Quantum capacitance and spin susceptibility of HgTe quantum wells

Ulrich Zuelicke

School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand

in collaboration with:
T Kernreiter & M Governale *Victoria University of Wellington*
E M Hankiewicz *Universität Würzburg, Germany*

Phys. Rev. X **6**, 021010 (2016); Phys. Rev. B **93**, 241304(R) (2016)

TE WHARE WĀNANGA O TE ŪPOKO O TE IKA A MĀUI
VICTORIA
UNIVERSITY OF WELLINGTON

DODD-WALLS CENTRE
for Photonic and Quantum Technologies

The MacDiarmid Institute
for Advanced Materials and Nanotechnology

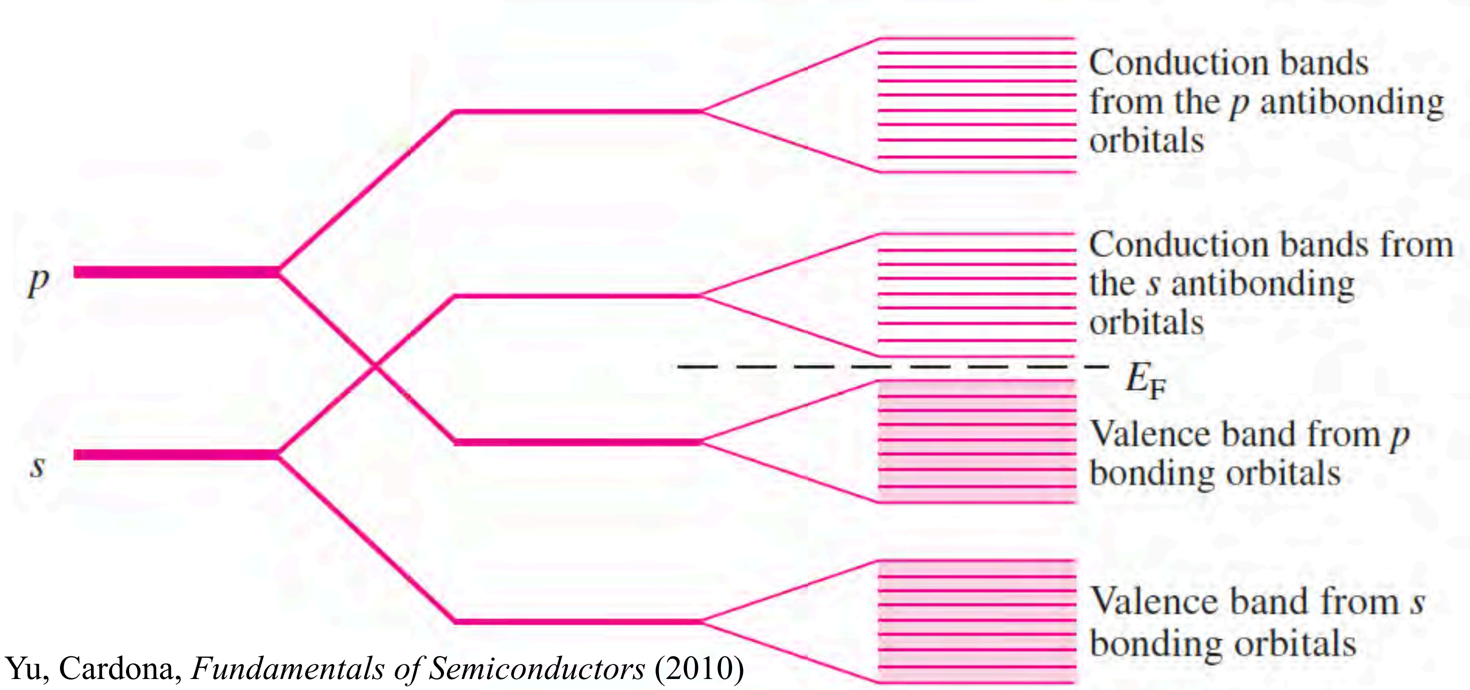
Outline

- Introduction & Motivation
  - – topological insulators: more than just the edge states!
  - – our model system: HgTe/CdTe quantum well
- Theoretical method
  - – band structure from BHZ model Hamiltonian
  - – calculate thermodynamic DOS, spin susceptibility, …
- Results
  - – importance of virtual inter-band processes
  - – distinct physical properties of topological regime
- Conclusions

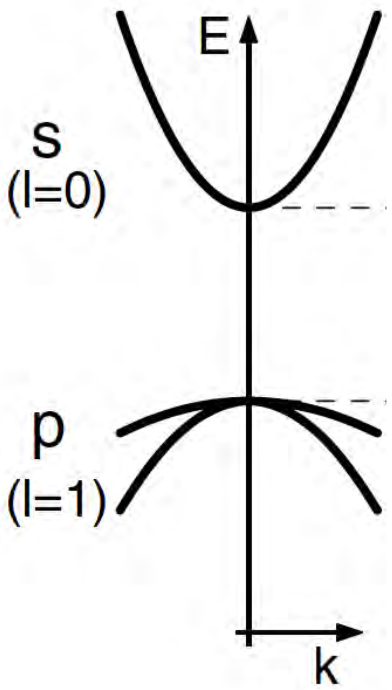
Introduction & Motivation

Electronic structure of crystalline solids

- atomic levels broaden into bands in solid material
  - – character of bands reflects that of atomic orbitals
- (anti-)bonding levels → (conduction) valence bands



