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Some Recent Results using SERGIS

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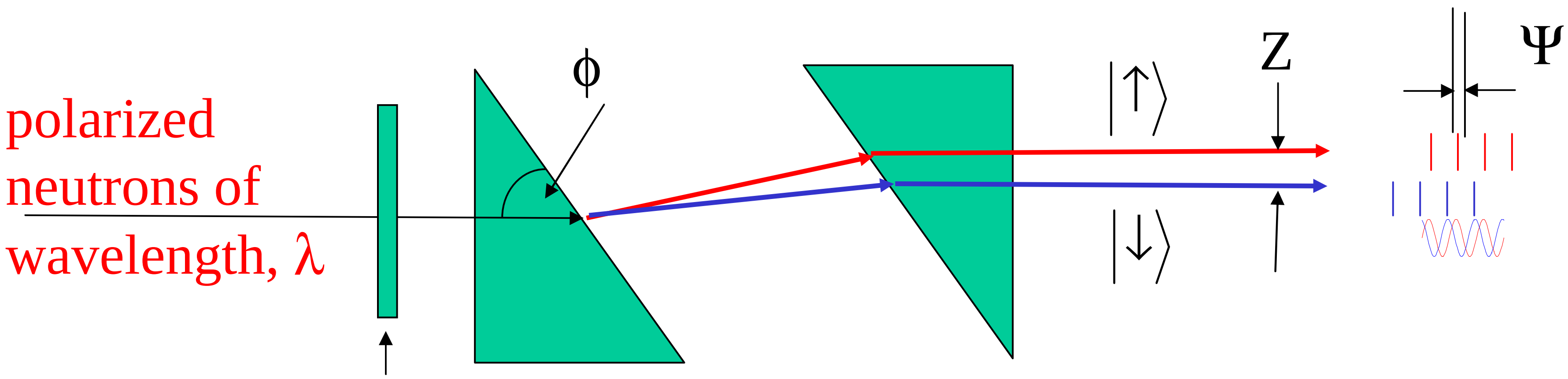
INDIANA UNIVERSITY

The next-generation neutron-scattering facility for the United States

SNS

Splitting Neutron Polarization States

- Birefringent prisms for neutrons are simply appropriately shaped magnetic-field regions



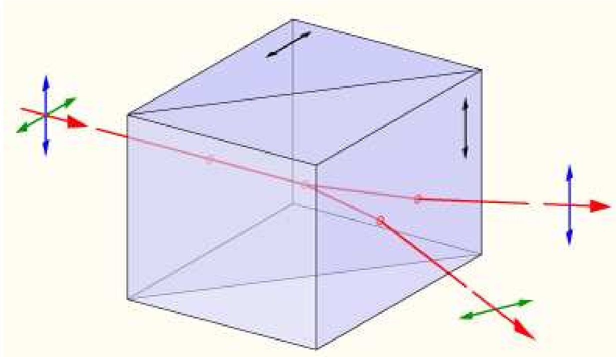
$\pi/2$ flipper produces

$$\left(|\uparrow\rangle + |\downarrow\rangle\right)/\sqrt{2}$$

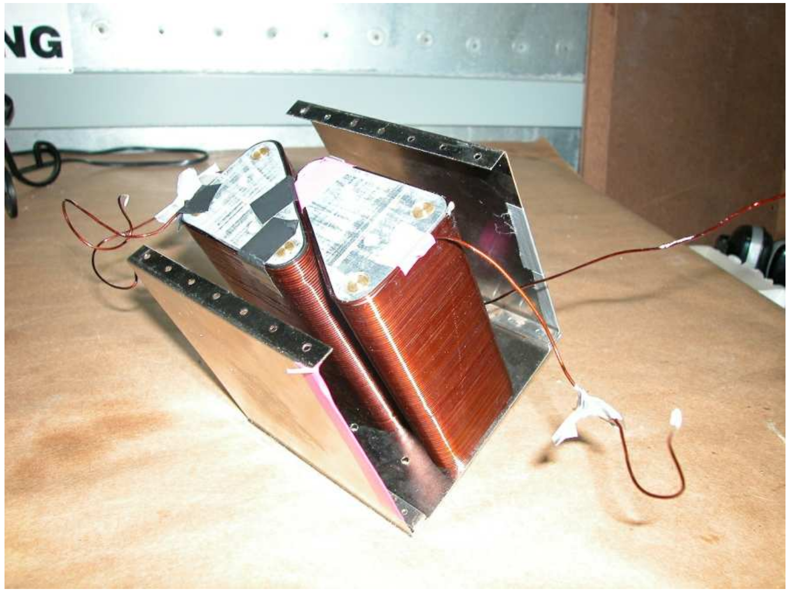
Snell's law relates Z and Ψ to ϕ

Wollaston Prism: Invented Early 19th Century

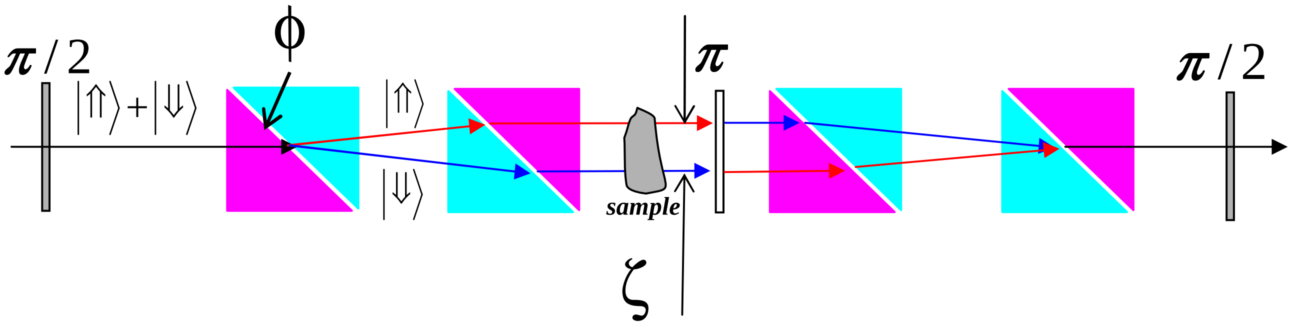
- *For light:* the refractive effect can be doubled by using a pair of prisms with perpendicular optic axes



