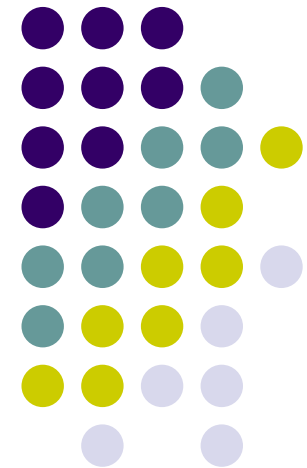


# NMR Diffraction and Diffusion Interference from Cells

Philip Kuchel & Guilhem Pages

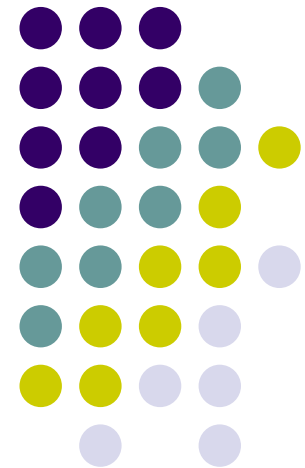


# Related posters

**D2** Levitz, P. Intermittent Brownian dynamics over strands

**E2** Gratz, M. and Galvasos, P. Methodical aspects of 2D NMR correlation spectroscopy under conditions of ultra high pulsed field gradients

**E3** Veil, S., Excoffier, G., Pages, G., Ziarelli, F., Delaurant, C., and Caldarelli, S. Combined use of pulsed gradient spin echo and high resolution magic angle spinning to investigate solute diffusion in the presence of chromatographic stationary phase



East or West we are  
all illuminated by science  
don't you agree!?

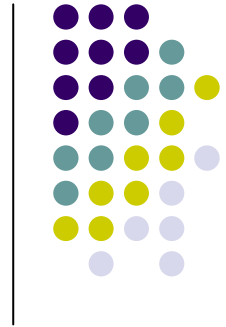
QuickTime™ and a  
TIFF (Uncompressed) decompressor  
are needed to see this picture.

It says here that your  
knowledge is *diffusing*  
to the West!

# Contents

- Red cells...motivation
- $q$ -Space analysis
- Flow diffraction
- Octagon-star model





QuickTime™ and a  
DivX 4.1.2 decompressor  
are needed to see this picture.





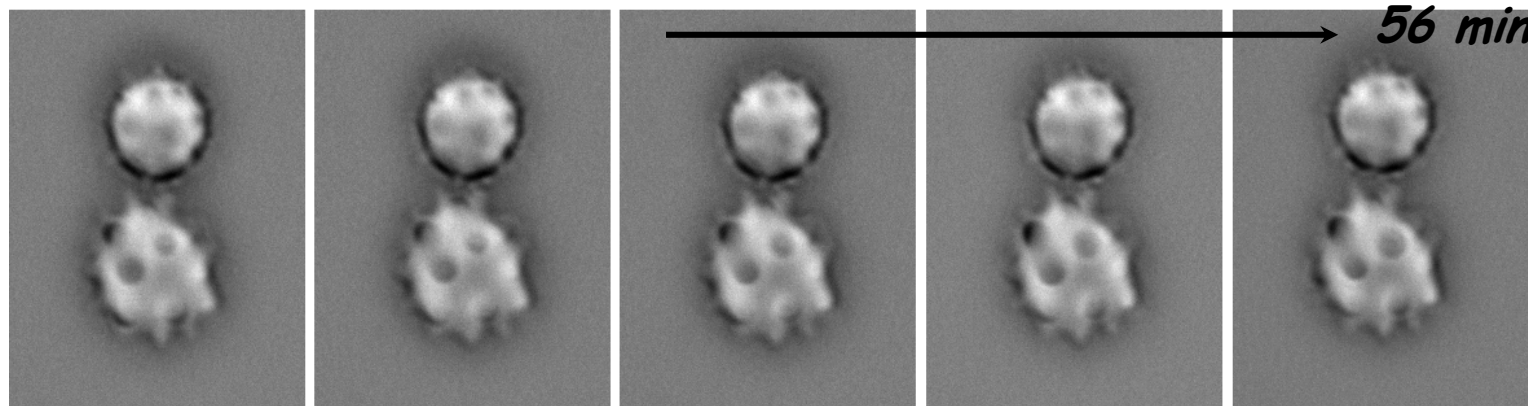
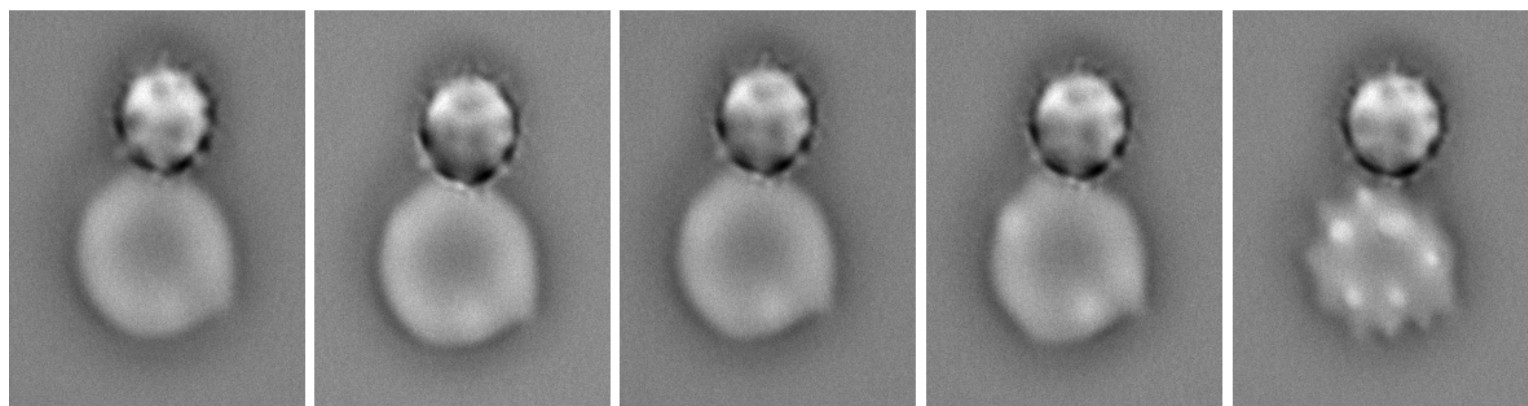
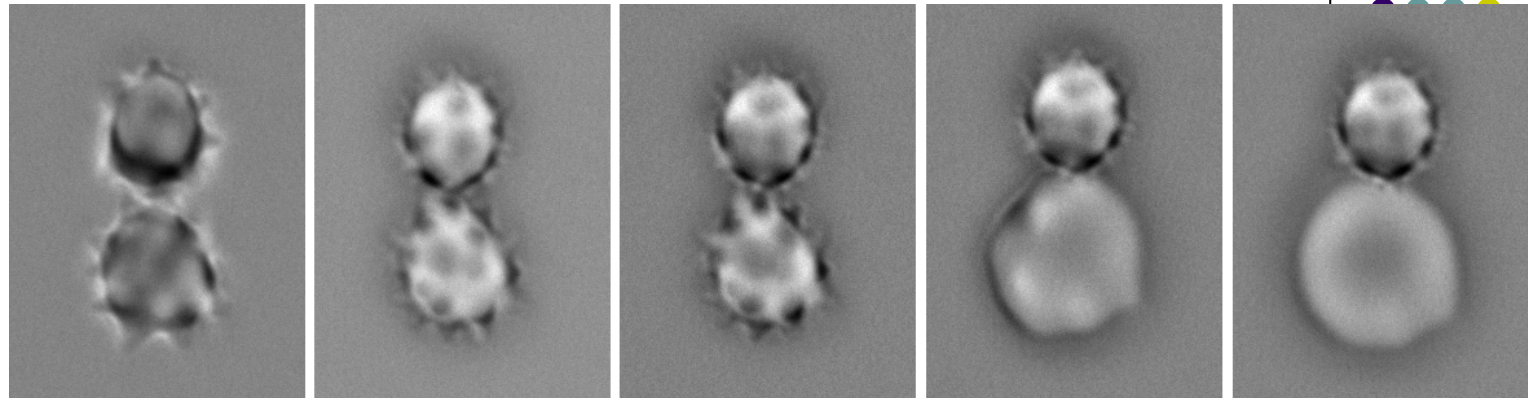
0 min

