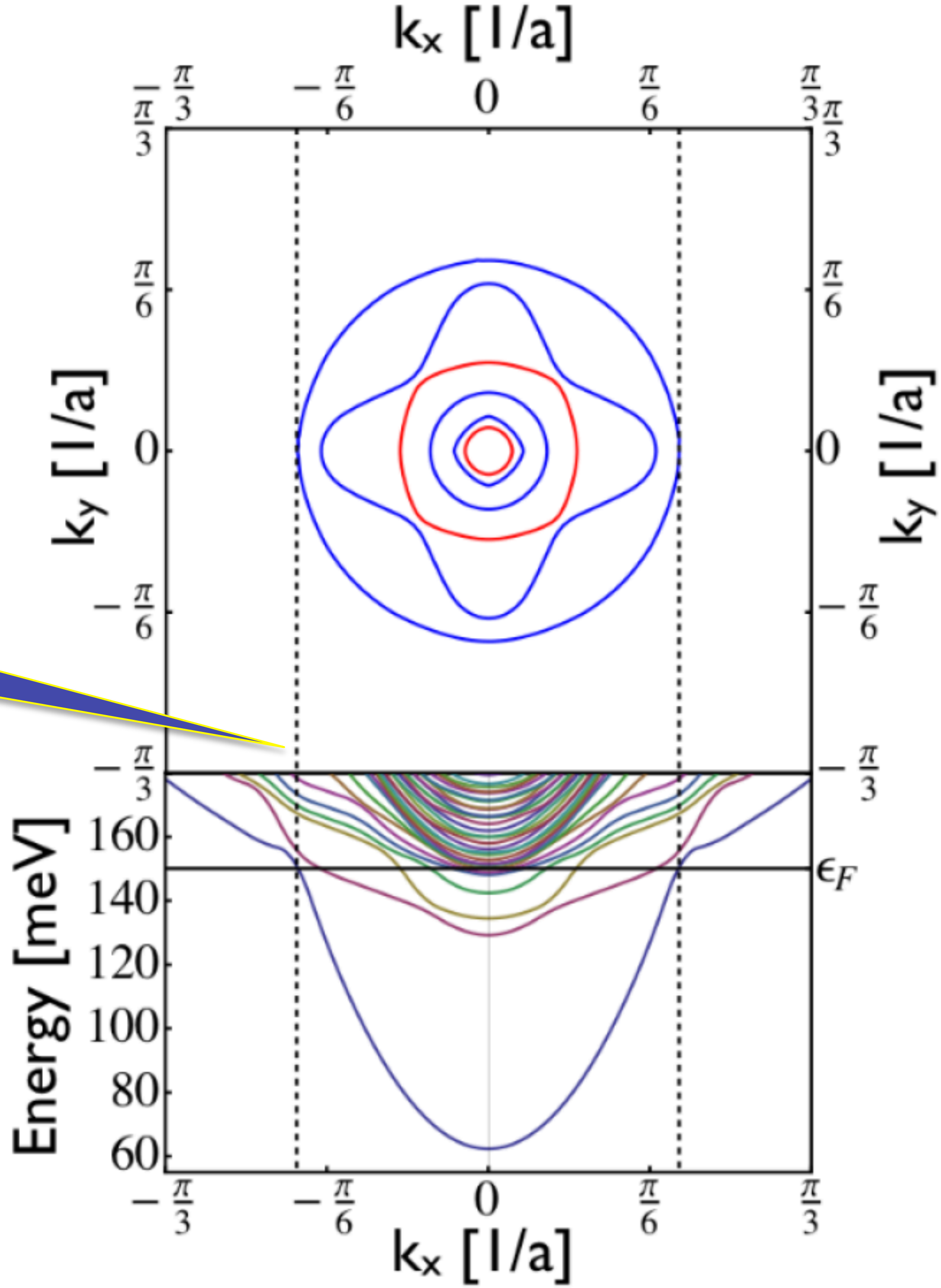
$$\boxed{w \sim \left(\frac{\hbar^2 \epsilon}{m 4\pi e^2 n_T}\right)^{1/3}}$$