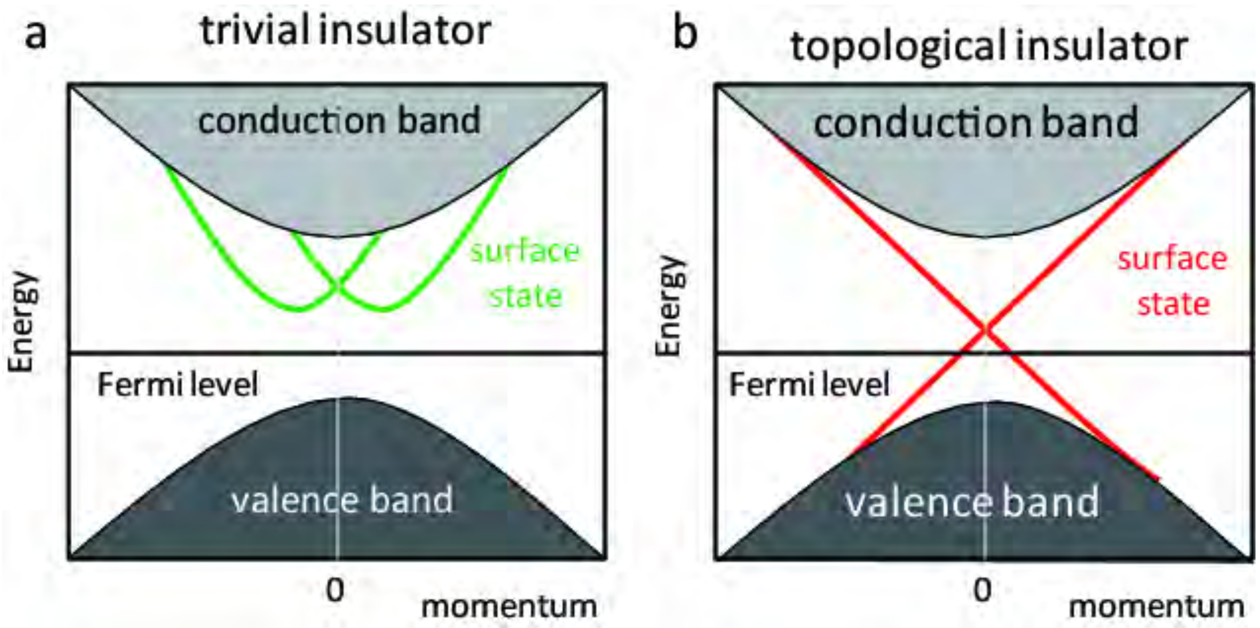
Yu, Cardona, *Fundamentals of Semiconductors* (2010)



Winkler et al. SST (2008)

Ordinary vs. topological insulator (TI)

- certain materials exist where order of bonding and anti-bonding bands is reversed: inverted bands
  - closing of gap required to go from normal type into the inverted situation: topologically distinct systems!
- gapless states emerge at the surface of a topological material (due to symmetry!)

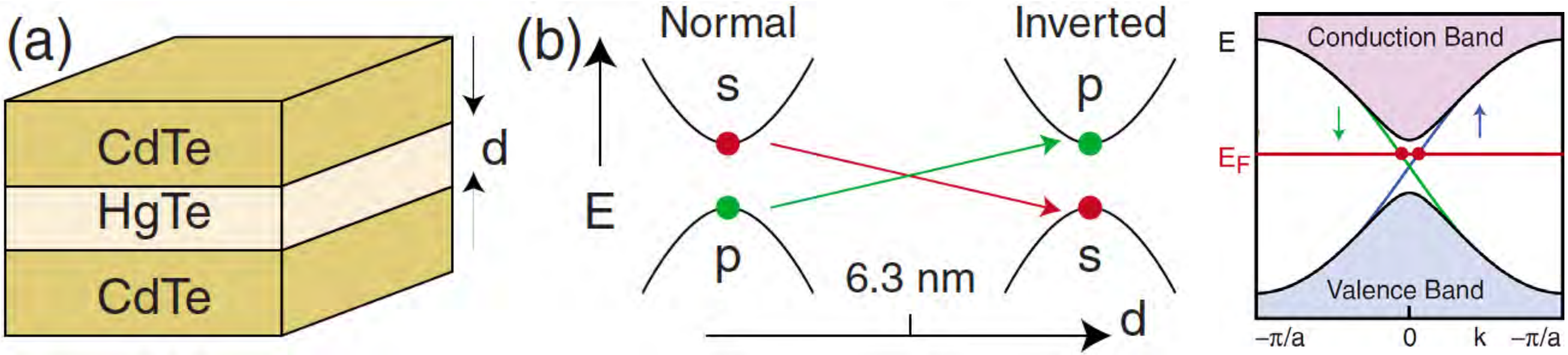


www.scholarpedia.org/article/Topological_insulators

2D TI “fruitfly system”: HgTe quantum well

- adjust quantum-well width to tune between the normal & inverted regimes (bulk HgTe inverted!)
- helical edge states in topological regime (Kramers degeneracy!) give rise to quantum spin Hall effect

Kane & Mele, PRL (2005)
Bernevig, Hughes & Zhang, Science (2006)
König et al., Science (2007); Roth et al., Science (2009), Brüne et al., Nat Phys (2012)

