Anomalous spin susceptibility and suppressed exchange energy of 2D holes

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Outline

• Introduction
  – basics of semiconductor band structure
  – valence-band states in the bulk: Heavy holes & light holes

• Quantum confinement and valence-band structure
  – strong coupling of spin and orbital degrees of freedom
  – valence-band splitting & valence-band mixing

• Physical ramifications of valence-band mixing
  – 2D holes are not like 2D conduction-band electrons!
  – density response, carrier-density controlled anisotropic spin susceptibility, suppression of exchange energy, ...

• Conclusions
Introduction: Semiconductor band structure & bulk-hole states
Band structure of common semiconductors

• quasi-free electrons in solids: energy bands
  – conduction band: orbital character of $l = 0$ (atomic s) state
  – valence band: has properties of $l = 1$ (atomic p) state

• spin-orbit coupling has the analogous effect as in atoms:
  – $l = 0$ & $s = \frac{1}{2}$ $\rightarrow$ $j = 1/2$
  – $l = 1$ & $s = \frac{1}{2}$ $\rightarrow$ $j = 3/2$, 1/2
    energy (fine-structure) splitting $\Delta$ between valence-band edges

• upper-most valence band: energy-split at finite $k$!

Valence-band states: Heavy & light holes

- effective-mass Hamiltonian for j = 3/2 valence band:
  \[
  \mathcal{H} = -\frac{\hbar^2}{2m_0} \left\{ \gamma_1 k^2 - \frac{2\gamma_s}{3} \left[ 3 \left( \mathbf{k} \cdot \mathbf{J} \right)^2 - k^2 \mathbf{J}^2 \right] \right\}
  \]

- choose spin-3/2 quantisation axis \( \parallel \mathbf{k} \), find energies
  \[
  E_{m_j}(\mathbf{k}) = -\frac{\hbar^2 k^2}{2m_0} \left( \gamma_1 - 2\gamma_s \left[ m_j^2 - \frac{5}{4} \right] \right)
  \]

- two branches:
  - heavy holes (HHs) having \( m_j = \pm 3/2 \)
  - light holes (LHs) having \( m_j = \pm 1/2 \)

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Interdependence of orbital motion and spin

- finite $\mathbf{k}$: fixed spin-$3/2$ projection $\parallel \mathbf{k}$ and splitting of $m_j = \pm 3/2$ & $m_j = \pm 1/2$ states: HH-LH splitting
- competition with magnetic field $\mathbf{B} \perp \mathbf{k}$
  - eg, $\mathbf{B} = B\mathbf{x}$: $B\hat{J}_x \equiv B(\hat{J}_+ + \hat{J}_-)$, hence Zeeman effect couples HH & LH states $\Rightarrow$ HH-LH mixing
  - unlike spin-1/2 case: a HH-LH mixed state is not a reoriented dipole; spin $3/2$ is much richer!
    Winkler, PRB (2004); PRB (2005)
  - unconventional Zeeman effect:
    HH states not split for large $|\mathbf{k}|$

Suzuki & Hensel, PRB (1974); Csontos & UZ, PRB (2007)

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Quantum confinement and valence-band structure
Quasi-2D hole systems in quantum wells

- band bending in semiconductor heterostructures realises textbook example of 2D quantum well
  - form 2D bound states in conduction & valence bands
  - different quantisation energy for HH and LH subbands

- HH-LH splitting of quasi-2D subband edges
  - fixes spin quantisation axis || growth direction
  - causes stiff response of the 2D HH states to in-plane $B$ fields


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2D holes are different from electrons

• HH-LH splitting: lowest 2D hole subband edge is HH-like and doubly degenerate \( m_j = \pm 3/2 \)
  – tempting to represent 2D holes states by pseudospin-\( \frac{1}{2} \) degree of freedom, equivalent to cond.-band electrons

• but states in lowest 2D hole band have finite \( m_j = \pm \frac{1}{2} \) amplitudes for finite \( k_\parallel \): HH-LH mixing!

\[
\Psi^{(2D)}_{el} = \begin{pmatrix} \chi_{\uparrow} \\ \chi_{\downarrow} \end{pmatrix} \iff \Psi^{(2D)}_{hh} = \begin{pmatrix} \chi_{\frac{3}{2}} \\ \chi_{\frac{1}{2}} \\ \chi_{-\frac{1}{2}} \\ \chi_{-\frac{3}{2}} \end{pmatrix}
\]
2D hole states exhibit a kind of `chirality´