- *For neutrons:* the refractive effect can be doubled by using a pair of triangular solenoids with opposite magnetic fields



Spin Echo Scattering Angle Measurement (SESAME)



- Neutron spin states are split and recombined by magnetic Wollaston prisms
- With no sample, the Larmor phase Ψ generated before sample is cancelled after the sample, independent of neutron incident angle, ϕ (spin echo)
- If scattering occurs, the phases generated before and after the sample are different (because ϕ is different) and the final neutron polarization is reduced
- The echo polarization is almost independent of the incident value of ϕ so we don't need to collimate the beam strongly

Expression for Final Neutron Polarization

- Final neutron polarization is given by the average of cos(Ψ_{tot}) over all neutrons scattered. When we work through the math we find:

$$\frac{P}{P_0} = e^{G(\zeta) - G(0)}$$

$$G(\zeta) = \frac{\lambda^2}{4\pi^2}\frac{1}{A}\int_{-\infty}^{\infty} dQ_y \int_{-\infty}^{\infty} dQ_z \frac{d\sigma\,(0,Q_y,Q_z)}{d\Omega}\cos(Q_y\zeta)$$

$$\zeta = c\lambda^2 BL\cot\phi$$ (λ = wavelength; other quantities on previous slide)

- ζ is approximately equal to the separation of rays in the previous slide

- ζ is only weakly dependent on beam collimation. For $\phi_0 = 32°$, and $\Delta\phi = \pm 0.5°$, $d\zeta/\zeta \sim \pm 2.5\%$

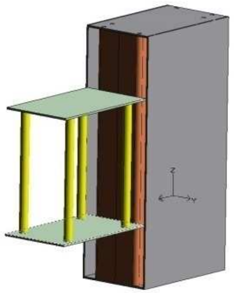
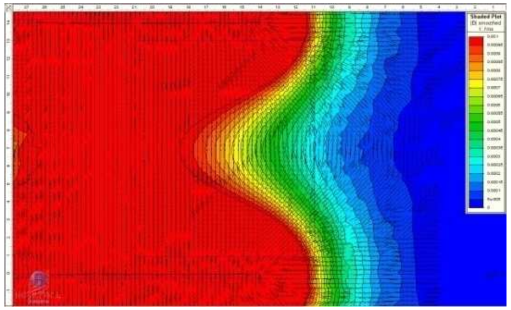
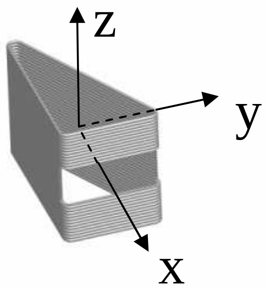
$$\frac{d\zeta}{\zeta} \approx \frac{2\Delta\phi}{\tan\phi_0}$$

Guide Fields

- Guide fields (or zero field) ensure spin transport between separated prisms & allow increase of spin echo length ($\zeta \sim L$)
- How should we design guide fields?

1. Make the guide field "constant" in space so that it adds to triangular fields?

– Very hard to ensure that all fields are parallel across sharp boundaries – leads to depolarization

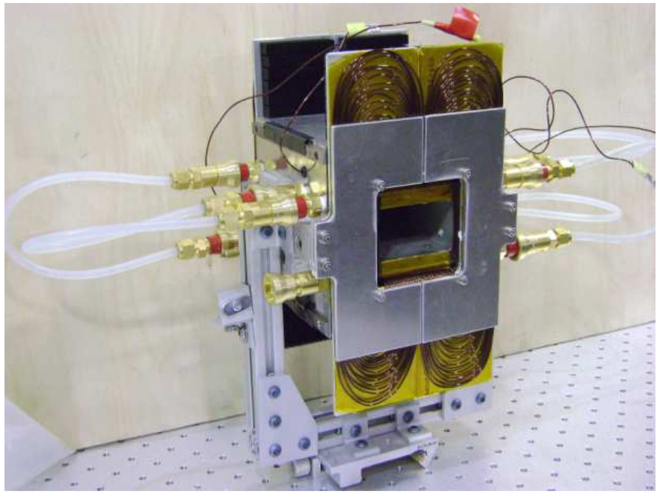




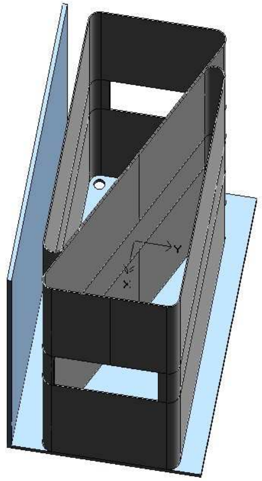
2. Make a gap in the face of the prism so that the field overlaps the guide field?