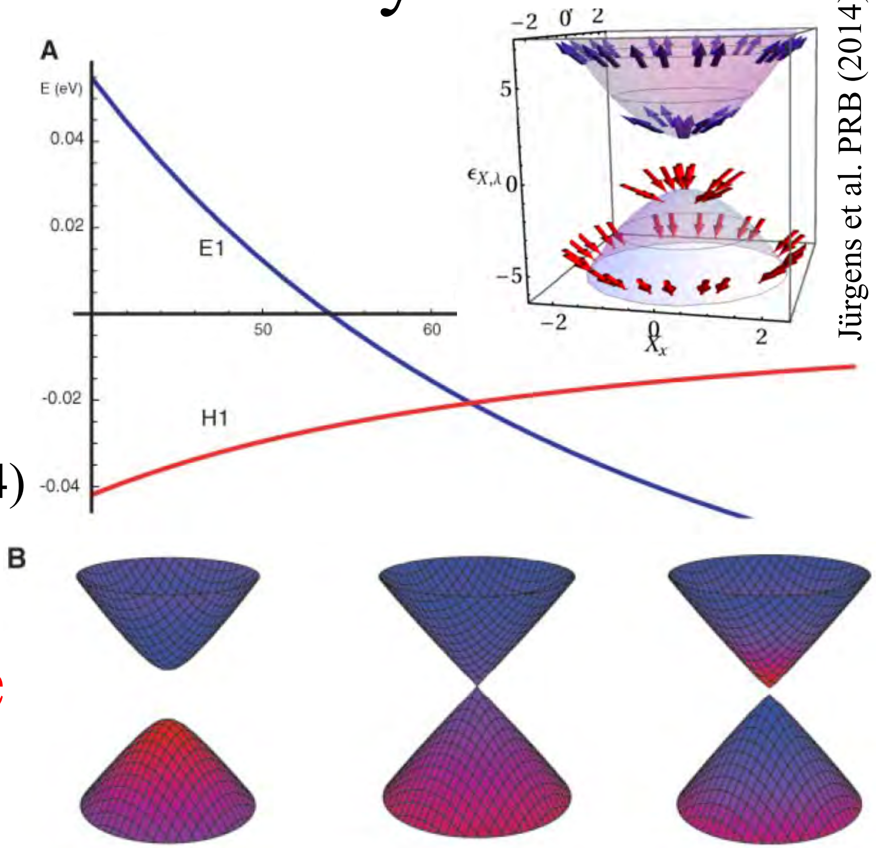


Hasan & Kane, RMP (2010)

Explore Schrödinger-Dirac-TI continuum

- HgTe/CdTe system facilitates controlled access to transitions between these three model systems!
- single-particle eigenstates have a pseudo-spin texture
  - band mixing leads to unusual charge-response properties

    Jürgens, Michetti & Trauzettel, PRB (2014)
- Topological order affecting collective-electron response properties?? Measurable!!



Jürgens et al. PRB (2014)

Bernevig, Hughes & Zhang, Science (2006)

Theoretical approach to studying the collective properties of 2D electrons in the HgTe/CdTe quantum-well system

TE WHARE WĀNANGA O TE ŪPOKO O TE IKA A MĀUI
VICTORIA
UNIVERSITY OF WELLINGTON

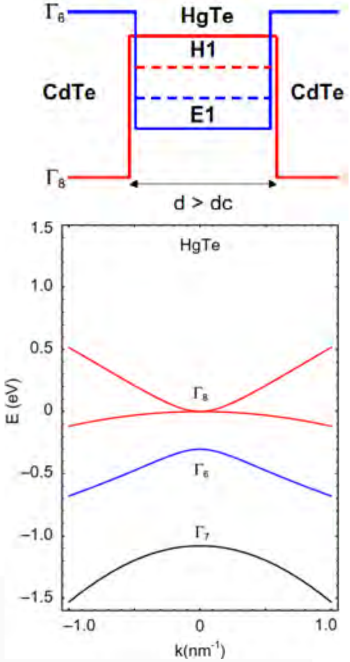
DODD-WALLS CENTRE
for Photonic and Quantum Technologies

The MacDiarmid Institute
for Advanced Materials and Nanotechnology

Effective four-band (BHZ) model

- relevant physics involves states near the band gap
  - Γ_6 (j=1/2): conduction band in normal regime
  - Γ_8 (j=3/2): heavy (m_j=±3/2) and light (m_j=±1/2) holes
  - hybridised Γ_6 & light-hole Γ_8 states form En subbands
- effective 4-band description for 2D E1/H1bands:

$$\mathcal{H}(k_x,k_y)=\begin{pmatrix} M-Bk^2 & Ak_- & 0 & 0 \\ Ak_+ & -M+Bk^2 & 0 & 0 \\ 0 & 0 & M-Bk^2 & -Ak_+ \\ 0 & 0 & -Ak_- & -M+Bk^2 \end{pmatrix}$$



Bernevig, Hughes & Zhang, Science (2006)

- relevant real spin given in terms of $\Gamma_6 \otimes \Gamma_8$ basis representation: $\hat{S}_i(\gamma)=\dfrac{\hat{\sigma}_i}{2}\otimes(\gamma\hat{J}_i)$
  - γ: Γ_8/Γ_6 couplg. ratio

Many-particle properties of interest

- thermodynamic density of states: $D_{\mathrm{T}} \equiv \partial n / \partial \mu$
  - renormalised by Coulomb interactions (Fock term)
  - intra- and inter-band contributions + 2D form factor

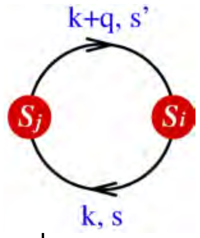
$$\Sigma^{(s)}_{k\pm} = -2\pi C \int \frac{d^2k'}{(2\pi)^2}\, n_{\mathrm{F}}(E^{(s)}_{\mathbf{k}'\pm}) \int dz \int dz'\, \frac{e^{-|\mathbf{k}-\mathbf{k}'||z-z'|}}{|\mathbf{k}-\mathbf{k}'|} \left[\psi^{(s)}_{\mathbf{k}'\pm}(z)^{\dagger} \cdot \psi^{(s)}_{\mathbf{k}+}(z)\right] \left[\psi^{(s)}_{\mathbf{k}+}(z')^{\dagger} \cdot \psi^{(s)}_{\mathbf{k}'\pm}(z')\right]$$