- Luttinger Hamiltonian contains terms that couple intrinsic spin to orbital motion: $\hat{J}_+^2 (k_x - ik_y)^2 + \text{H.c.}$
- in axial approx: general state has the form

$$\Psi^{(2D)}_{nk}(r) = e^{i \mathbf{k} \cdot \mathbf{r}} \xi_{nk}(z) \equiv e^{i \mathbf{k} \cdot \mathbf{r}} e^{-i \hat{J}_z \theta_k}$$

- compare with graphene:

$$\mathcal{H} \propto \sigma_+ (k_x - ik_y) + \text{H.c.}$$

$$\Psi^{(g)}_{\sigma, k}(r) = e^{i \mathbf{k} \cdot \mathbf{r}} e^{-i \frac{\sigma z}{2} \theta_k} \begin{pmatrix} 1 \\ \sigma \end{pmatrix}$$
Physical ramifications of valence-band mixing

I. Warm-up: Density response

Density response of the electron gas

• elementary property of conductors: charge carriers screen impurity potentials

\[ \delta n(r) = \int \frac{d^2 q}{(2\pi)^2} e^{i q \cdot r} \chi(q) V_{\text{ext}}(q) \]

• can express general susceptibility \( \chi(q) \) in terms of result \( \chi_0(q) \) for non-interacting system (Lindhard)

\[ \chi(q) = \frac{\chi_0(q)}{1 - v_q[1 - G(q)]\chi_0(q)} \]

Giuliani & Vignale, *Quantum Theory of the Electron Liquid*

• universal \( \chi_0(q) \) for parabolic band dispersion
Lindhard function of 2D hole gases

• 2D electron system: universal 2D result applies
  Giuliani & Vignale, *Quantum Theory of the Electron Liquid*

• lowest 2D hole subband: HH-LH mixing matters!
  – density-dependent 2D-hole Lindhard function!
  – important deviations in the high-density limit

\[ r^*_s = 4, 6, 8, \infty \]
Physical ramifications of valence-band mixing

II. Spin response

Spin susceptibility of 2D hole gases

• ordinary **electron** system: spin response tied to the density response (Lindhard): \( \chi_{ij}(q) = \chi_0(q)\delta_{ij} \)
  
  Giuliani & Vignale, *Quantum Theory of the Electron Liquid*

• 2D **holes**: interplay of HH-LH splitting and HH-LH mixing causes **density-dependent** anisotropy!
  
  – low density: **easy axis** \( \parallel z \) (q-well growth) direction
    
    Kernreiter, Governale & UZ, PRL (2013)
  
  – as expected from HH-LH splitting (cf. behaviour of Zeeman splitting/g-factor!)

\[
\chi_{ii}(q) = \chi_{0}(q)\delta_{ii}
\]
Spin susceptibility of 2D hole gases cont’d

- for higher densities: unexpectedly rich behaviour exhibited by 2D holes due to HH-LH mixing
  Kernreiter, Governale & UZ, PRL (2013)
  - easy-plane response dominant at intermediate density
  - easy-axis again at high densities + structure at finite $q$

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Effective $g$ factor for 2D holes

- hole-spin couples to magnetic field: $\mathcal{H}_Z = 2\kappa \mu_B \mathbf{B} \cdot \hat{\mathbf{J}}$
- paramagnetic response: $\chi_{P,j} = (2\kappa \mu_B)^2 \chi_{jj}(\mathbf{q} = 0)$
- Pauli susceptibility: $\chi_{P,j} = \left( \frac{g_j \mu_B}{2} \right)^2 \chi_0(\mathbf{q} = 0)$
  
  - $\propto$ Lindhard function/DOS
  - used by experimentalists to extract a 2D-hole $g$ factor
    
    Chiu et al., PRB (2011)

- this motivates definition
  
  Kernreiter, Governale & UZ, PRL (2013)

$$g_j = 4\kappa \sqrt{\frac{\chi_{jj}(\mathbf{q} = 0)}{\chi_0(\mathbf{q} = 0)}}$$
Carrier-mediated magnetic (RKKY) interaction