4 min

16 min

*Echinocytes  
under DIC  
Microscopy*

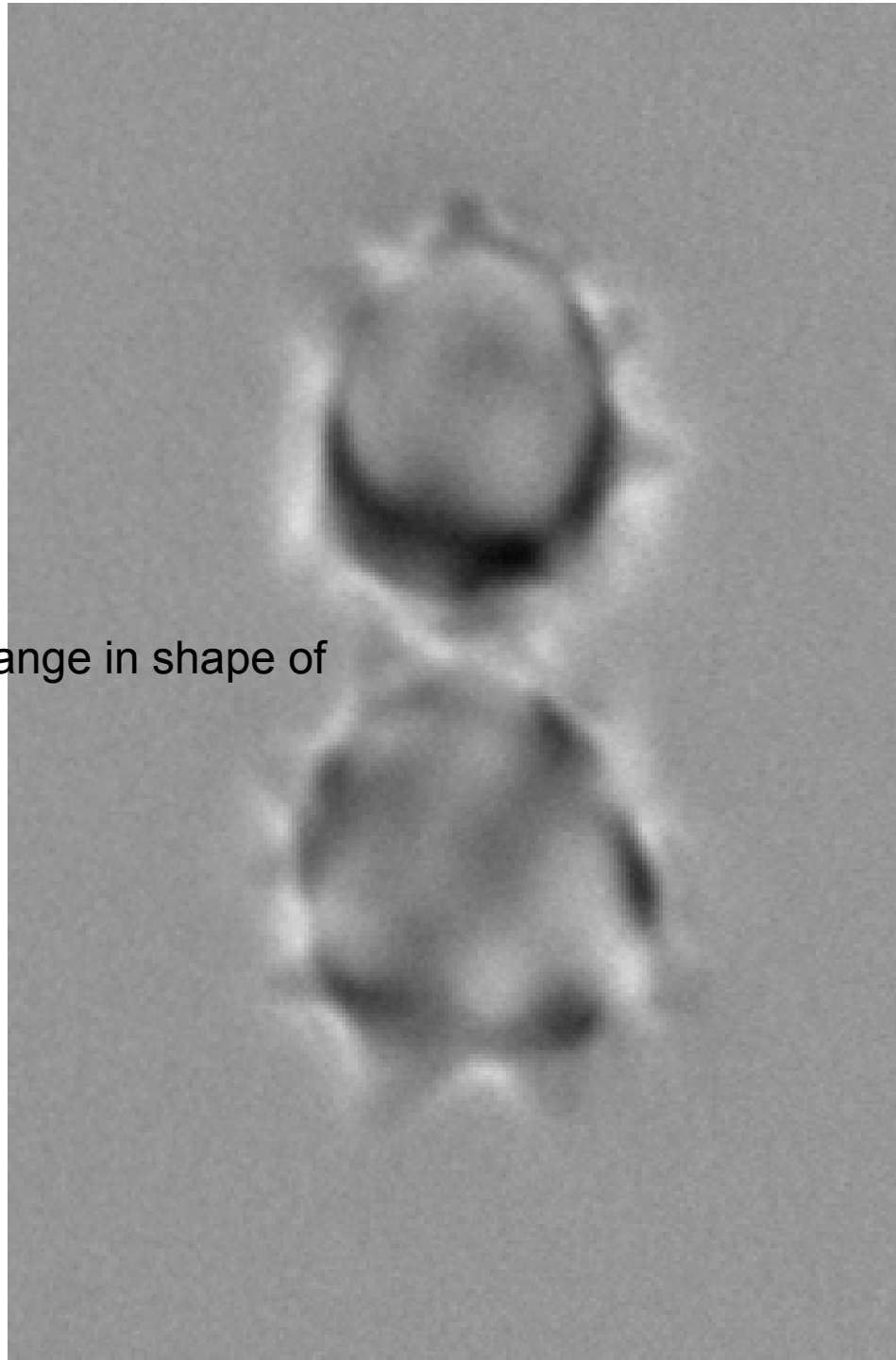
*...showing  
echinocyte  
to discocyte  
reversion  
and back  
again*



56 min

*Echinocytes  
under DIC  
microscopy*

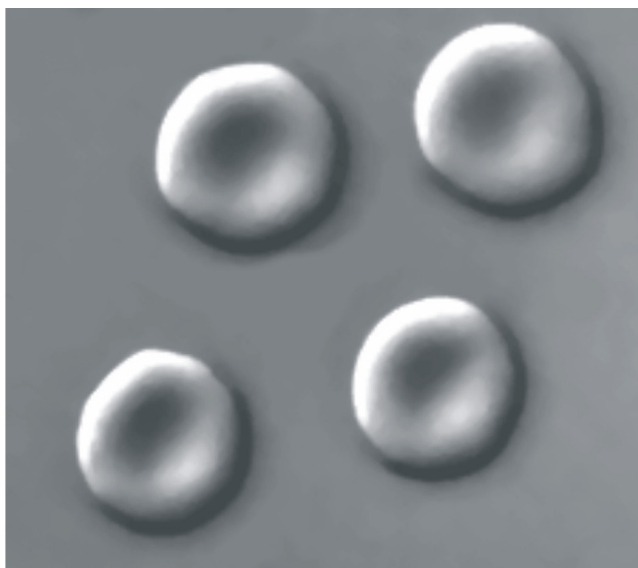
Movie showing change in shape of  
red blood cell





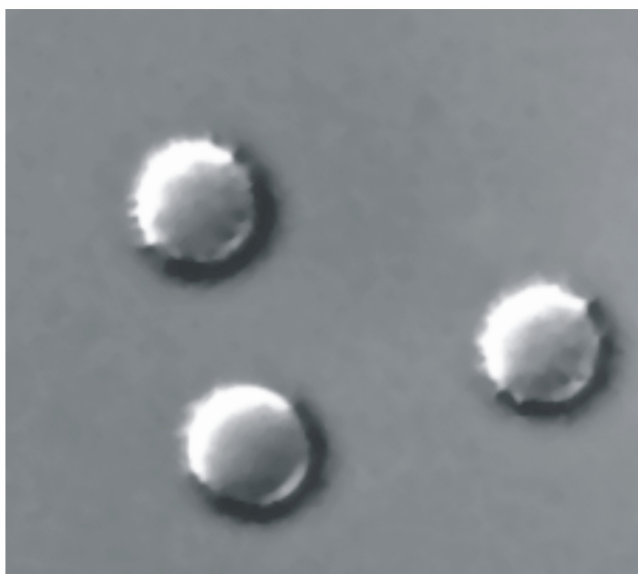
*Discocytes*

(a)



*Spherocytes*

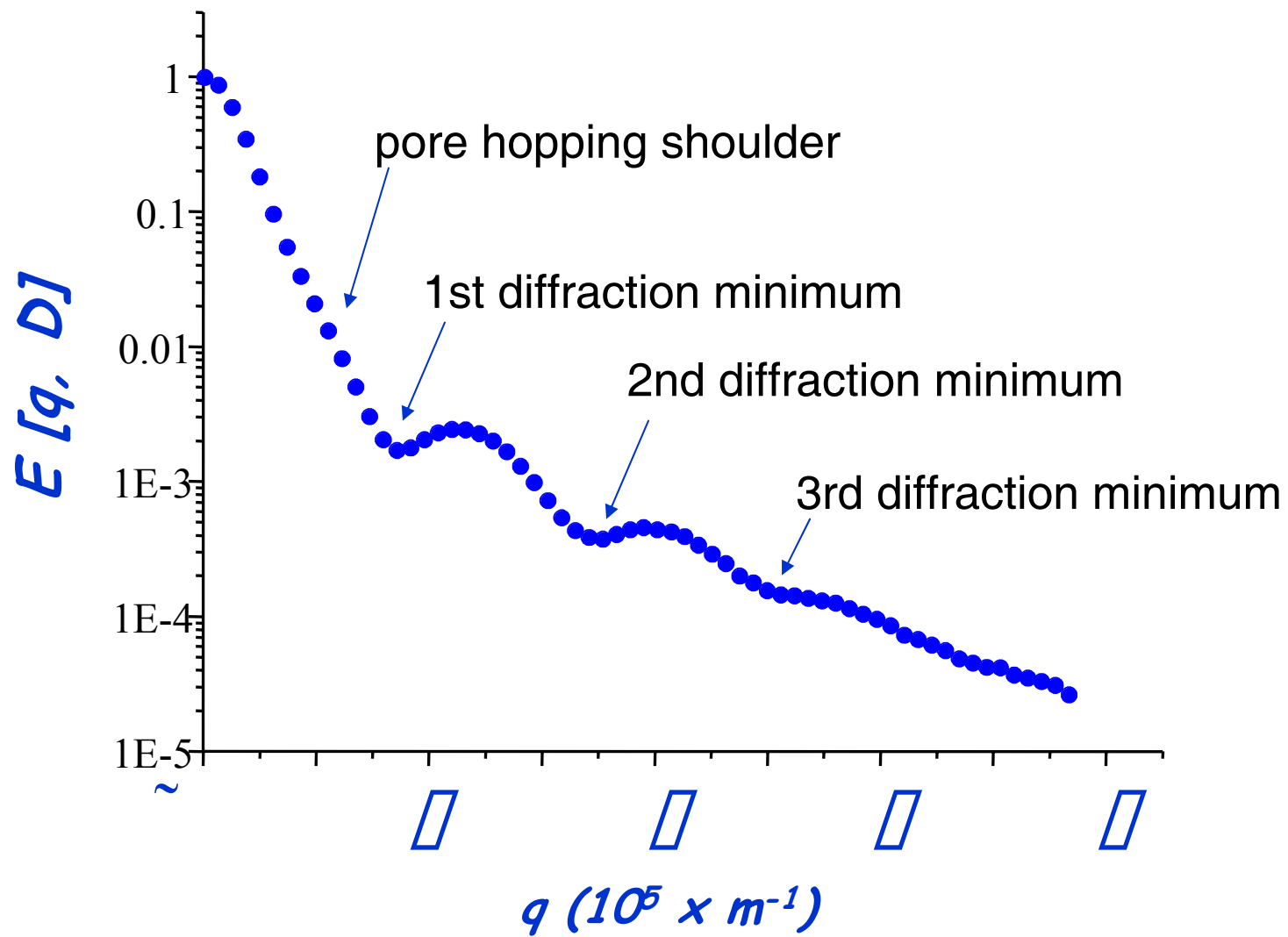
(b)