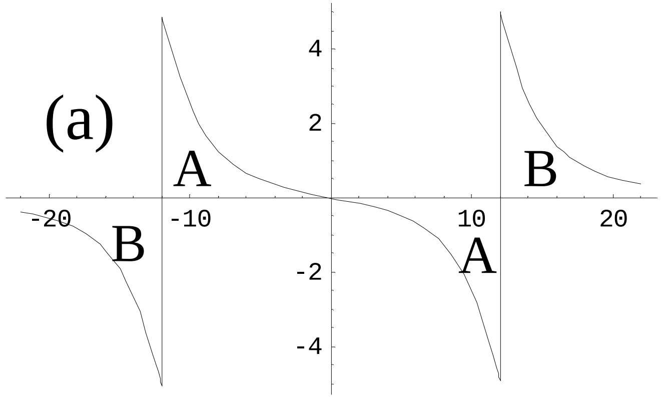
– Gaps in the faces of triangle coils allow fields to "spill out" and avoid neutron depolarization at sharp field boundaries

– But what do gaps do to field-integrals for equivalent neutrons?

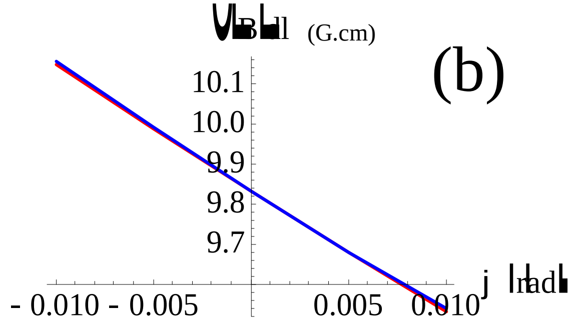
Gapped Triangular Prisms







Difference between (a) fields and (b) field-integrals of gapped and closed prisms



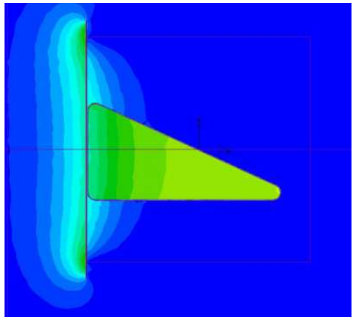
- Suppose we model the coils as an infinite intact solenoid plus current sheets at the gaps
  - For a neutron travelling along the optic axis, the field integral of a gapped coils is the same as that of closed coils because the marked areas (A & B) are equal
  - For off-axis neutrons, there is almost no difference between the field-integrals of gapped and closed prisms

Bottom Line

- Verify model by comparing with measured fields
  - It works
- Can now compute field overlaps of neighboring coils exactly
- Can compute Larmor phase aberrations (i.e. differences in field integral for equivalent neutrons) along any path in the absence of scattering
  - Overall aberration is zero for paths parallel to optic axis and thru sample center
  - “zero” results from cancellations that result from symmetry
- Can compute phase aberrations when scattering occurs
  - Aberrations give rise to uncertainty in spin echo length
  - Uncertainty is dominated by aberrations associated with ungapped coils – gaps add essentially nothing

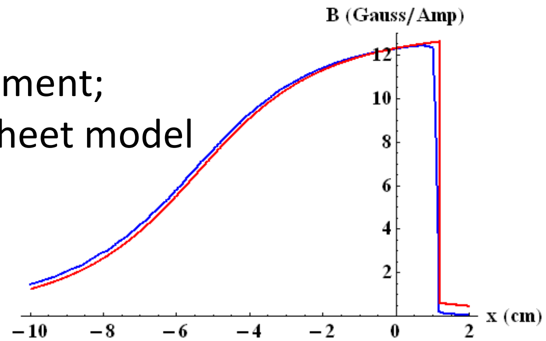
Does the Current Sheet Model Work?

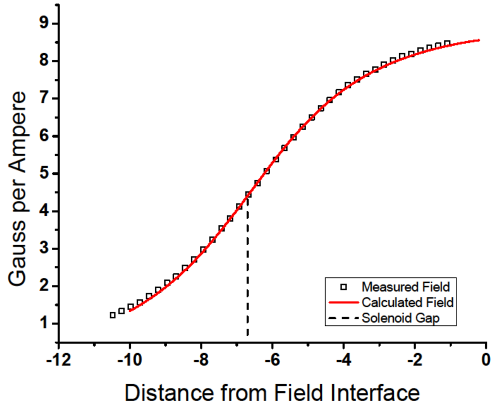
- FE for full system, including mu-metal, gives same field shape as current-sheet model inside coil
- Current-sheet model agrees with measured data quite well
- Only discrepancy is inside neighboring coil