- spin susceptibility:

$$\chi_{ij}(\mathbf{R}, z; \mathbf{R}', z') = \lim_{\eta \to 0^+} \left\{ -\frac{i}{\hbar} \int_0^{\infty} dt\; e^{-\eta t} \langle [S_i(\mathbf{R}, z; t)\,,\, S_j(\mathbf{R}', z'; 0)] \rangle \right\}$$

  - collective spin response of many-electron system

$$\chi_{ij}(\gamma; \mathbf{q}; z, z') = \sum_{\alpha,\beta,s,s'} \int \frac{d^2k}{(2\pi)^2}\, \mathscr{W}^{(s,s')}_{ij(\mathbf{k},\mathbf{k}+\mathbf{q},\alpha,\beta)}(\gamma; z, z')\, \frac{n_{\mathrm{F}}(E^{(s)}_{\mathbf{k}\alpha}) - n_{\mathrm{F}}(E^{(s')}_{\mathbf{k}+\mathbf{q}\beta})}{E^{(s)}_{\mathbf{k}\alpha} - E^{(s')}_{\mathbf{k}+\mathbf{q}\beta} + i\hbar\eta}$$

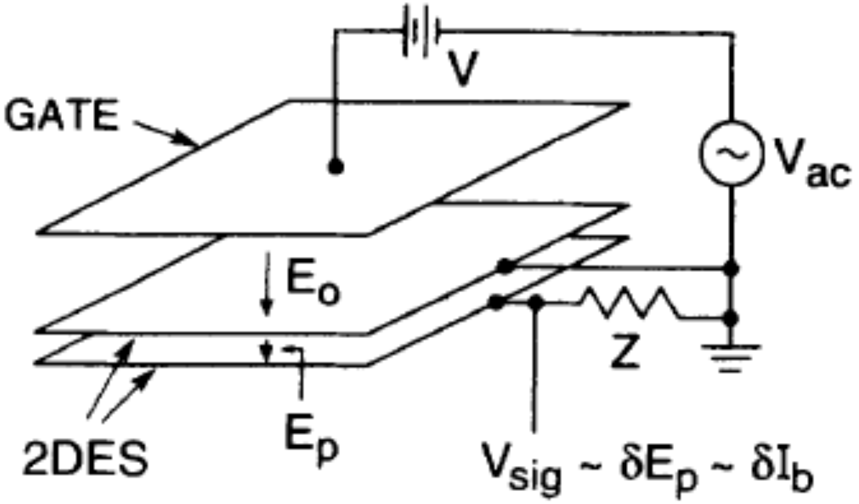


$$\mathscr{W}^{(s,s')}_{ij(\mathbf{k},\mathbf{k}+\mathbf{q},\alpha,\beta)}(\gamma; z, z') = \left[\psi^{(s)}_{\mathbf{k}\alpha}(z)\right]^{\dagger} \cdot \left[\hat{S}_i(\gamma)\, \psi^{(s')}_{\mathbf{k}+\mathbf{q}\beta}(z)\right] \left[\psi^{(s')}_{\mathbf{k}+\mathbf{q}\beta}(z')\right]^{\dagger} \cdot \left[\hat{S}_j(\gamma)\, \psi^{(s)}_{\mathbf{k}\alpha}(z')\right]$$

Relation to physical observables

- thermodynamic DOS: quantum capacitance

$$\frac{A}{C_{\mathrm{tot}}} = \frac{d}{\kappa\epsilon_0} + \frac{1}{e^2 D_{\mathrm{T}}}$$

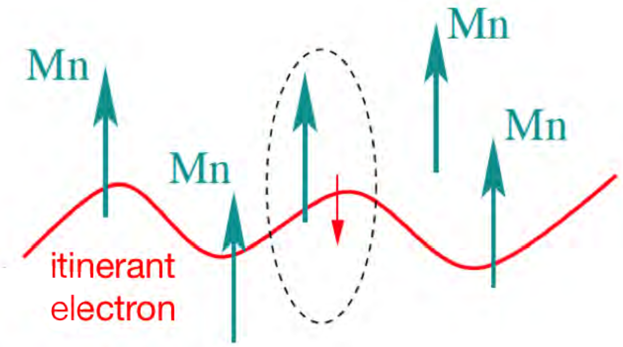


Eisenstein et al. PRL (1992)

- spin susceptibility: carrier-mediated (RKKY) exchange interac. of localised magnetic impurities

$$H_{\mathrm{RKKY}}^{(\alpha\beta)} = -G^2 \sum_{i,j} I_i^{(\alpha)}\, I_j^{(\beta)}\, \chi_{ij}\left(\mathbf{R}_\alpha, \mathbf{R}_\beta\right)$$