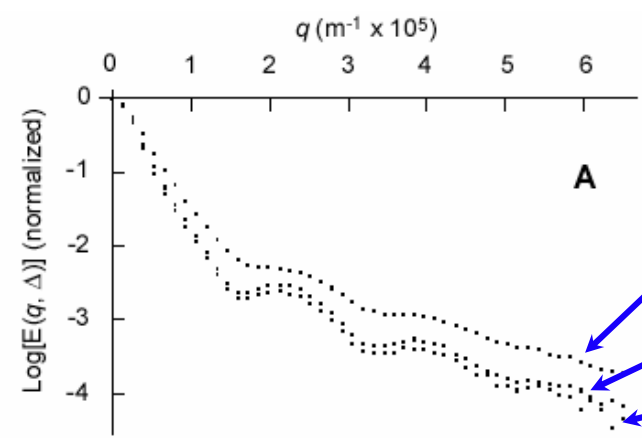




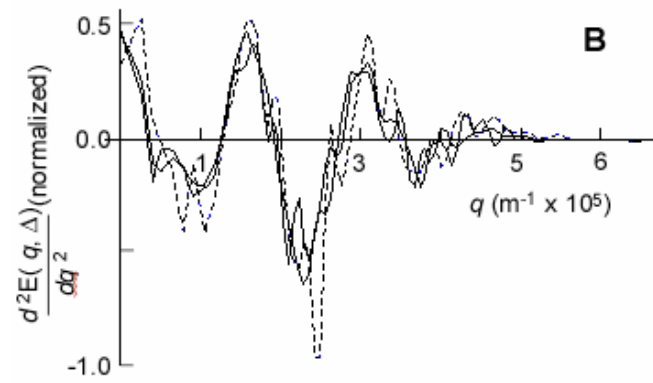


*Tracking red cell shape transformation  
in packed samples over time courses of  
minutes*

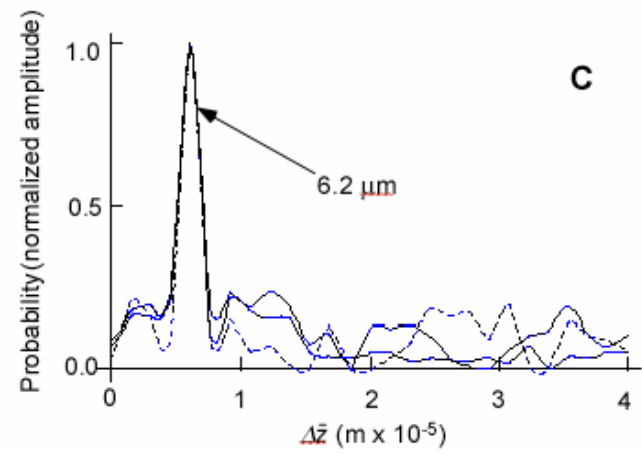




Ht = 58%  
48%  
41%



Second derivative

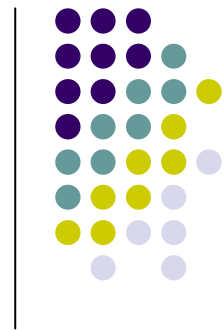


Fourier transform

*Unbalanced bipolar pulses in STE...rapid signal acquisition*

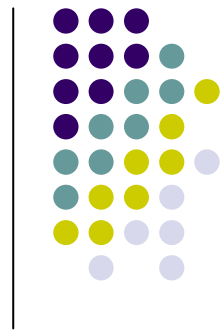


QuickTime™ and a  
TIFF (uncompressed) decompressor  
are needed to see this picture.



Movie showing change in shape of the q-space  
plot  
QuickTime™ and a  
decompressor  
are needed to see this picture.

$q$



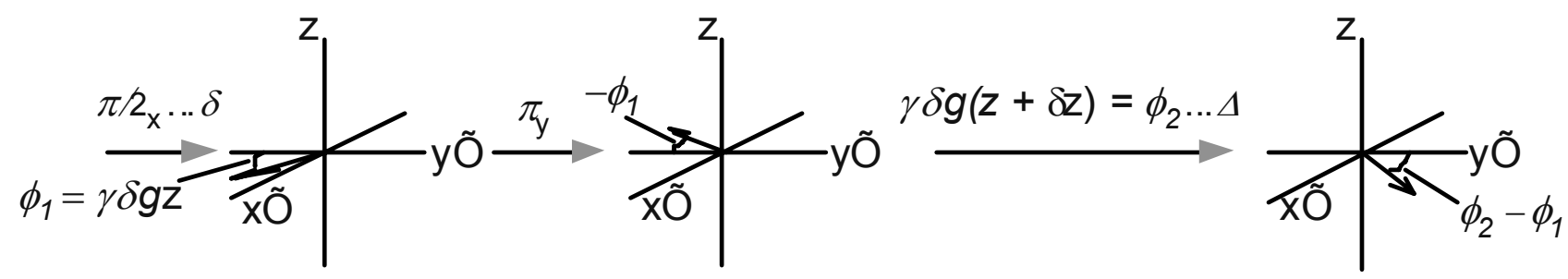
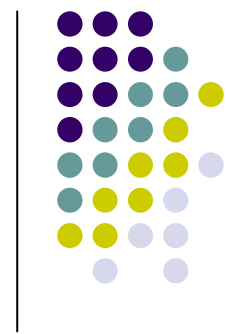
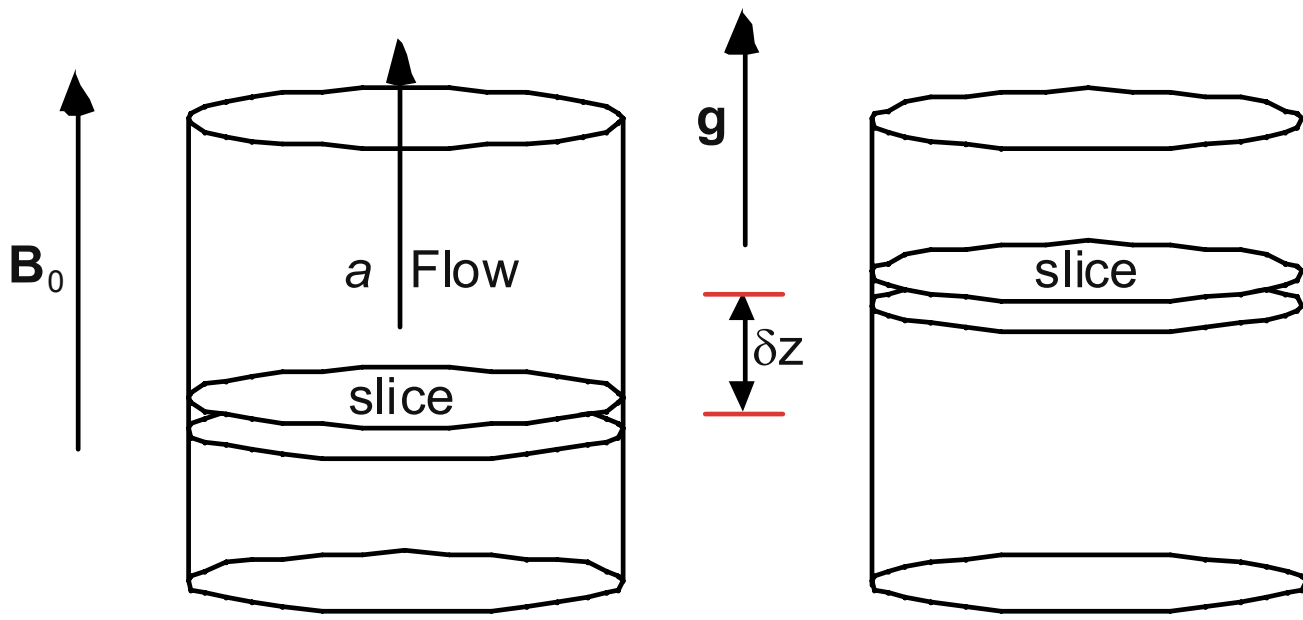
Movie showing change in shape of the mean cell diameter