Field calculated by FE with extended current sheets

Blue:- Finite Element;
Red:- Current-sheet model

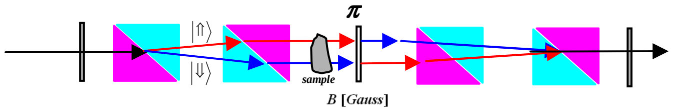


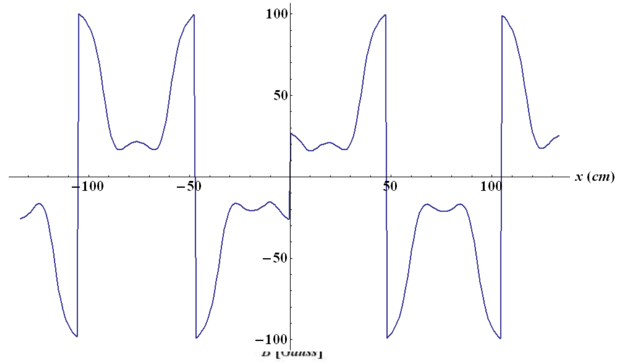


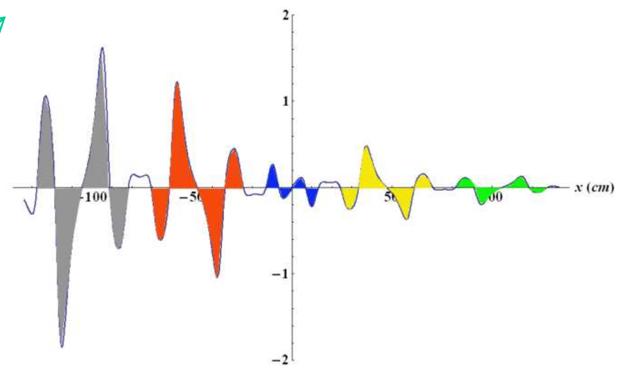
Model & data

Cancelling Field-Integral Aberrations

- Exploit symmetry to cancel aberrations in *B.L*
- Place “equivalent” field elements symmetrically about each pi flipper so that local cancellation is maximized
  - Guide fields designed like our flippers *decrease* aberrations *wrt* no guides
  - Changing the guide-field design can reduce the aberrations at $2\theta = 0$ even further
  - Contribution of gaps to spin-echo-length resolution is negligible compared to resolution obtained with closed prisms







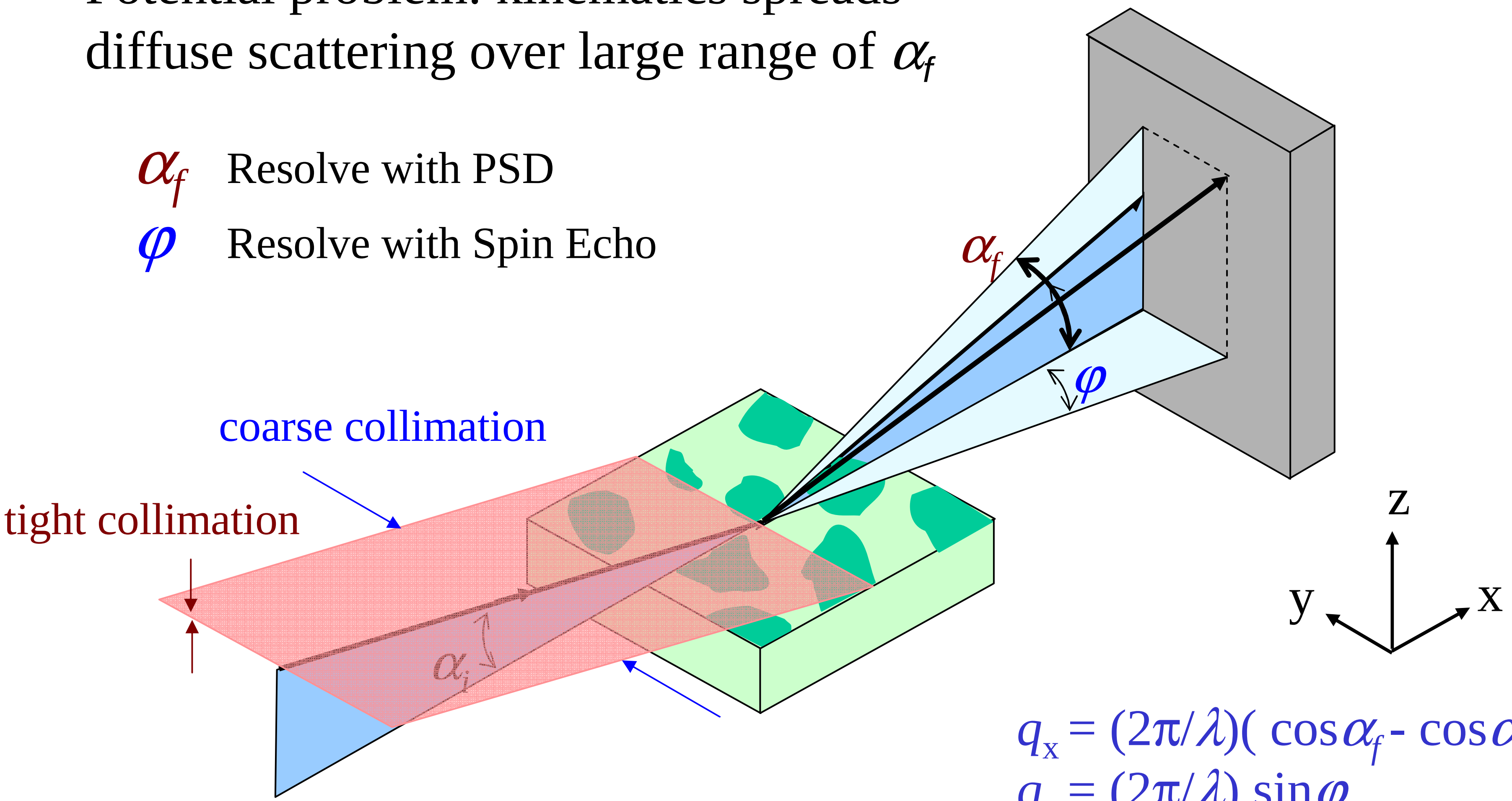
Upper plot shows field modulus. Lower plot is difference between field modulus in Gauss on axis and a trajectory with y = 0, z = -1 cm, $\phi = 0$, $\psi = 0.3°$. Grey integral is slightly +ve, red is slightly –ve: sum is very slightly +ve. Sum on right side is very slightly –ve. Near cancellation around a pi flipper, between adjacent pi’s & across central pi. Cancellation is exact if $\phi = \psi = 0$