- charge carriers in conductors can mediate exchange interaction of localised magnetic impurities (spins)
- coupling depends on carriers’ spin susceptibility $\chi_{ij}$

$$H_{\text{RKKY}}^{(\alpha\beta)} = -G^2 \sum_{i,j} S_i^{(\alpha)} S_j^{(\beta)} \chi_{ij}(\mathbf{R}_\alpha, \mathbf{R}_\beta)$$

- electron gas: $\chi_{ij}$ is isotropic in spin space; Heisenberg magnet
- 2D hole gas, only HH-LH splitting taken into account: $\chi_{zz} \gg \chi_{xx,yy} \approx 0$; Ising magnet

Haury et al., PRL (1997); Wurstbauer et al., Nat. Phys. (2010)
RKKY interaction/magnetism for 2D holes

- perform **mean-field analysis** of RKKY exchange-coupling Hamiltonian ⇒ Curie temperature $T_C$

$$T_C^{(\perp,\parallel)} = \frac{S(S + 1)}{3} \frac{G^2 n_{\text{imp}}}{k_B} \frac{d}{|\chi_{zz,xx}(q = 0)|}$$

- HH-LH mixing: important even for lowest subband
  - easy-axis/easy-plane transitions (+helical magnetism?)

Kernreiter, Governale & UZ, PRL (2013)

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Physical ramifications of valence-band mixing

III. Exchange energy

Taking account of Coulomb interactions

- perturbatively for electron gas: change of ground-state energy
  
  \[ E_{gs} \approx \langle FS | \mathcal{H}_0 + \mathcal{H}_{\text{int}} | FS \rangle = E_0 + E_H + E_X \]
  
  – consider exchange-energy contribution \( E_X \)

- general expression for 2D system:
  
  \[ \frac{E_X}{N} = -\frac{1}{2\rho} \sum_{n,n'} \int \frac{d^2 k}{(2\pi)^2} \int \frac{d^2 k'}{(2\pi)^2} V_{kk'}^{(nn')} n_F(E_{n'k'}) n_F(E_{nk}) \]
  
  – matrix element of two-particle interaction potential affected by quantum-well state:
  
  \[ V_{kk'}^{(nn')} = \frac{e^2 / 2\epsilon\epsilon_0}{|k - k'|} \sum_{\nu,\nu'} F_{kk',\nu\nu'}^{(nn')} \]
Previously known results & a puzzle

• for strictly 2D electron system:  
  \[ \frac{E_{X}^{(0)}}{N} = -\frac{e^2}{\epsilon \epsilon_0} \frac{k_F}{3\pi^2} \]
  Chaplik, JETP (1971); Stern, PRL (1973)

• quasi-2D system with parabolic subbands: finite width \( d \) results in reduction of exchange effects  
  Betbeder-Matibet et al., PRL (1994)
  \[ \frac{E_{X}^{(EMA)}}{N} = \frac{E_{X}^{(0)}}{N} \Lambda^{(EMA)}(k_Fd) \]

• curious experimental observation: seemingly no exchange effects in 2D hole systems  
  Winkler et al., PRB (2005)
Exchange in `spin-orbit-coupled´ systems

• idea: `chirality´/spinor structure of electronic states affects Coulomb matrix element/form factor
  – spin-rotationally invariant case: can use global quantization axis for spin; exchange matrix element only finite between states with same spin projection
  – in systems with spin-momentum locking (2D system with Rashba spin splitting): no global quantization axis exists; average spin overlap of eigenstates reduced ⇒ exchange reduced (?)

\[
V_{kk'}^{(nn')} = \frac{e^2}{2\varepsilon\varepsilon_0} \sum_{\nu,\nu'} F_{kk',\nu\nu'}^{(nn')}
\]
Exchange reduction in model 2D hole system

- Rashba spin splitting has almost no effect on 2D-electron exchange energy
  (Chesi & Giuliani, PRB (2007, 2011))
- in contrast: HH-LH mixing in 2D hole systems results in significant reduction
  – exchange suppression correlated w/ spinor mixture
  (Kernreiter et al. PRB (2013))
Conclusions

• quantum confinement of holes introduces HH-LH splitting and HH-LH mixing
  – HH-LH mixing renders properties of confined holes to be much different from conduction electrons

• differences relevant even in single-2D-subband limit and in the absence of magnetic fields
  – carrier-density-controlled anisotropy of spin response
  – significant suppression of exchange energy

• presented work has resulted from collaboration with M. Governale, T. Kernreiter, R. Winkler