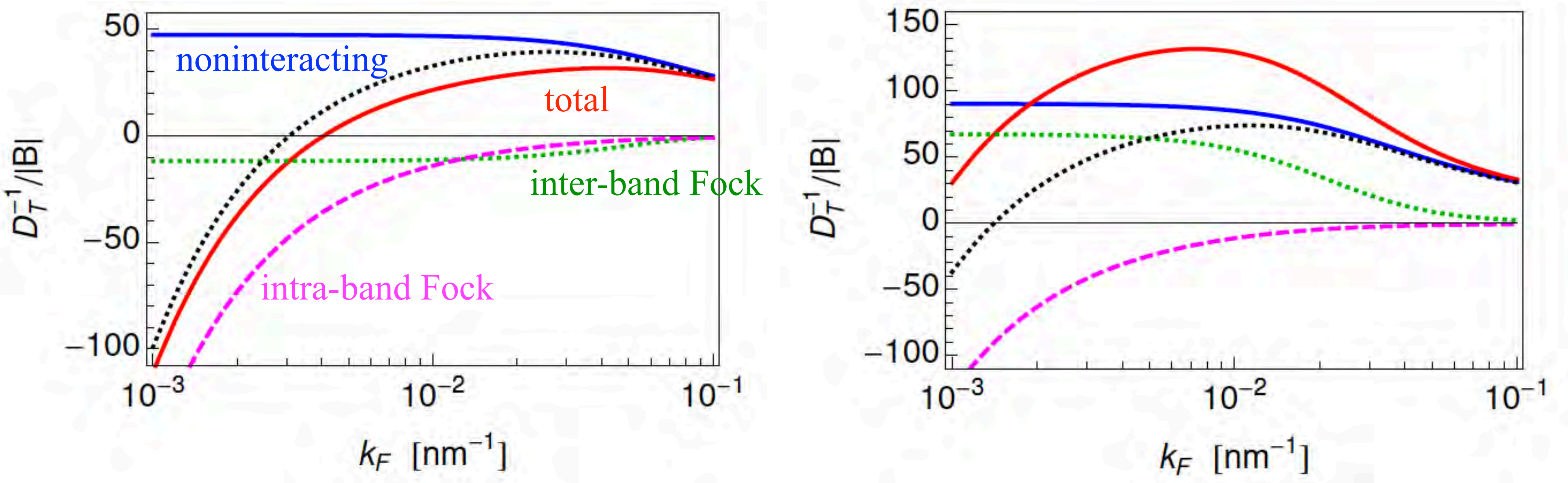
$$T_{\mathrm{C}}^{(\perp,\parallel)} = \frac{I(I+1)}{3}\,\frac{G^2}{k_{\mathrm{B}}}\,\frac{n_{\mathrm{imp}}}{d}\;\left|\bar{\chi}_{zz,xx}(\mathbf{q}=0)\right|$$



Results

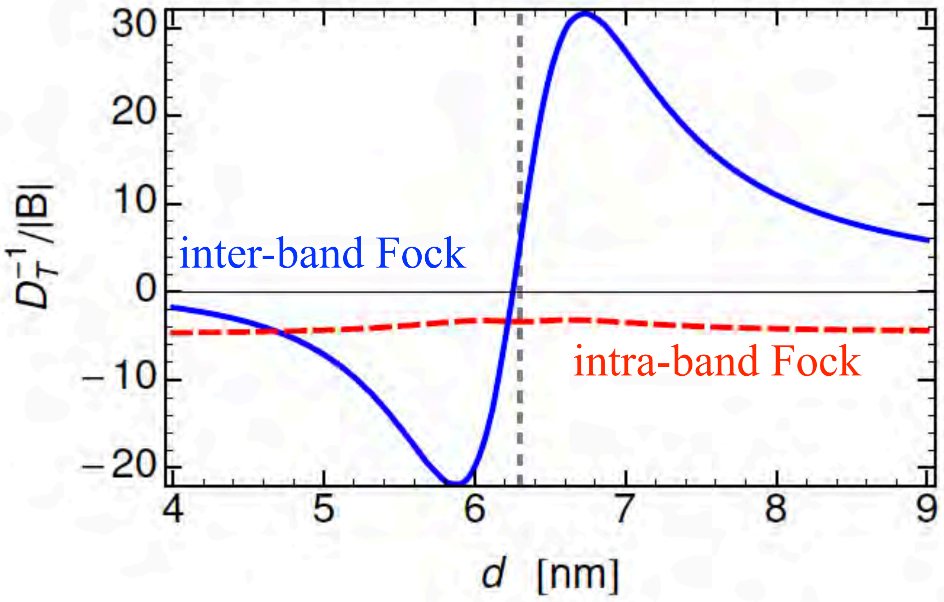
Thermodynamic DOS

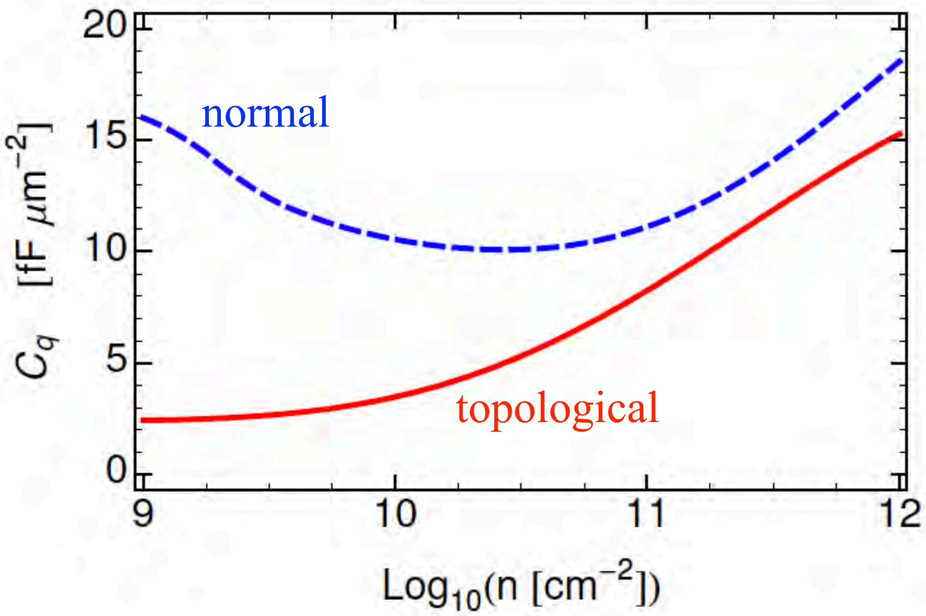
- normal regime: similar to ordinary 2D el. system
  - in particular also tendency to negative compressibility!
- topological regime: different due to inter-band contribution, suppressed negative compressibility!