Low-Carrier Densities



Khalsa PRB (2012)

Higher Carrier Densities



n=7 x 10^{13} cm^{-2}

Stengel PRL (2011)
Khalsa PRB (2012)

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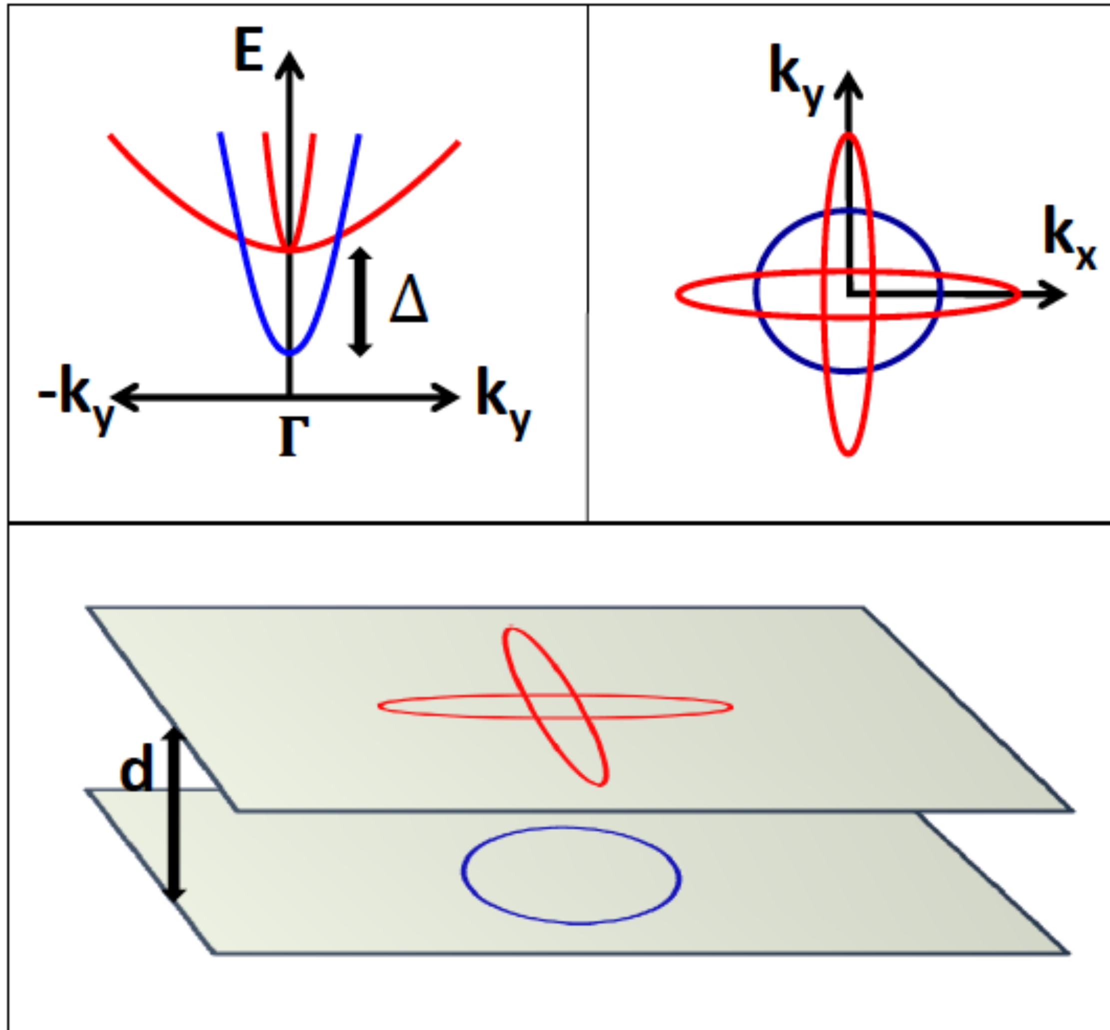
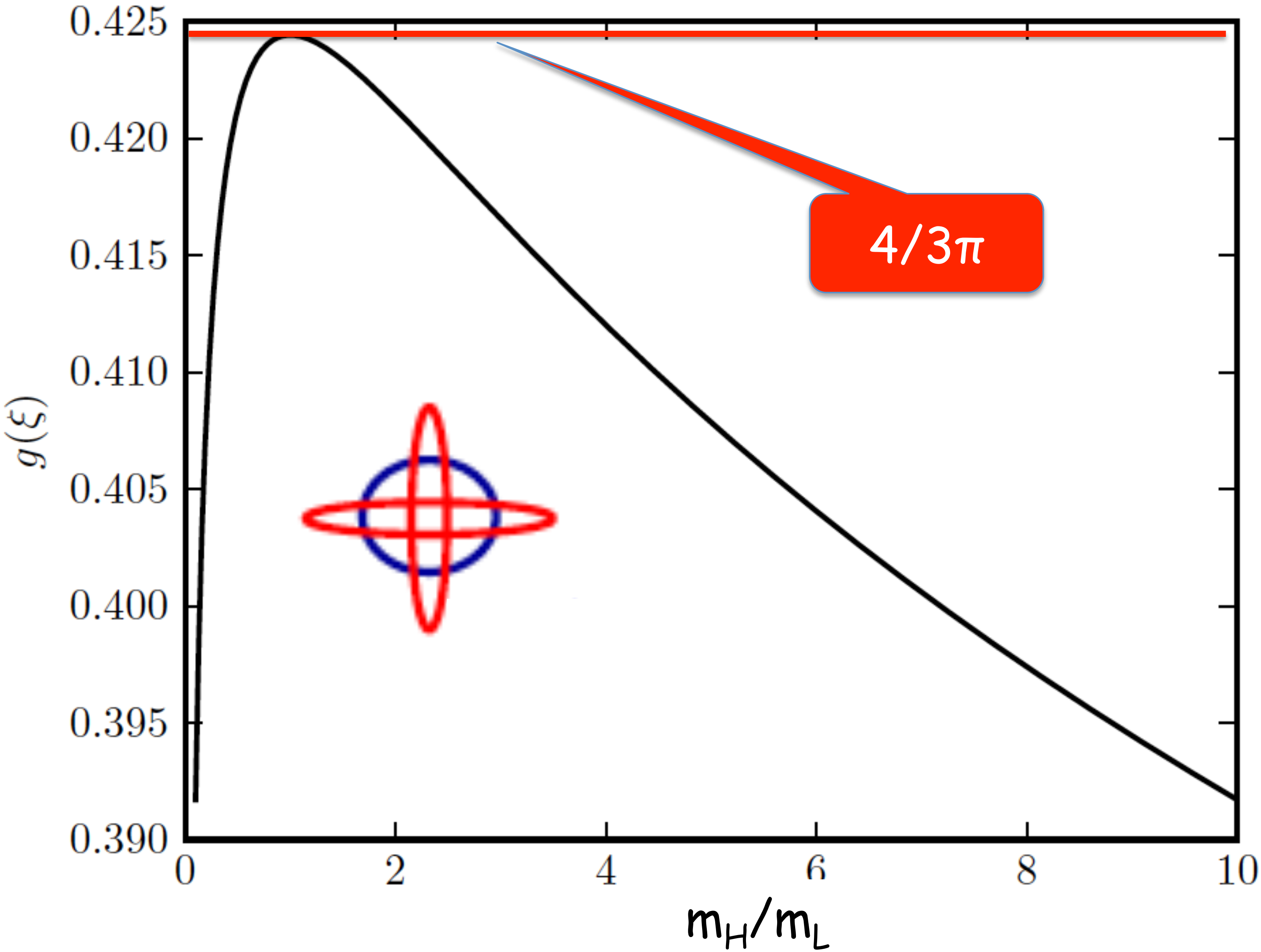