Geometry at grazing incidence

Potential problem: kinematics spreads diffuse scattering over large range of α_f

α_f Resolve with PSD

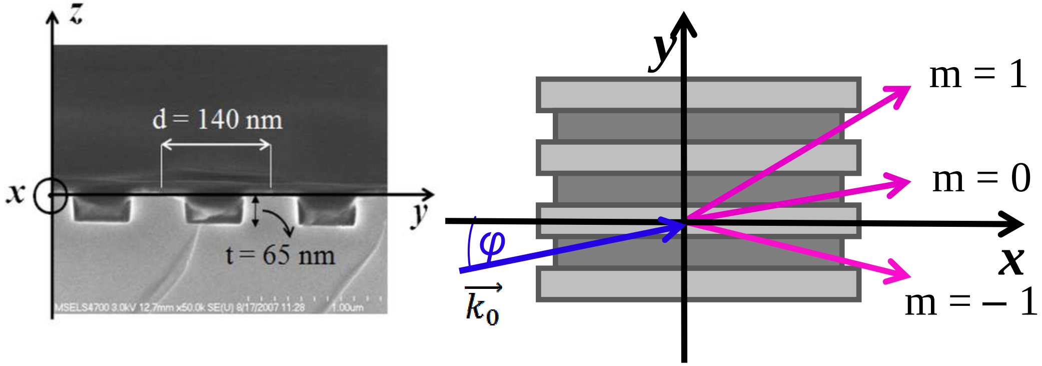
φ Resolve with Spin Echo

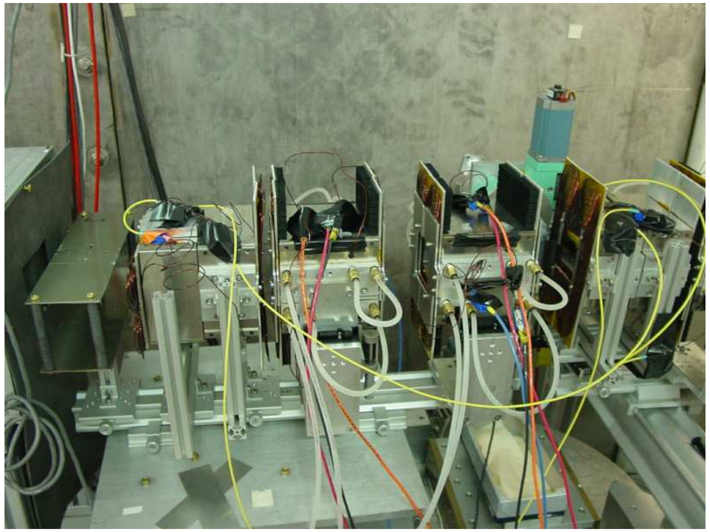


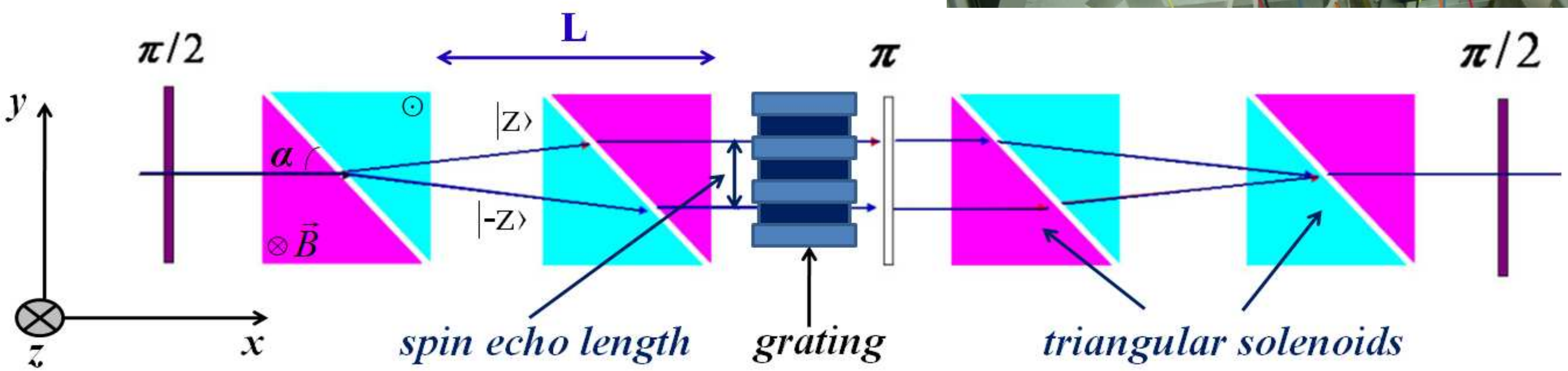
$q_x = (2\pi/\lambda)(\cos\alpha_f - \cos\alpha_i)$
$q_y = (2\pi/\lambda)\sin\varphi$

SERGIS Measurements of a Diffraction Grating

- First, let's look at something we understand (or do we?).