Implication for quantum capacitance

- inter-band exchange-renormalisation of thermodynamic DOS varies strongly through transition
- quantum capacitance heralds topological phase!
  - in both magnitude and density dependence





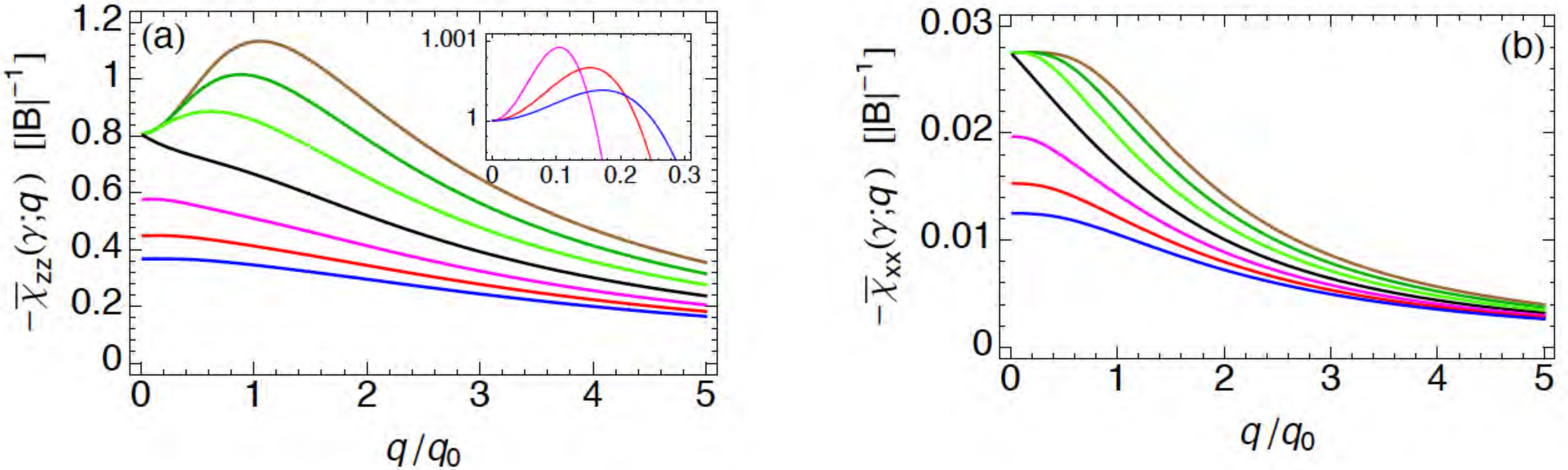
TE WHARE WĀNANGA O TE ŪPOKO O TE IKA A MĀUI VICTORIA UNIVERSITY OF WELLINGTON

DODD-WALLS CENTRE for Photonic and Quantum Technologies

The MacDiarmid Institute for Advanced Materials and Nanotechnology

Spin susceptibility: Undoped system

- vary gap parameter $\xi_M = M \cdot |B|/A^2 = -0.3, \ldots, 0.3$



  - finite at $q = 0$; independent of ξ_M in topological regime

- analytic result for static uniform spin susceptibility

$$\overline{\chi}^{(\mathrm{int})}_{xx,zz}(\gamma;\mathbf{q}=0) = -\frac{\mathcal{C}^2_{x,z}(\gamma)}{16\pi|B|}\,\frac{1}{1+4\xi_{\mathrm{M}}\Theta(\xi_{\mathrm{M}})}$$

TE WHARE WĀNANGA O TE ŪPOKO O TE IKA A MĀUI
VICTORIA
UNIVERSITY OF WELLINGTON

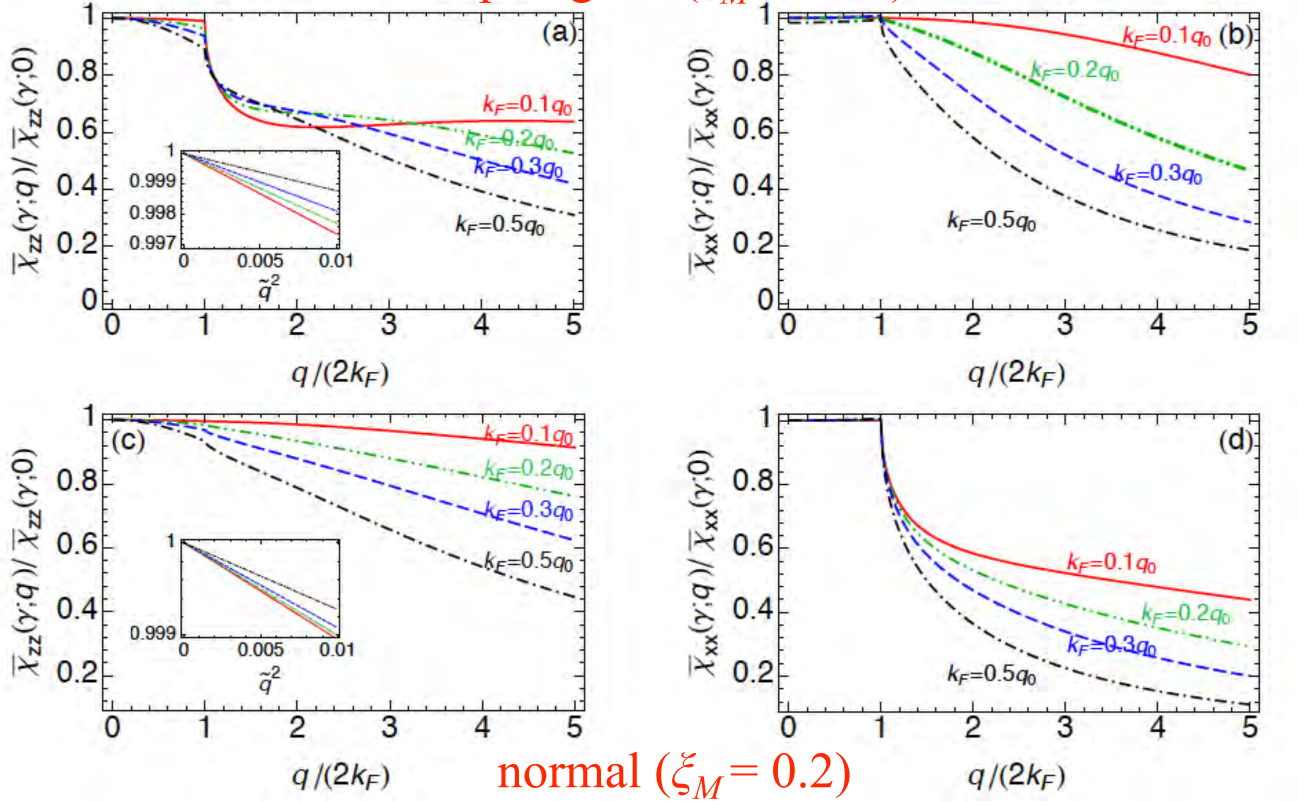
DODD-WALLS CENTRE
for Photonic and Quantum Technologies