Exchange Energy of Elliptical Band

$$
\begin{aligned}
\varepsilon_{\mathrm{E},1,\mathrm{x}}(n_{\mathrm{E},1}) &= \frac{1}{2}\int \frac{d^2q}{(2\pi)^2}\frac{2\pi e^2}{\kappa q}\left[S_{\mathrm{HF}}\left(\frac{q}{2\sqrt{2\pi n_{\mathrm{E},1}}}\mathcal{F}_\xi(\theta)\right)-1\right] \\
&= -\frac{e^2}{\kappa}\sqrt{2\pi n_{\mathrm{E},1}}\int_0^{2\pi}\frac{d\theta}{2\pi}\int_0^{1/\mathcal{F}_\xi(\theta)} dx\,\left\{1-\frac{2}{\pi}\left[\arcsin(x\mathcal{F}_\xi(\theta))+x\mathcal{F}_\xi(\theta)\sqrt{1-x^2\mathcal{F}_\xi^2(\theta)}\right]\right\} \\
&\equiv -\frac{e^2}{\kappa}\sqrt{2\pi n_{\mathrm{E},1}}\; g(\xi)\ .
\end{aligned}
$$

Exchange Energy



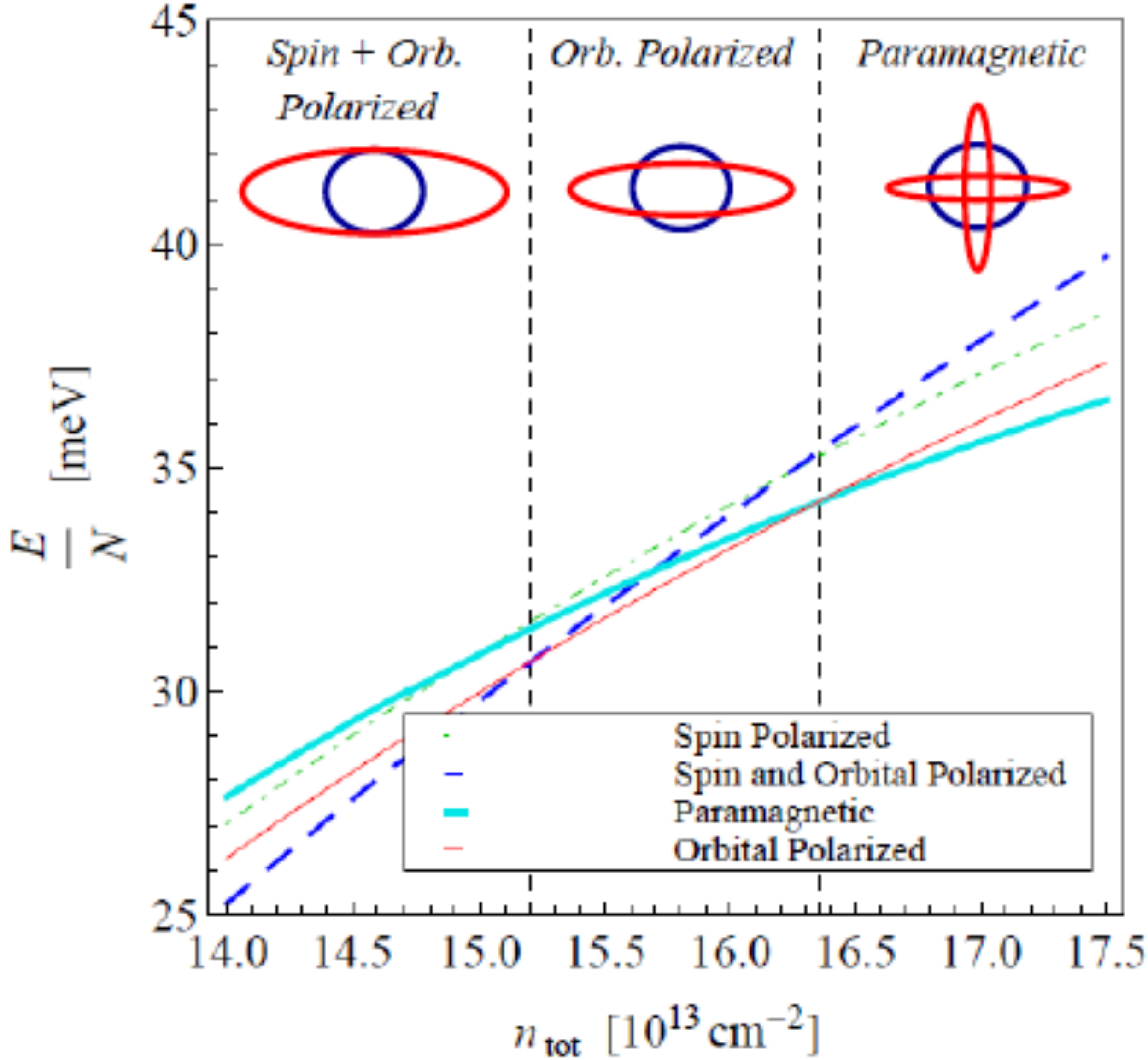
Bloch-Stoner Instability

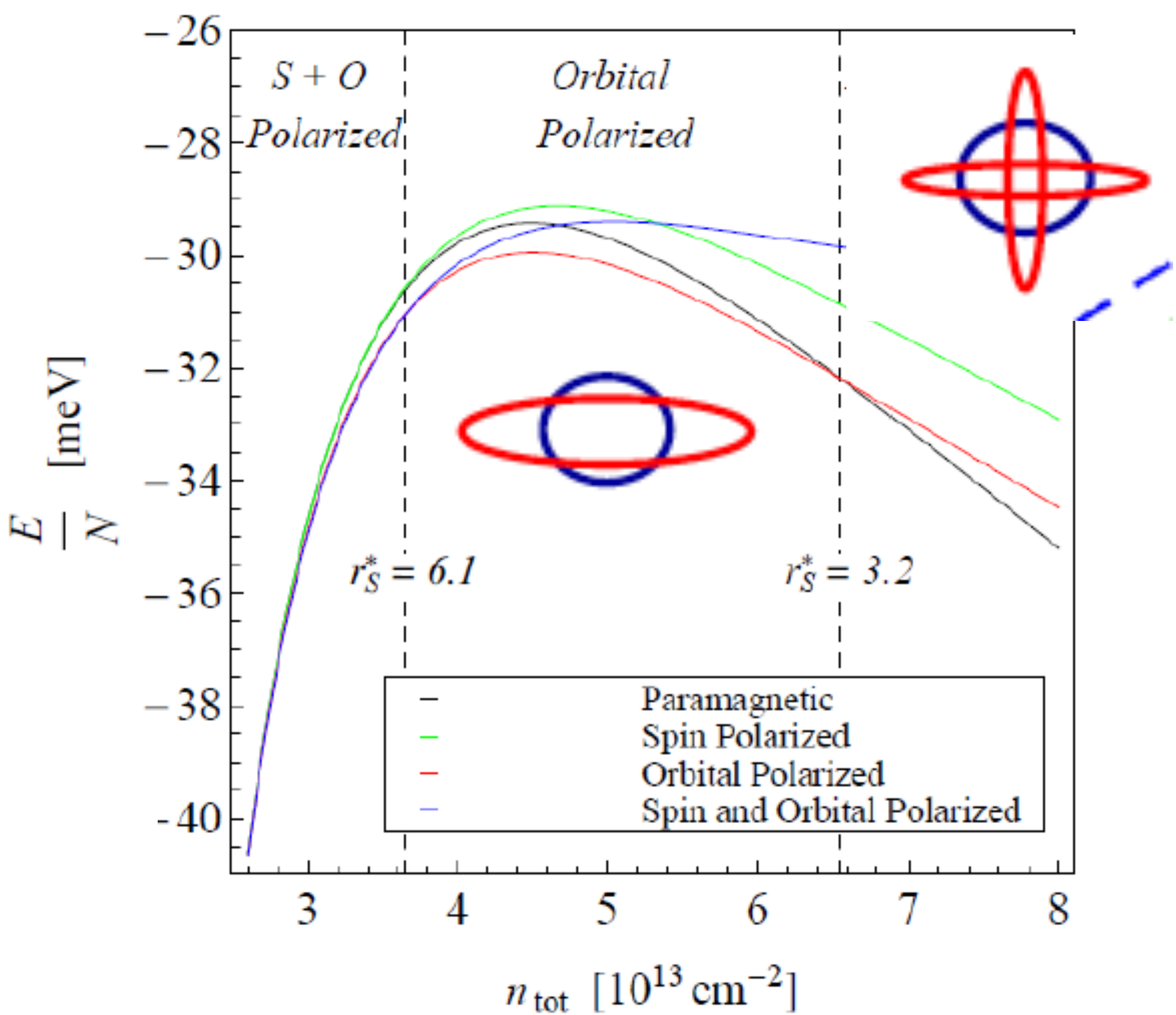
$$\boxed{\mathcal{E}_0(n_{\rm E}, p_{\rm E}, n_{\rm C}) = \pi \frac{\hbar^2 n_{\rm E}^2}{4 m_{\rm DOS}} \frac{(1+p_{\rm E})^2 + (1-p_{\rm E})^2}{2} + \pi \frac{\hbar^2 n_{\rm C}^2}{2 m_{\rm C}}}$$