QuickTime™ and a decompressor are needed to see this picture.

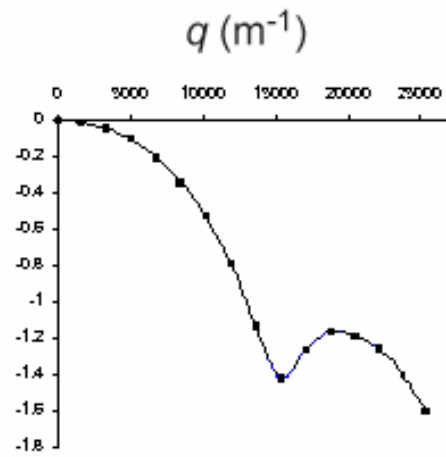
$z$  ( $\mu\text{m}$ )



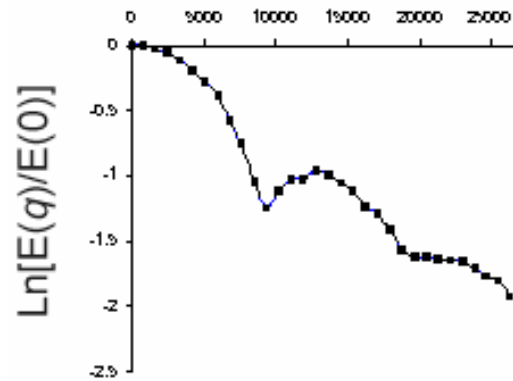
## *Flow diffraction*



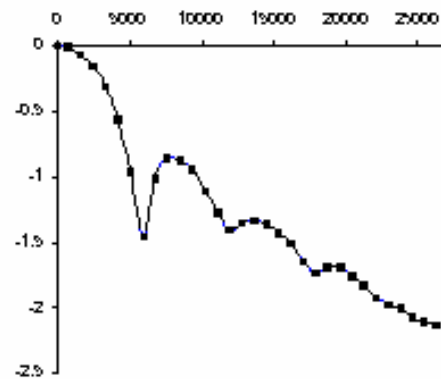




Flow rate =  $0.834 \text{ mm s}^{-1}$



$1.32 \text{ mm s}^{-1}$



$2.15 \text{ mm s}^{-1}$



Since the uniform linear flow-velocity is  $a \text{ m s}^{-1}$  then  $a = \delta z / \Delta$ ; and by definition  $\mathbf{q} = (1/2\pi) \gamma \delta \mathbf{g}$  so the change in phase angle brought about by flow is:

$$\begin{aligned}\Delta\phi &= 2 \pi q \delta z \\ &= 2 \pi q a \Delta\end{aligned}$$

Hence, the normalized signal  $S[q, \Delta]$  is proportional to,

$$S[q, \Delta] \propto \sin^2[2 \pi q a \Delta] / (2 \pi q a \Delta)^2$$

$$q_{\min, n} = n / (2 a \Delta)$$

$$a = n / (2 q_{\min, n} \Delta)$$



$$E[\mathbf{g}, \Delta] = \int \rho[\mathbf{r}_0] \Delta \exp[i \delta \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_0)] d\mathbf{r} d\mathbf{r}_0$$

$$E[\mathbf{q}, \Delta] = \iint \rho[\mathbf{r}_0] P[\mathbf{r}_0 | \mathbf{r}_0 + \mathbf{R}, \Delta] \exp[i 2 \pi \mathbf{q} \cdot \mathbf{R}] d\mathbf{r}_0 d\mathbf{R}$$

$$\bar{P}[\mathbf{R}, \Delta] = \int \rho[\mathbf{r}_0] P[\mathbf{r}_0 | \mathbf{r}_0 + \mathbf{R}, \Delta] d\mathbf{r}_0$$

$$E[\mathbf{q}, \Delta] = \int \bar{P}[\mathbf{R}, \Delta] \exp[i 2 \pi \mathbf{q} \cdot \mathbf{R}] d\mathbf{R}$$

$$\bar{P}[\mathbf{R}, \Delta] = \int E[\mathbf{q}, \Delta] \exp[-i 2 \pi \mathbf{q} \cdot \mathbf{R}] d\mathbf{q}$$

$$E[\mathbf{q}, \infty] = \int \rho[\mathbf{r}_0] \exp[i 2 \pi \mathbf{q} \cdot \mathbf{r}_0] d\mathbf{r}_0 \int \rho[\mathbf{r}] \exp[i 2 \pi \mathbf{q} \cdot \mathbf{r}] d\mathbf{r}$$

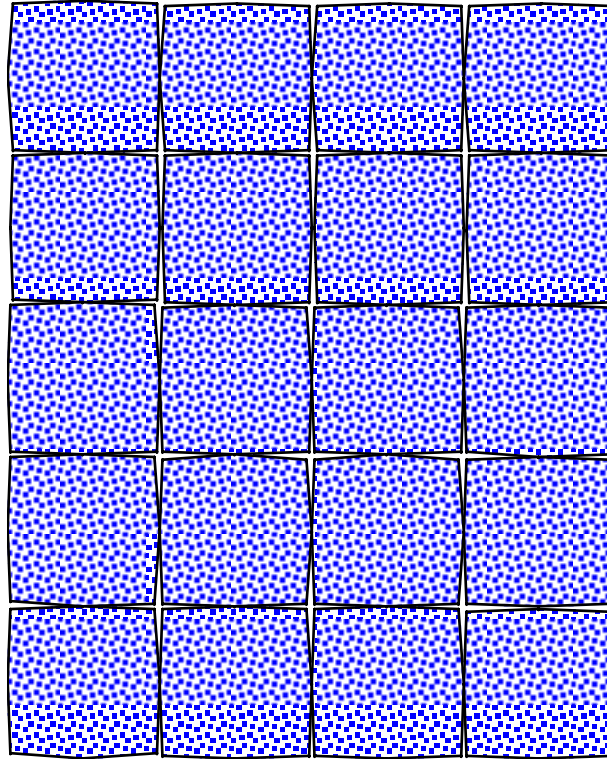
$$E[\mathbf{q}, \infty] = S^*[\mathbf{q}] S[\mathbf{q}] = |S[\mathbf{q}]|^2$$