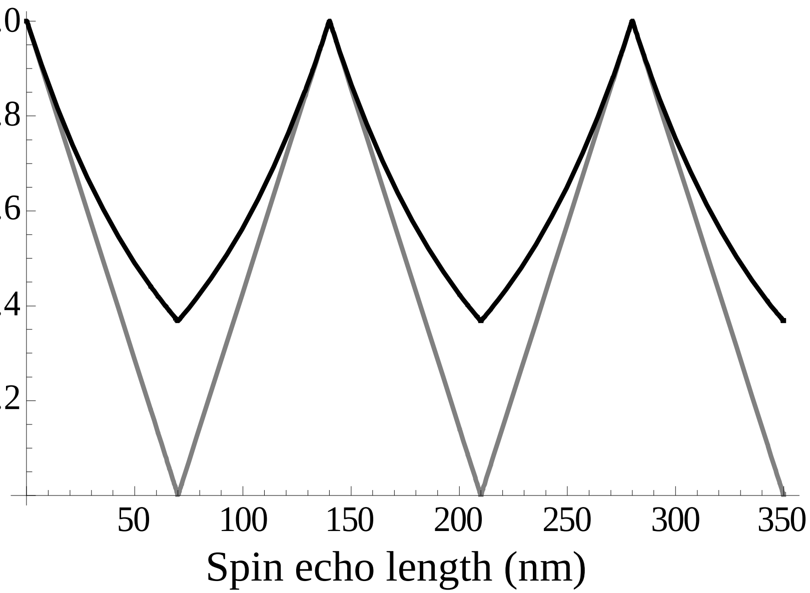




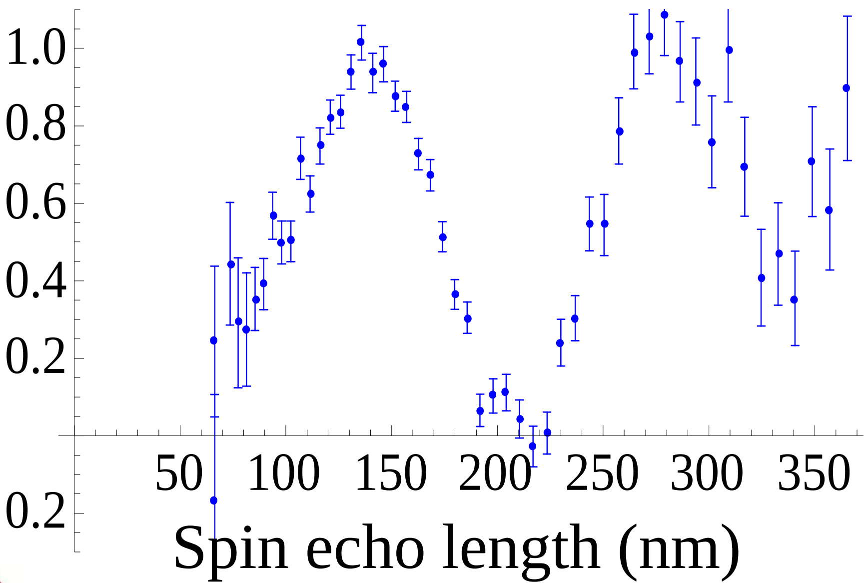


What should we expect?

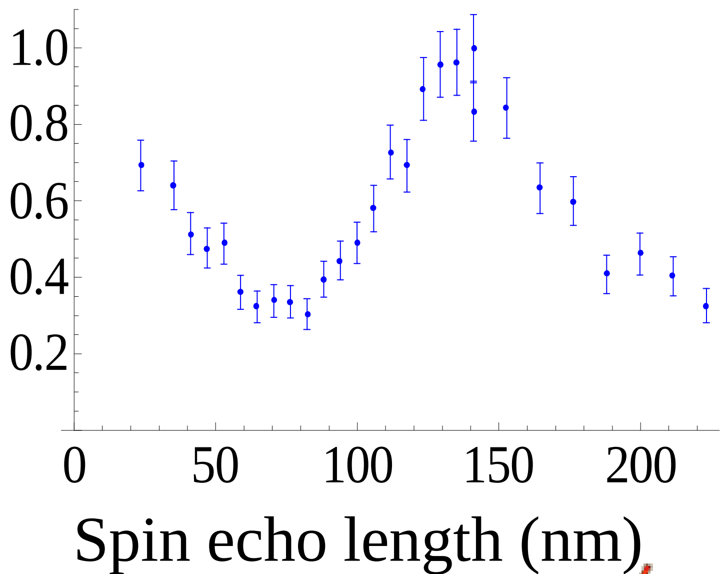
- P/P_0 is the FT of S(Q)
- Within DWBA, S(Q) ~ FT of height-height correlation function
- So, P/P_0 should look like the height auto-correlation function?



On *ASTERIX* at *LANSCE*

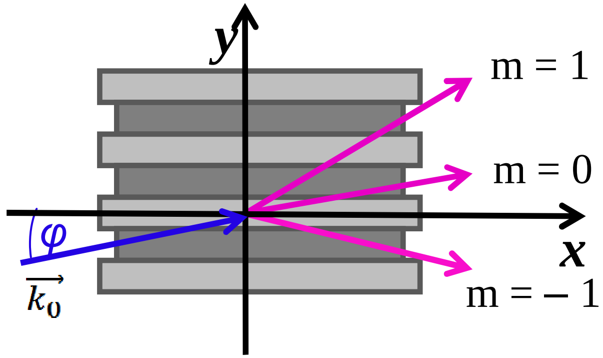


On *AND/R* at *NCNR*

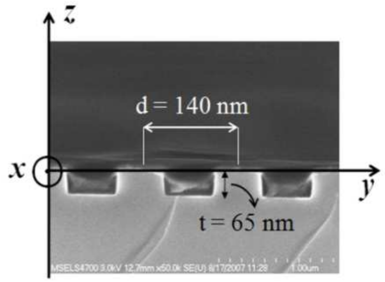


Exact Dynamical Theory Calculation by Rana Ashkar

- Expand wavefunction in terms of Bloch waves
- Solve boundary conditions at interfaces between air, modulated layer and substrate