$$\boxed{\mathcal{E}_{\rm x}(n_{\rm E}, p_{\rm E}, n_{\rm C}) = -g(\xi) \frac{e^2}{\kappa} n_{\rm E} \sqrt{\pi n_{\rm E}} \frac{(1+p_{\rm E})^{3/2} + (1-p_{\rm E})^{3/2}}{2} - \frac{4}{3\pi} \frac{e^2}{\kappa} n_{\rm C} \sqrt{2\pi n_{\rm C}}}$$

$$\boxed{n_{\rm E}^\star \equiv \frac{1}{a_{\rm DOS}^2} \frac{16}{\pi} g^2(\xi)(3 - 2\sqrt{2})}$$

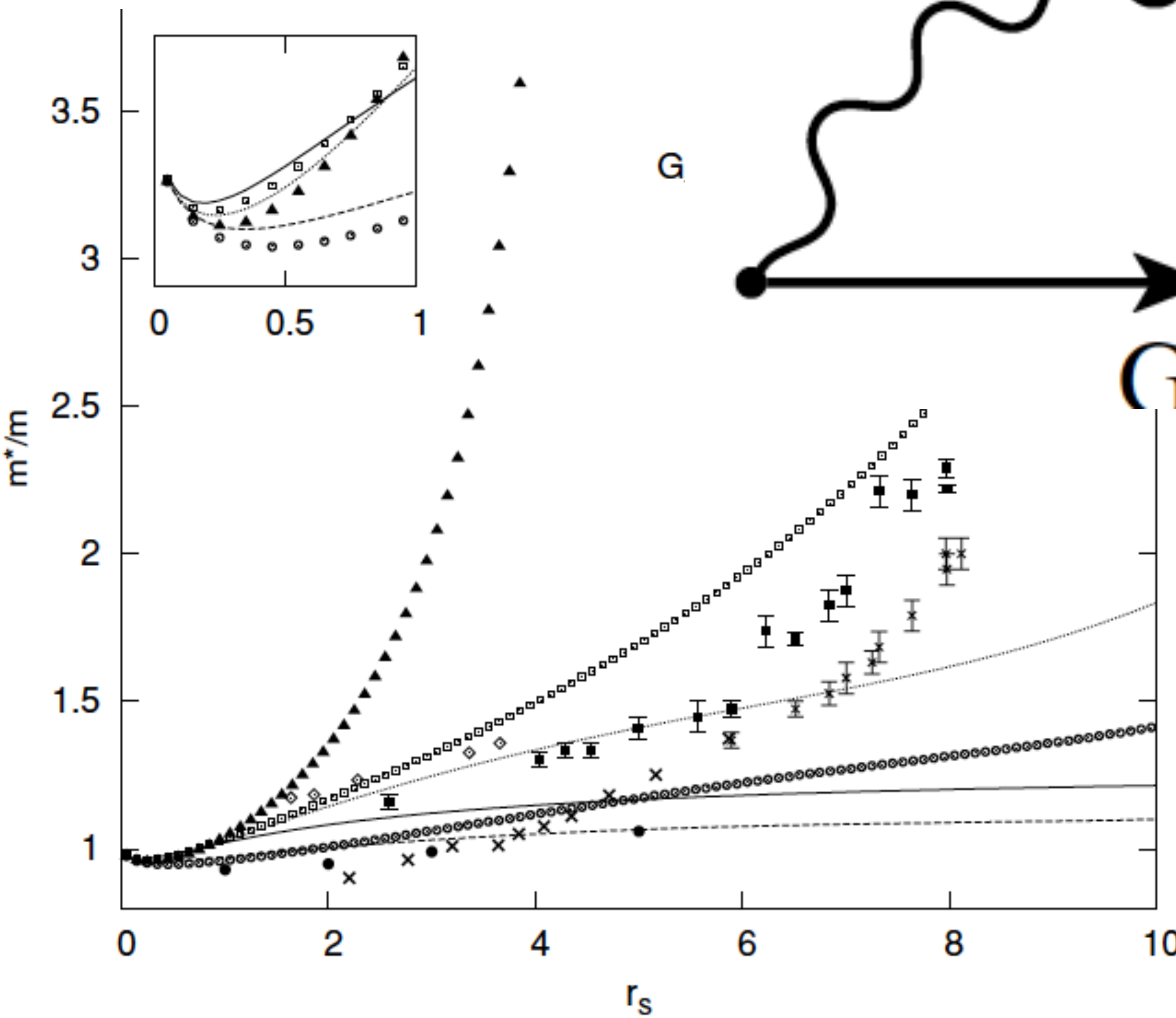
Spin & Orbital Polarization

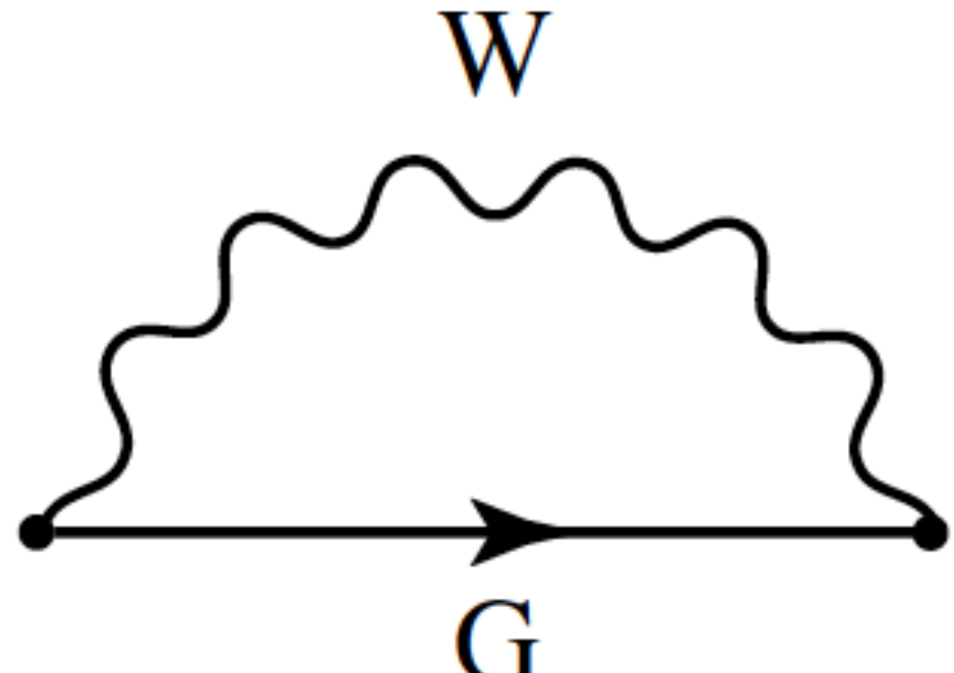


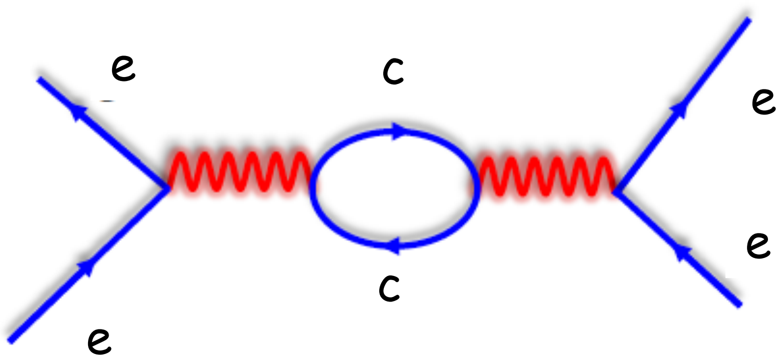


S + O Polarized
Orbital Polarized
$r_S^* = 6.1$
$r_S^* = 3.2$
$\frac{E}{N}$ [meV]
n_{tot} [$10^{13}\,\mathrm{cm}^{-2}$]
−26
−28
−30
−32
−34
−36
−38
-40
3
4
5
6
7
8
Paramagnetic
Spin Polarized
Orbital Polarized