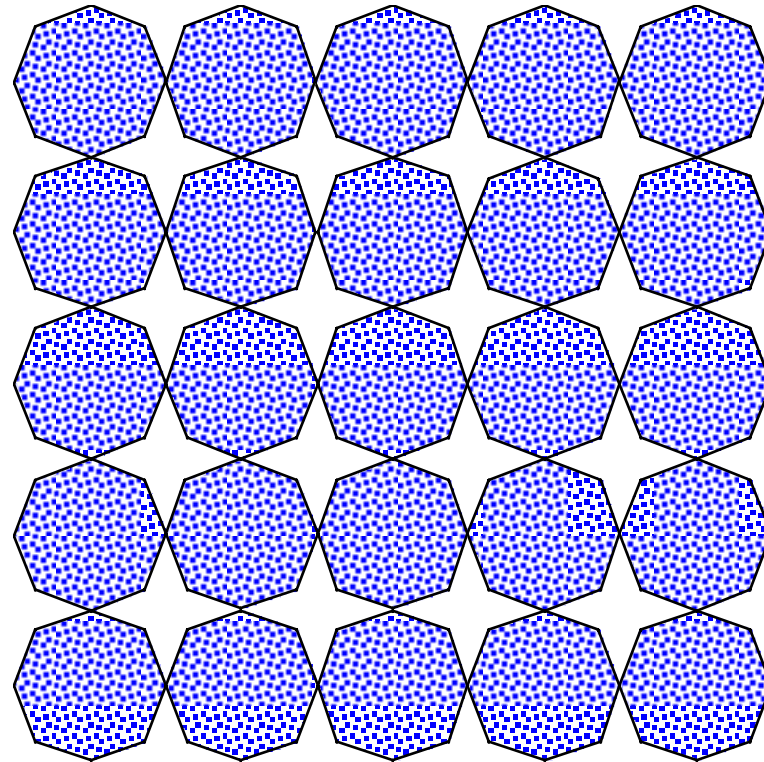


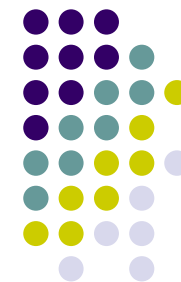
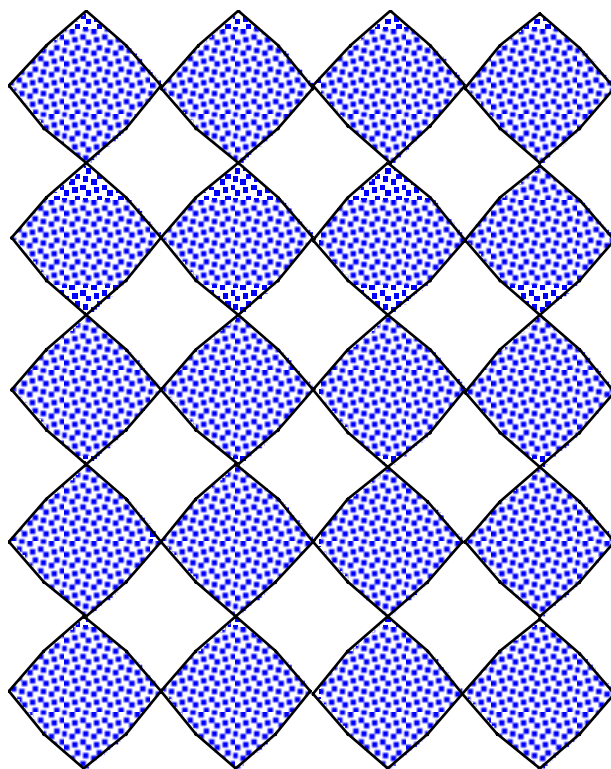
*A model of variable packing density*

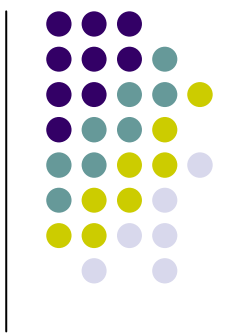
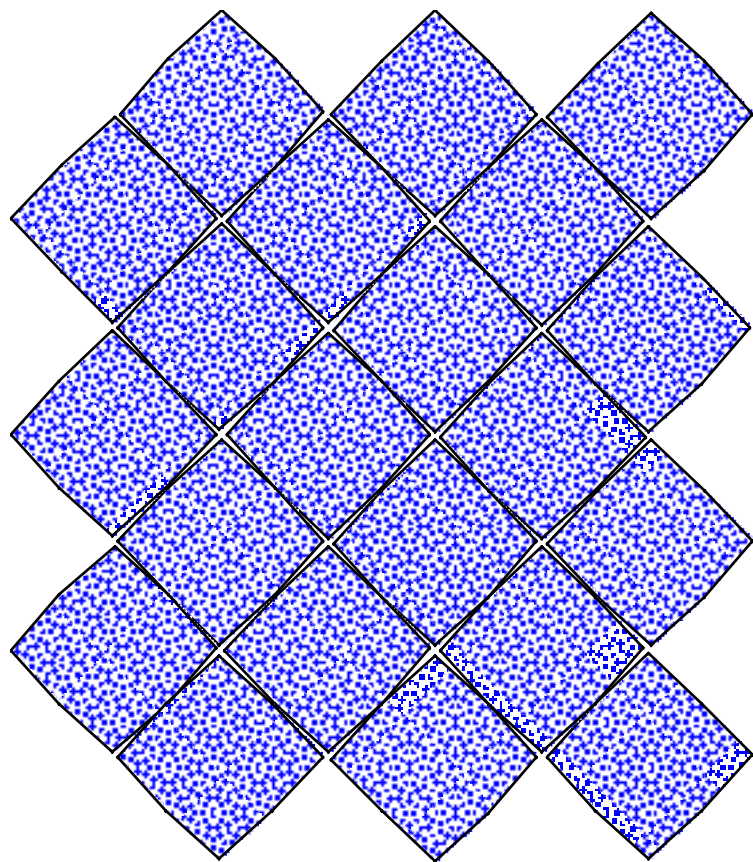
*q-space plot results*