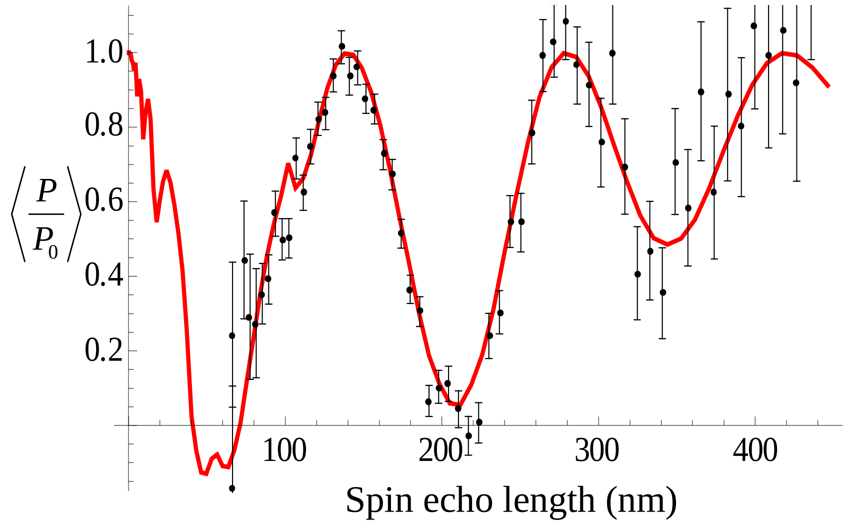


- Find: $$\frac{P(\zeta)}{P_0} = \sum_m \tilde{p}_m \cos(mg\zeta)$$
  where $g = 2\pi/d$, m is the order of Bragg reflection from the grating and the coefficients p_m are found from the calculation



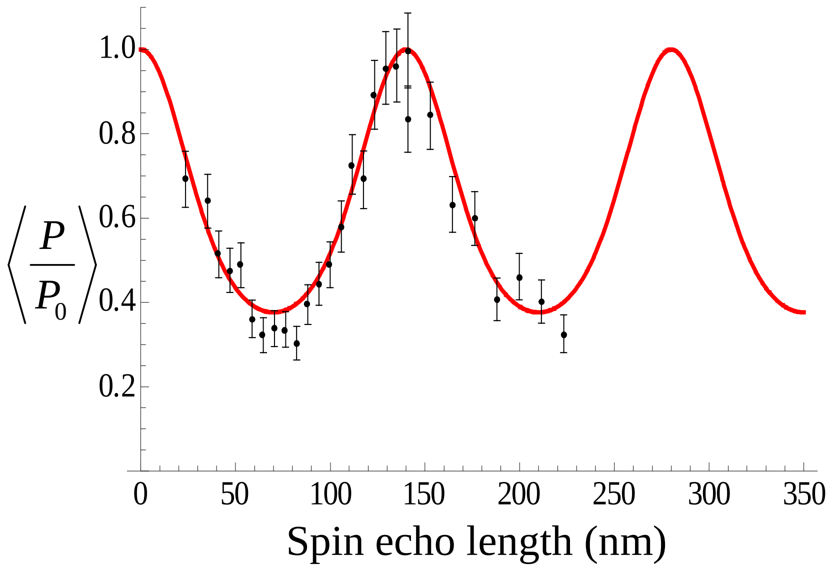
- The calculation is stable to any Bragg order and easily extended to other grating shapes
  – Mathematica code available