Spin and Orbital Polarized

Effective Mass Enhancement







Wigner Xtal of Heavy Electrons ?

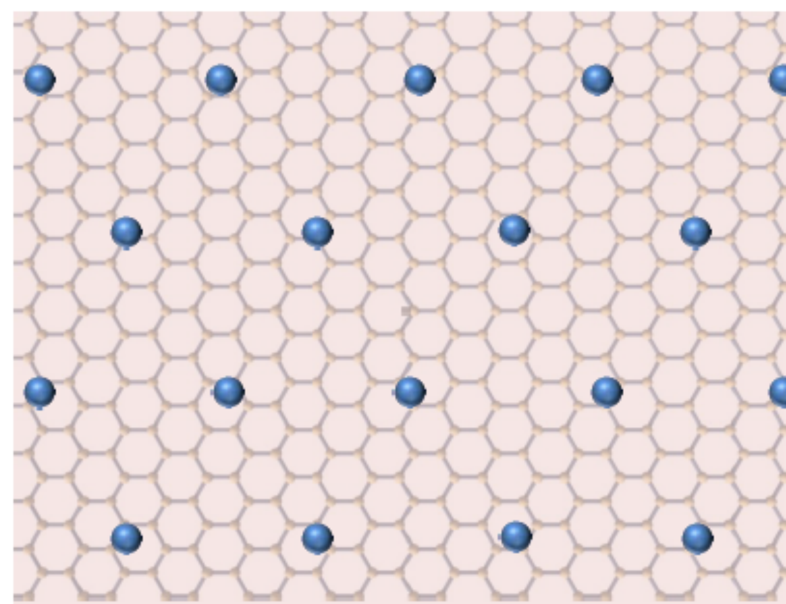
2D Wigner crystal Energy

$$\frac{E}{N} = \left(\frac{-2.212}{r_S} + \frac{1.59}{(r_S)^{\frac{3}{2}}}\right)$$

Electrostatic energy

Zero point energy

2D Wigner crystal



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