*...octagon-star system*

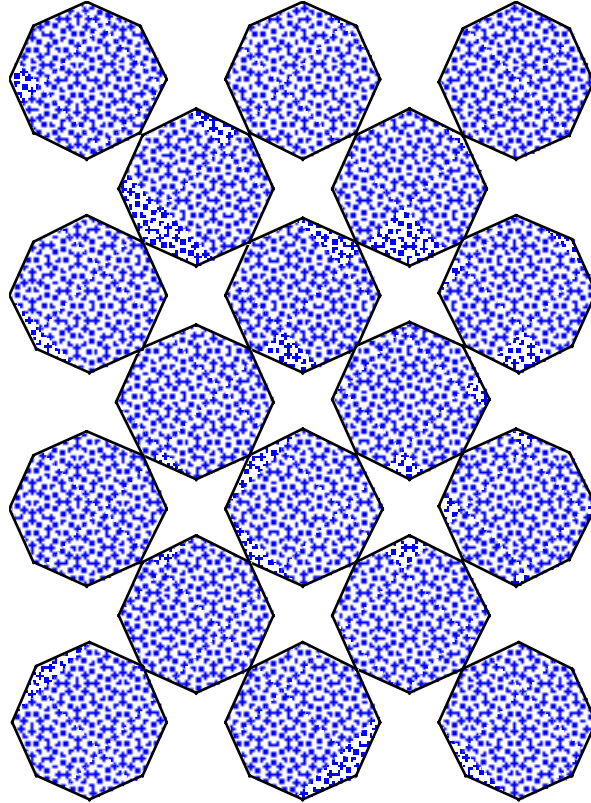


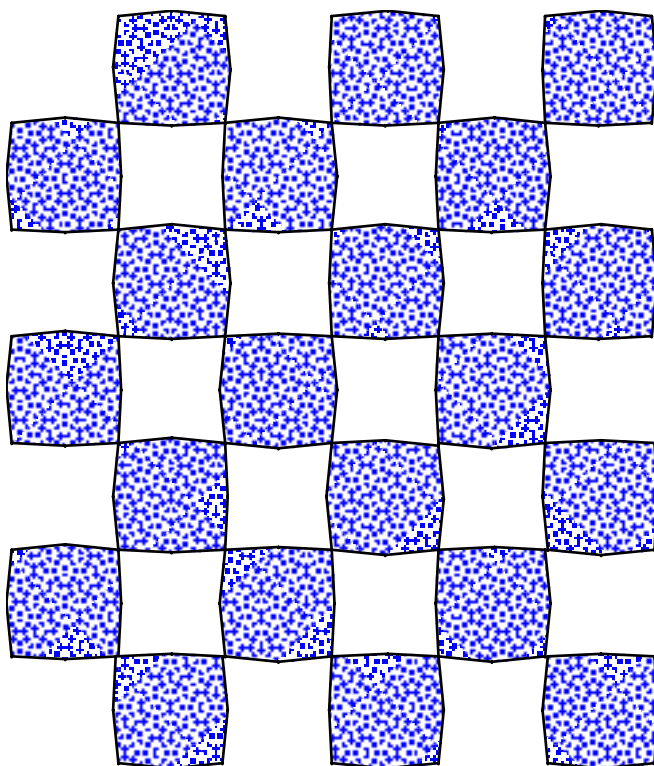




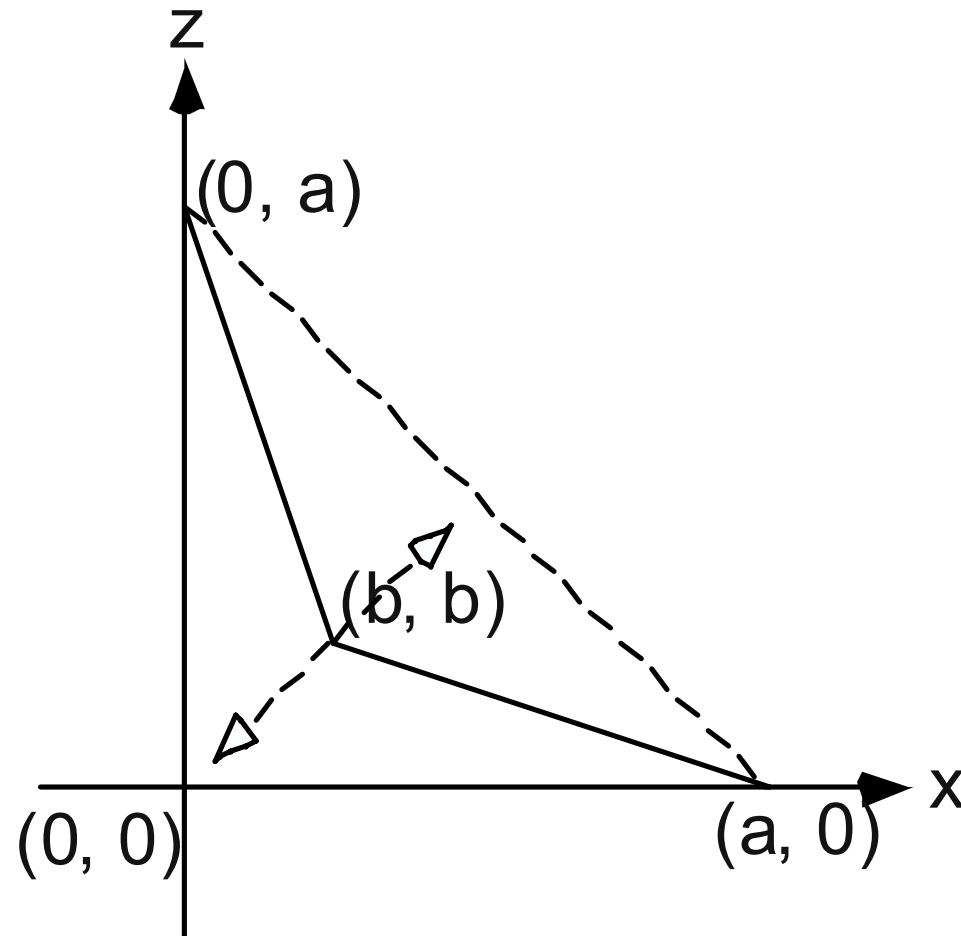




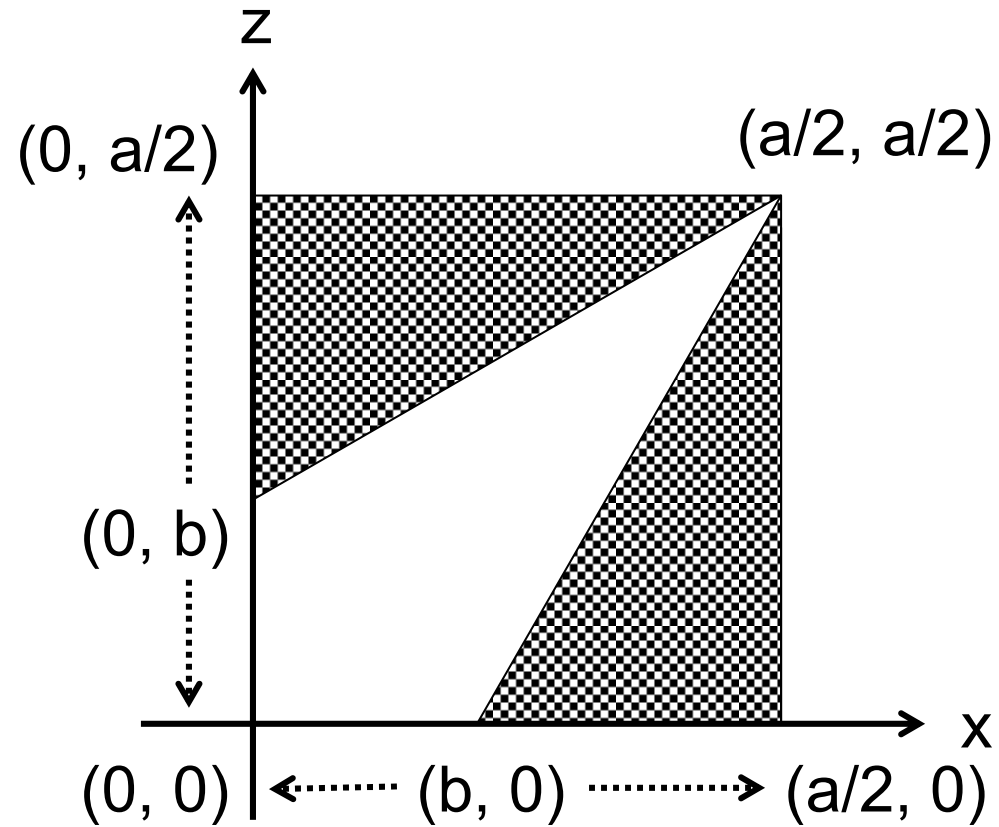




# Construction element for $q$ -space signal intensity for octagon-star model



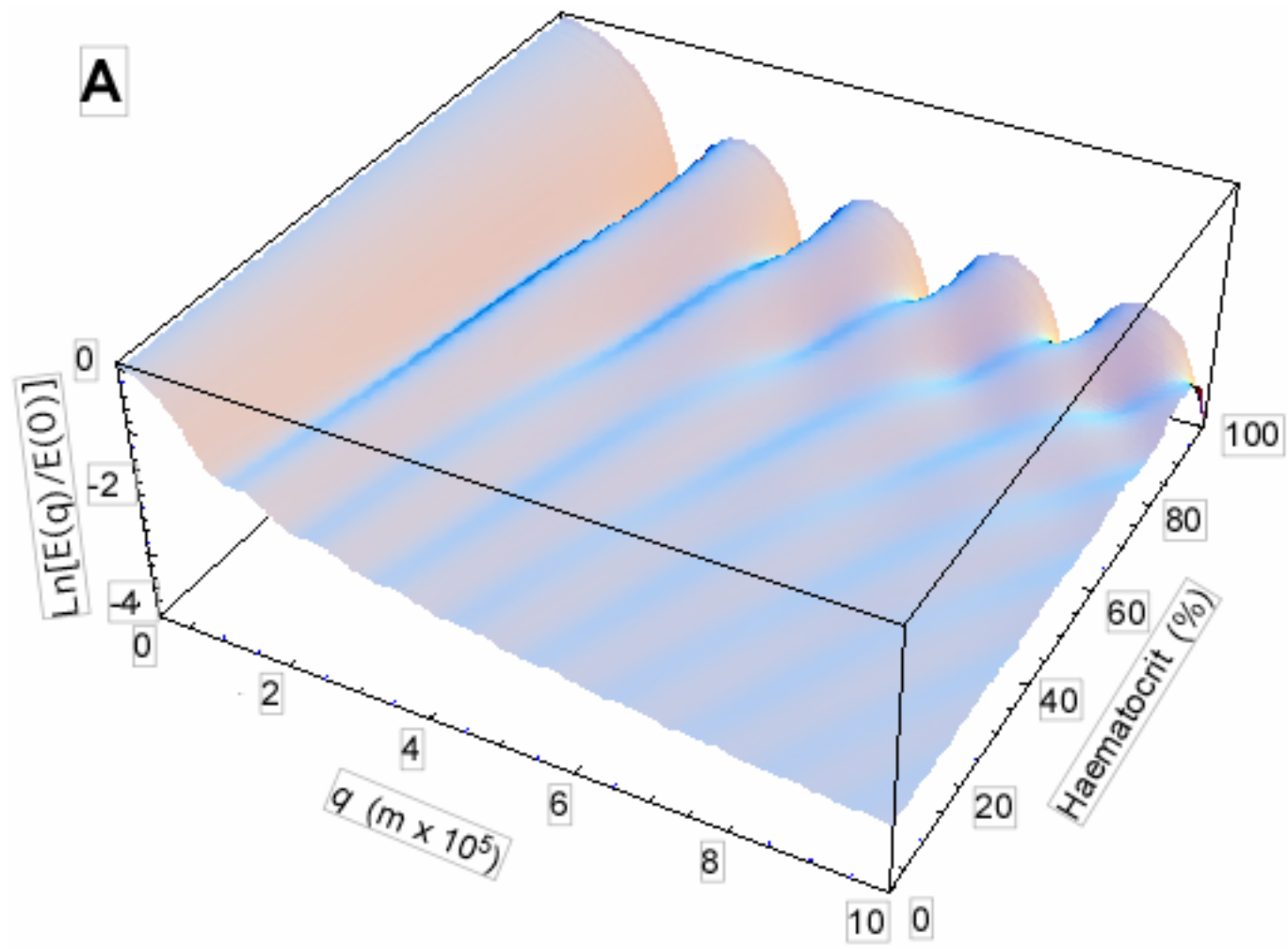
Construction element for  $q$ -space signal intensity for octagon-star model...90° rotation