The MacDiarmid Institute
for Advanced Materials and Nanotechnology

Susceptibility of electron-doped system

- sum of intrinsic & doping-dependent contributions
- complex dependence on parameters, density, …
- unconventional 2DEG response
  - band-mixing effects are strong!

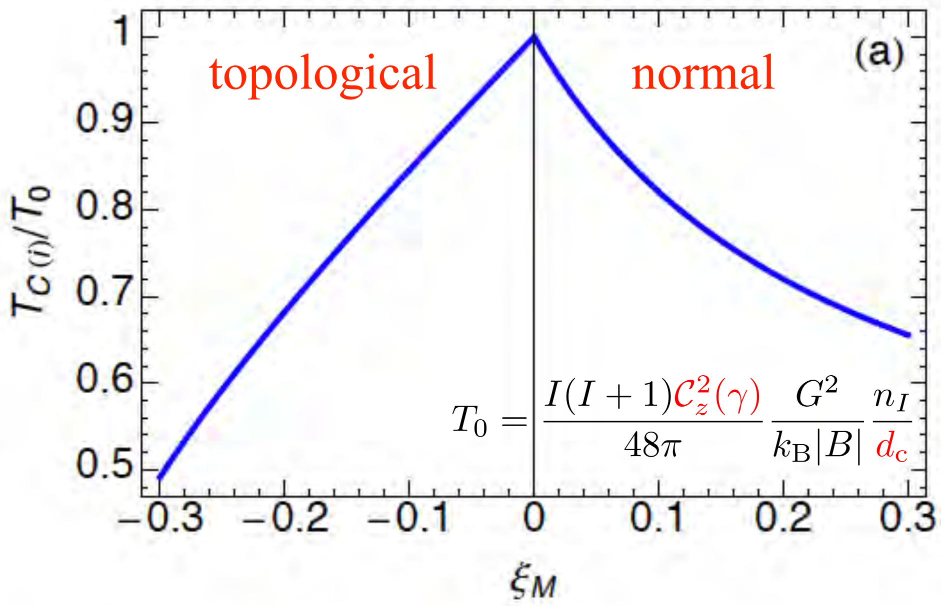
topological ($\xi_M = -0.2$)

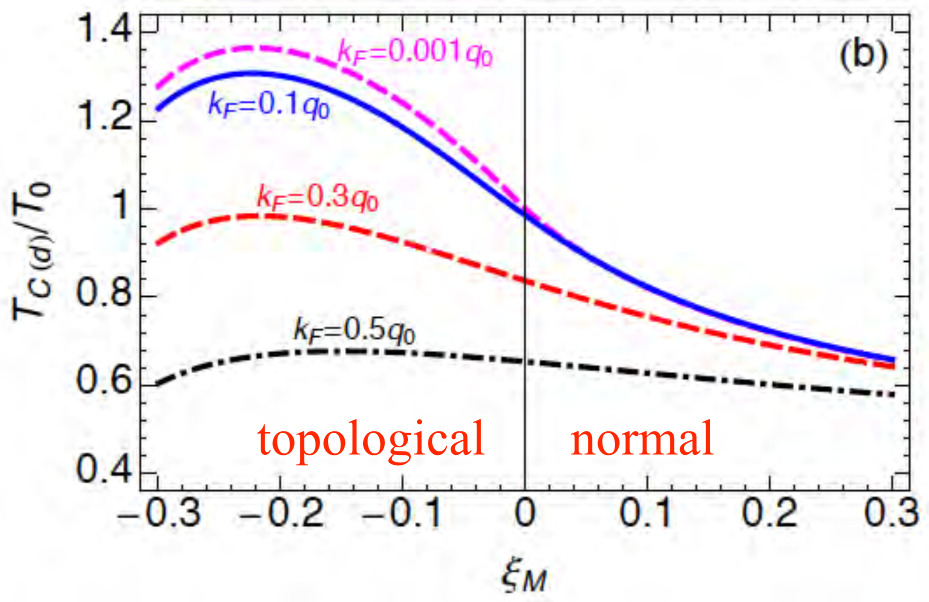


normal ($\xi_M = 0.2$)

Application: Carrier-mediated magnetism

- mean-field: uniform Ising magnetisation ($\chi_{zz} \gg \chi_{xx}$)
- clear asymmetry between topological and normal regimes, in both un-doped and doped cases!
- magnons: magnetism (un-)stable in (un-)doped case