Comparison with Experiment



Asterix Data

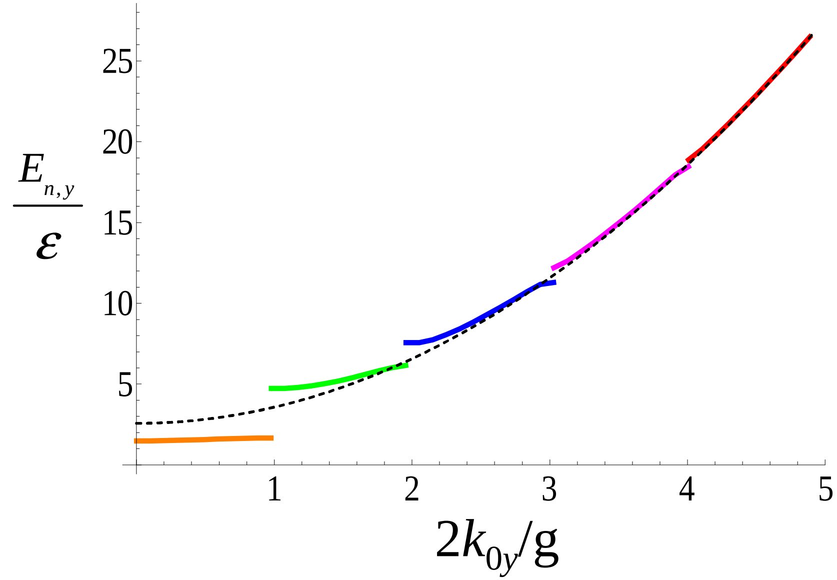
NIST data

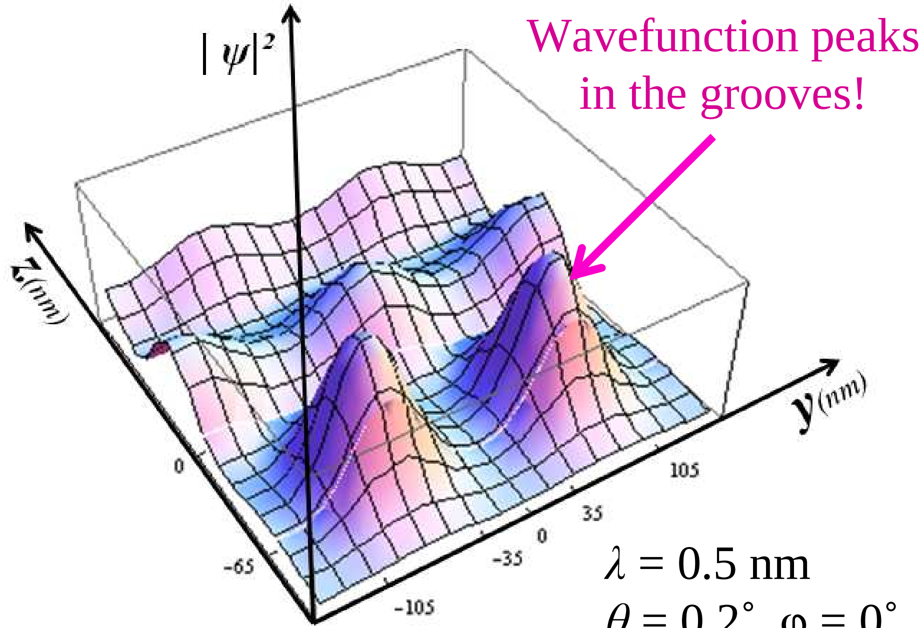


Predictions of the Theory

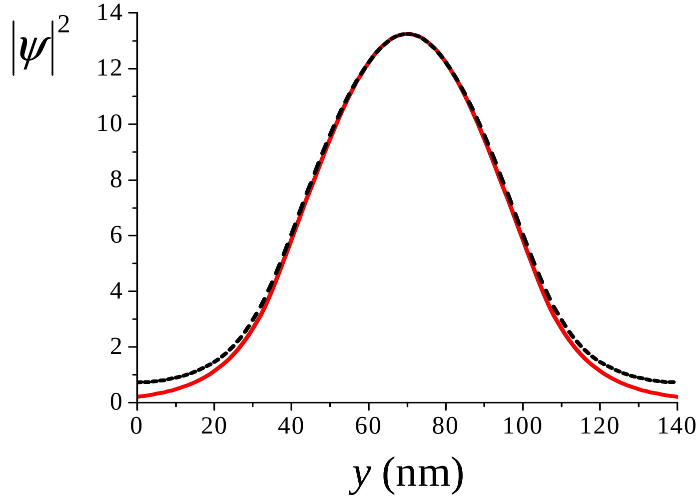
Theory predicts a band structure for neutrons in a 1D periodic potential that is close to tight-binding model.

Theory predicts the behavior of the neutron wavefunction in the vicinity of the grating.





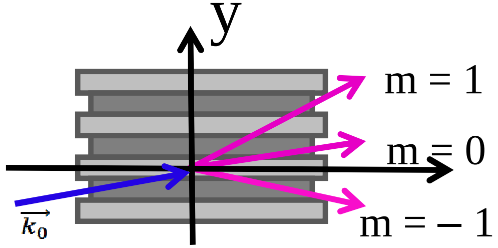
λ = 0.5 nm
θ = 0.2°, φ = 0°

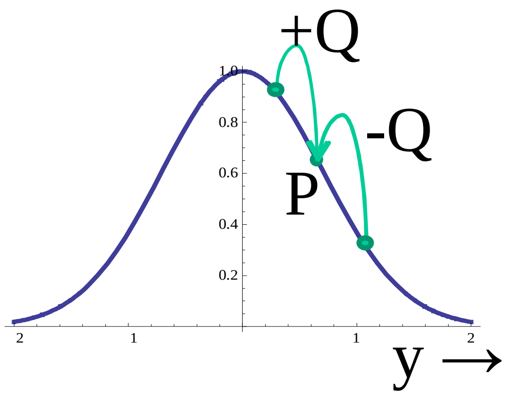


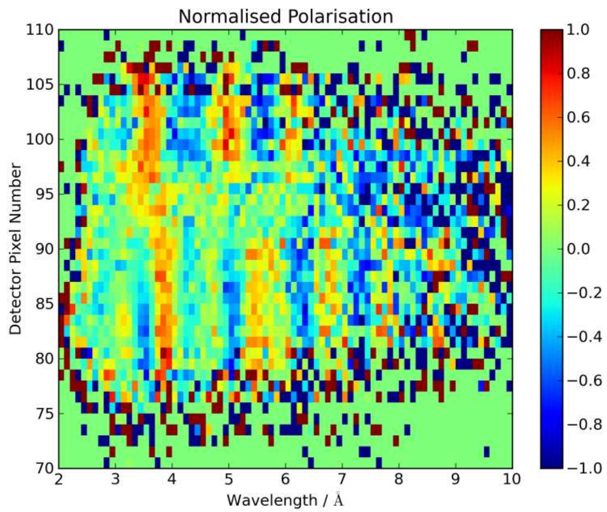
z = – 45 nm, λ = 0.5 nm and θ = 0.2°

The Sine Transform

- Set up detector with position sensitive direction along y
- Use a beam that is wide in y and set up echo so that $P_0 = 0$ with no sample
- Measure echo polarization as a function of detector position
- Anti-symmetric echo about detector center (if sample is lined up)
- Subtract polarizations on opposite sides of detector
- Result should be $G(\zeta) = \frac{\lambda^2}{4\pi^2}\frac{1}{A}\int_0^\infty dQ_y \int_{-\infty}^{\infty} dQ_z \frac{d\sigma\,(0,Q_y,Q_z)}{d\Omega} Q_y \sin(Q_y\zeta)$







Questions & Conclusions

- Can we use the fact that the wave function peaks in the grooves to examine structures in the grooves?
- Can we examine competitions between grating induced order and "natural" periodicity of an overlayer?
- Can we measure the lotus leaf effect?
- Does the exact dynamical theory work in all cases?
- Under what circumstances do other theories like the DWBA and the Phase Object Approximation work?
- Does the fact that we can see grating structure actually mean that we can do SERGIS successfully with other samples or do we need to invent dark-field SESANS?

END