# Expression for $q$ -space signal intensity from stars alone

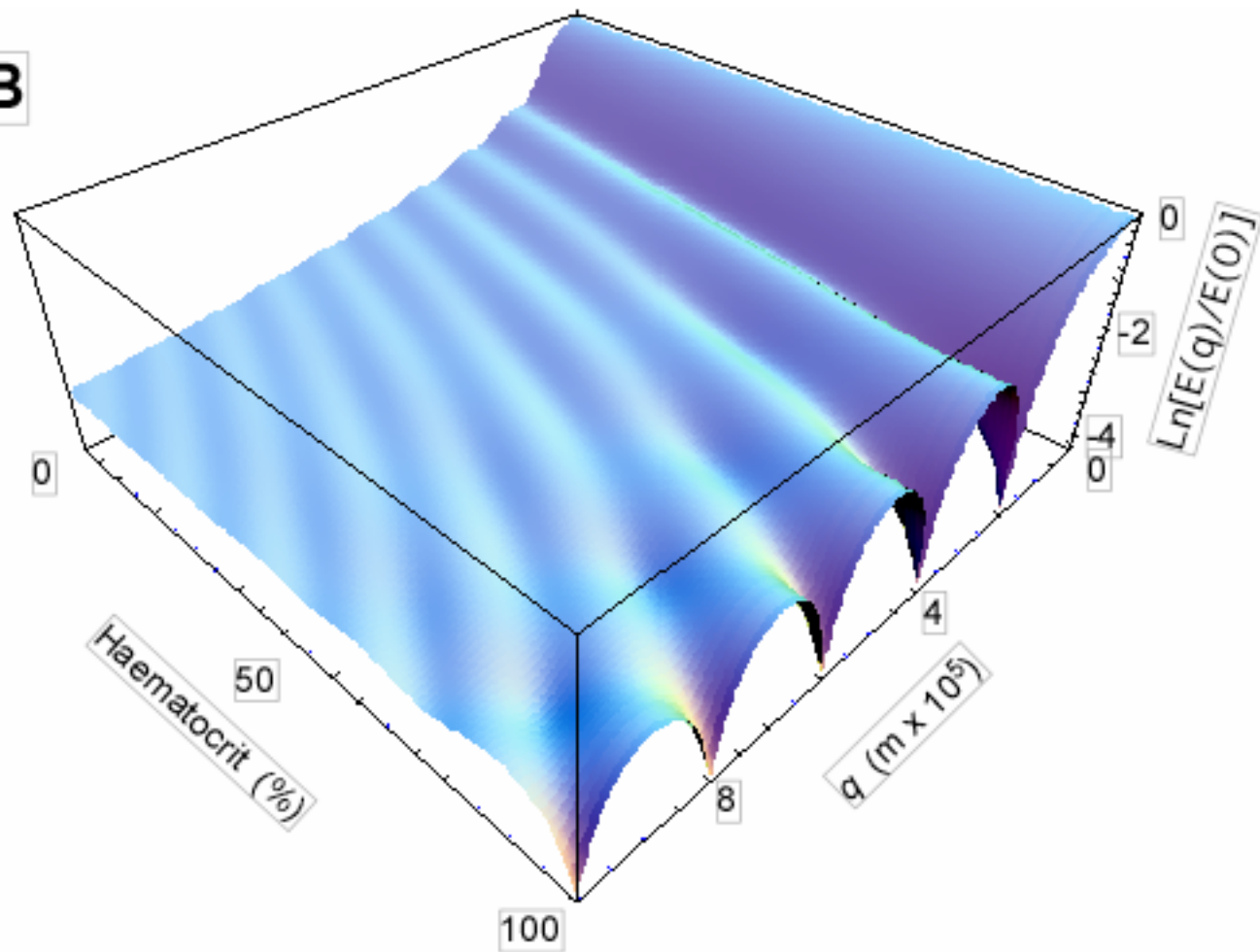


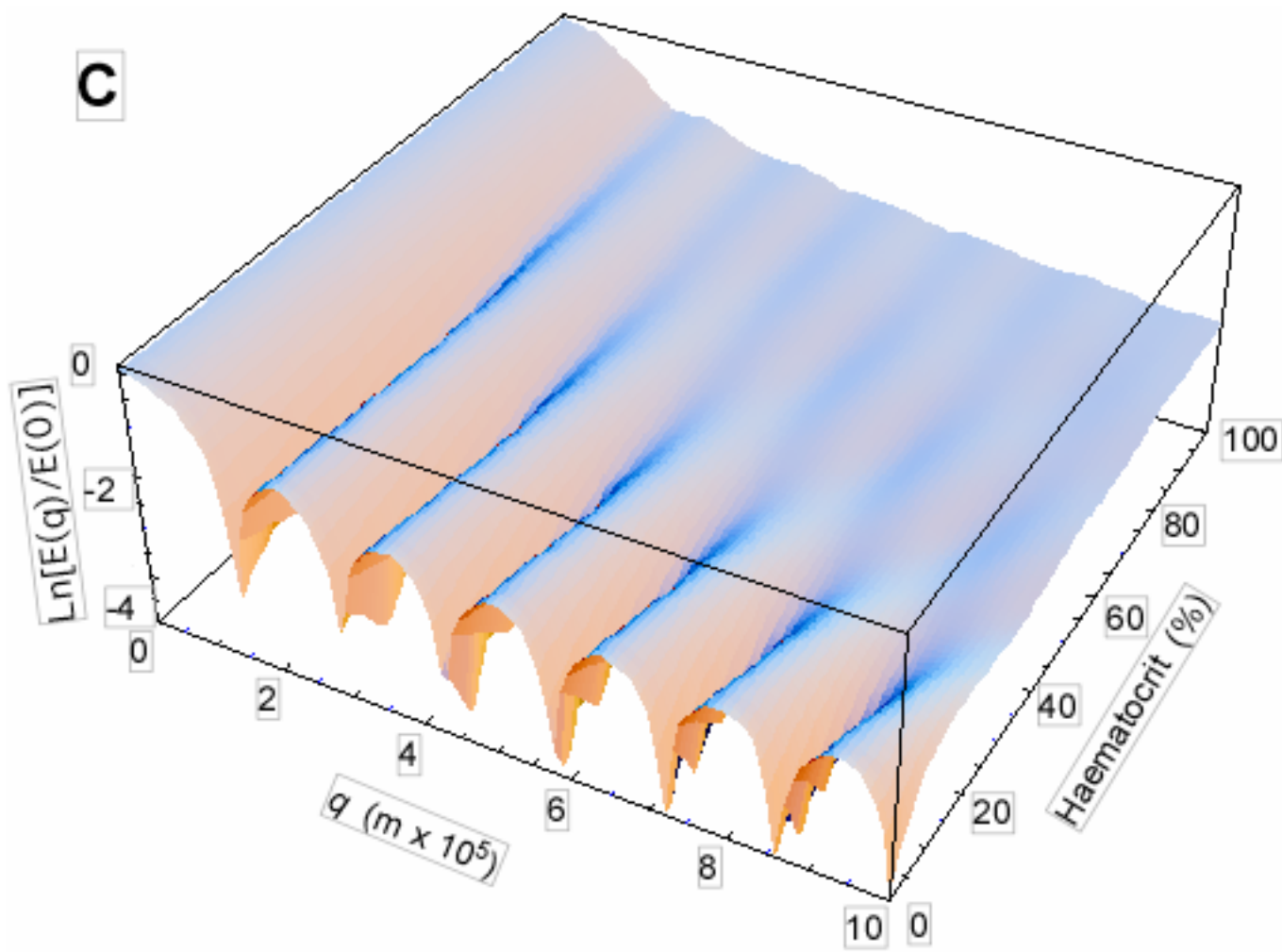
$$E_{star}[q, \infty] = \frac{1}{8a^2(a-2b)^2\pi^4q^4} \times \left( \begin{aligned} &a^4 - 4a^3b + 20a^2b^2 - 32ab^3 + 16b^4 + 2a^2(a-2b)^2b^2\pi^2q^2 - a^2(a-2b)^2\cos[2b\pi q] + \\ &4(a-b)b \left( (a-2b)^2\cos[a\pi q] - a \left( a\cos[(a-2b)\pi q] + 2(a-2b)b\pi q\sin[a\pi q] \right) \right) + \\ &2a^3(a-2b)b\pi q\sin[2b\pi q] \end{aligned} \right)$$