Application: Collective-electron *g* factor

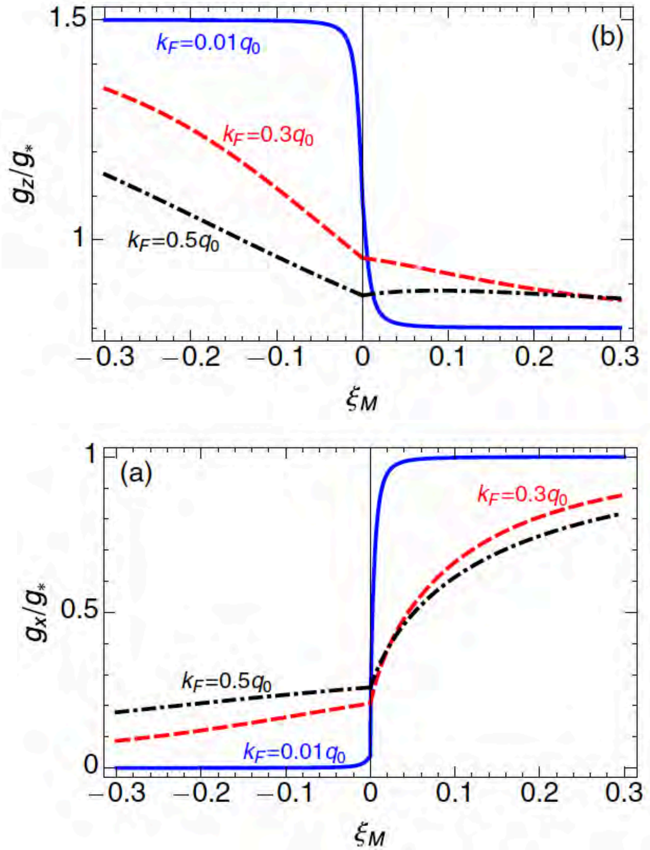
- relate calculated paramagnetic spin susceptibility to Pauli susceptibility: yields collective *g* factor

$$\mathcal{H}_{\mathcal{B}} = g_* \, \mu_{\mathrm{B}} \sum_j \mathcal{B}_j \, \hat{S}_j(-2\kappa/g_*)$$

$$g_j = g_* \sqrt{4 \, \frac{\overline{\chi}^{(\mathrm{dop})}_{jj}(-2\kappa/g_*; q)}{\overline{\chi}_0(q)} \Bigg|_{q=0}}$$

  - experimentally relevant measure for Zeeman splitting in a many-electron systems with spin-orbit coupling

Kernreiter, Governale, UZ, PRL (2013)

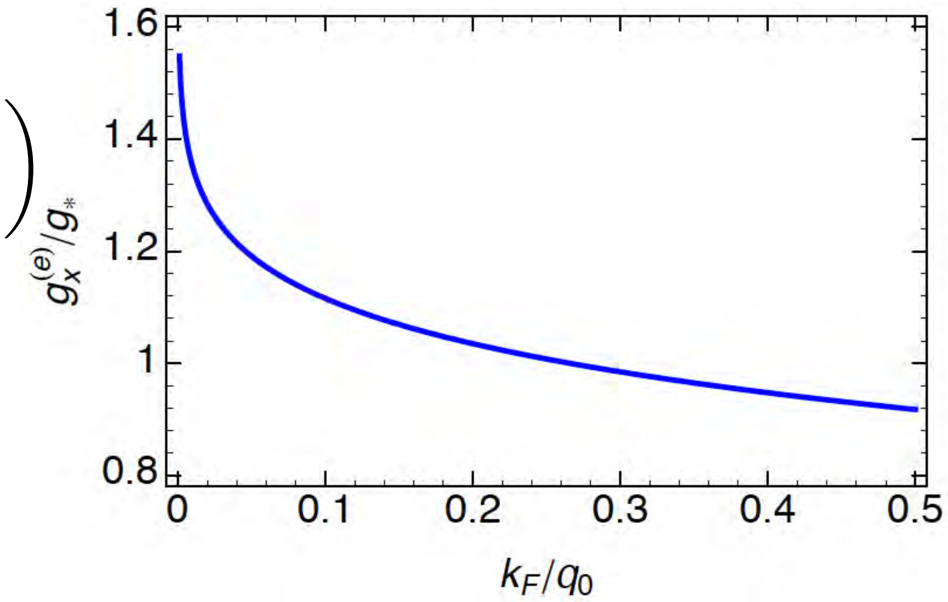


Spin response of helical edge states

- calculated spin susceptibility of helical edge states based on their quantum description Zhou et al. PRL (2008)
- derived collective 1D edge-electron *g* factors
  - constant for ⊥ plane:

$$\frac{g_z^{(\mathrm{e})}}{g_*} = -\frac{4\kappa}{g_*} + \frac{1-\mathcal{C}_{\mathrm{LH}}}{2}\left(1+\frac{2\kappa}{g_*}\right)$$

  - nontrivially density-dependent in-plane



- probe w/ superconducting proximity effect Hart et al., Nat Phys (‘14); Pribiag et al., Nat Nano (‘15)

Conclusions

- comprehensive study of many-electron properties in HgTe quantum-well 2D electron system
- distinctive features in topological regime revealed
  - thermodynamic DOS: positive inter-band Fock term
  - intrinsic $q = 0$ spin susceptibility: no gap dependence
- considered physical implications
  - quantum capacitance/compressibility
  - carrier-mediated magnetism, effective g factor
- our study is focused on the HgTe quantum-well system, but conclusions valid more generally

Kernreiter, Governale, UZ & Hankiewicz, Phys. Rev. X **6**, 021010 (2016)
Kernreiter, Governale, UZ, Phys. Rev. B **93**, 241304(R) (2016)

TE WHARE WĀNANGA O TE ŪPOKO O TE IKA A MĀUI
VICTORIA
UNIVERSITY OF WELLINGTON

DODD-WALLS CENTRE
for Photonic and Quantum Technologies

The MacDiarmid Institute
for Advanced Materials and Nanotechnology