**B**







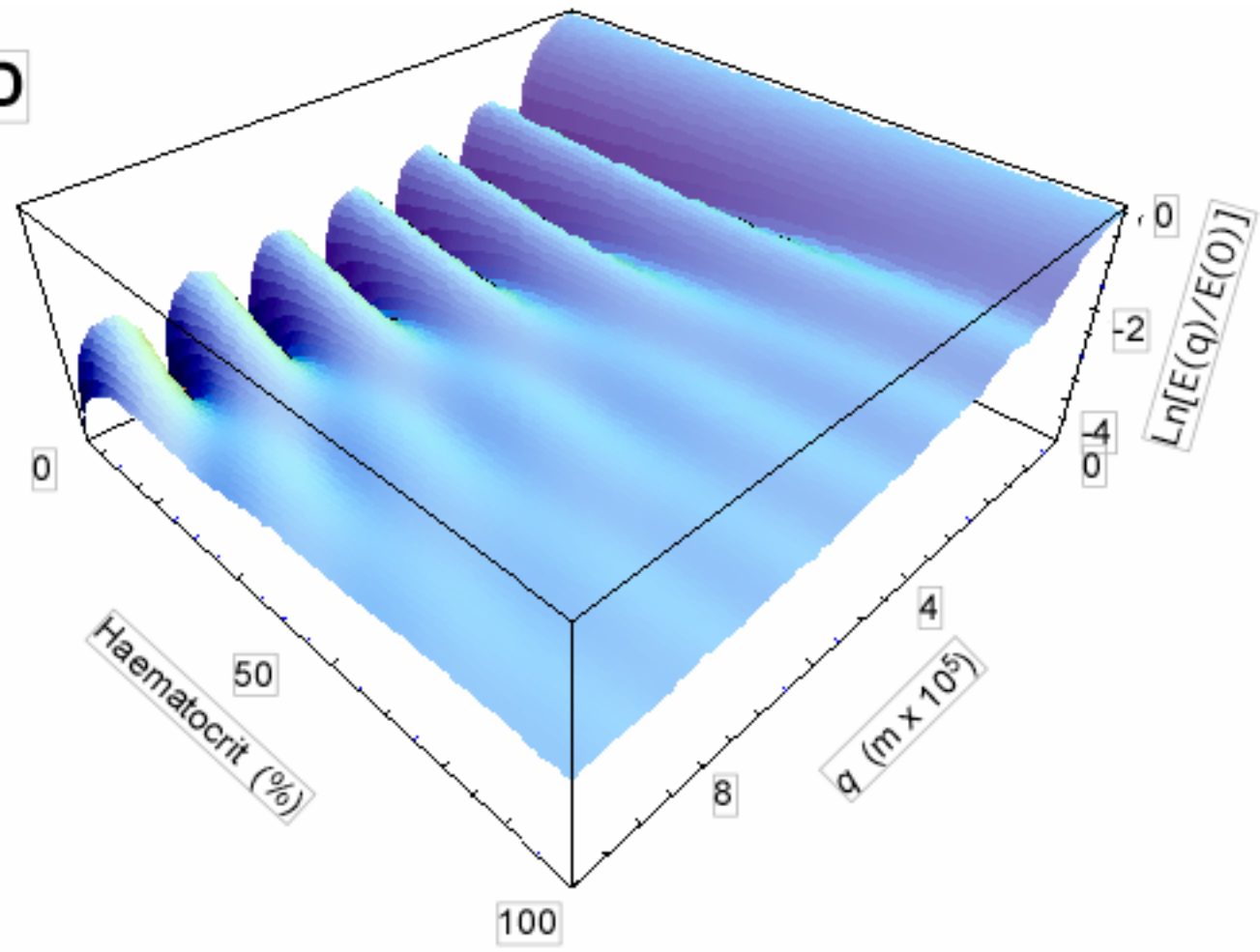
$q$ -space plot from octagon-star system as  $Ht$  increases



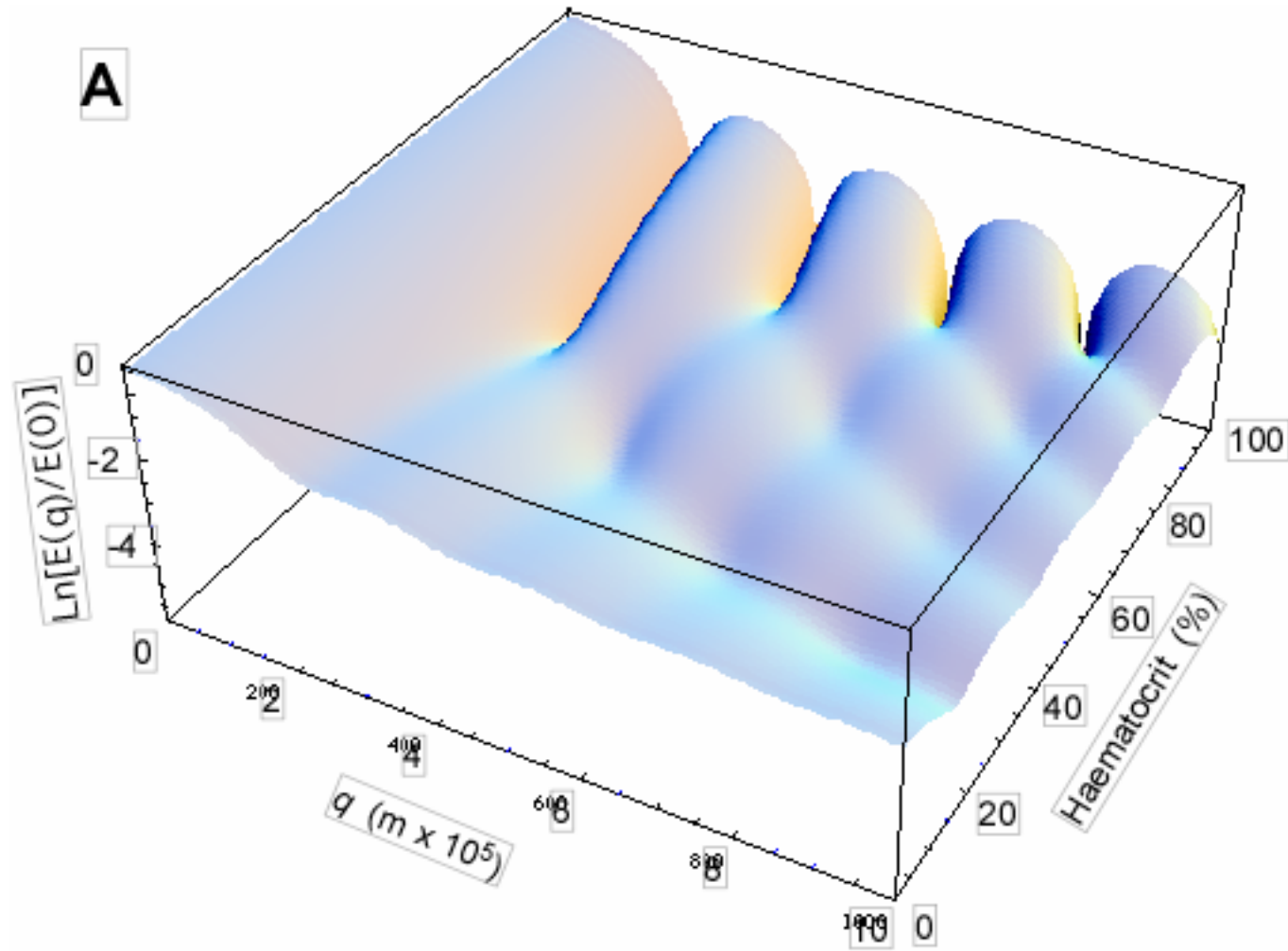
QuickTime™ and a  
decompressor  
are needed to see this picture.

Movie showing change in shape of the  $q$ -space  
plot-function as  $Ht$  is increased

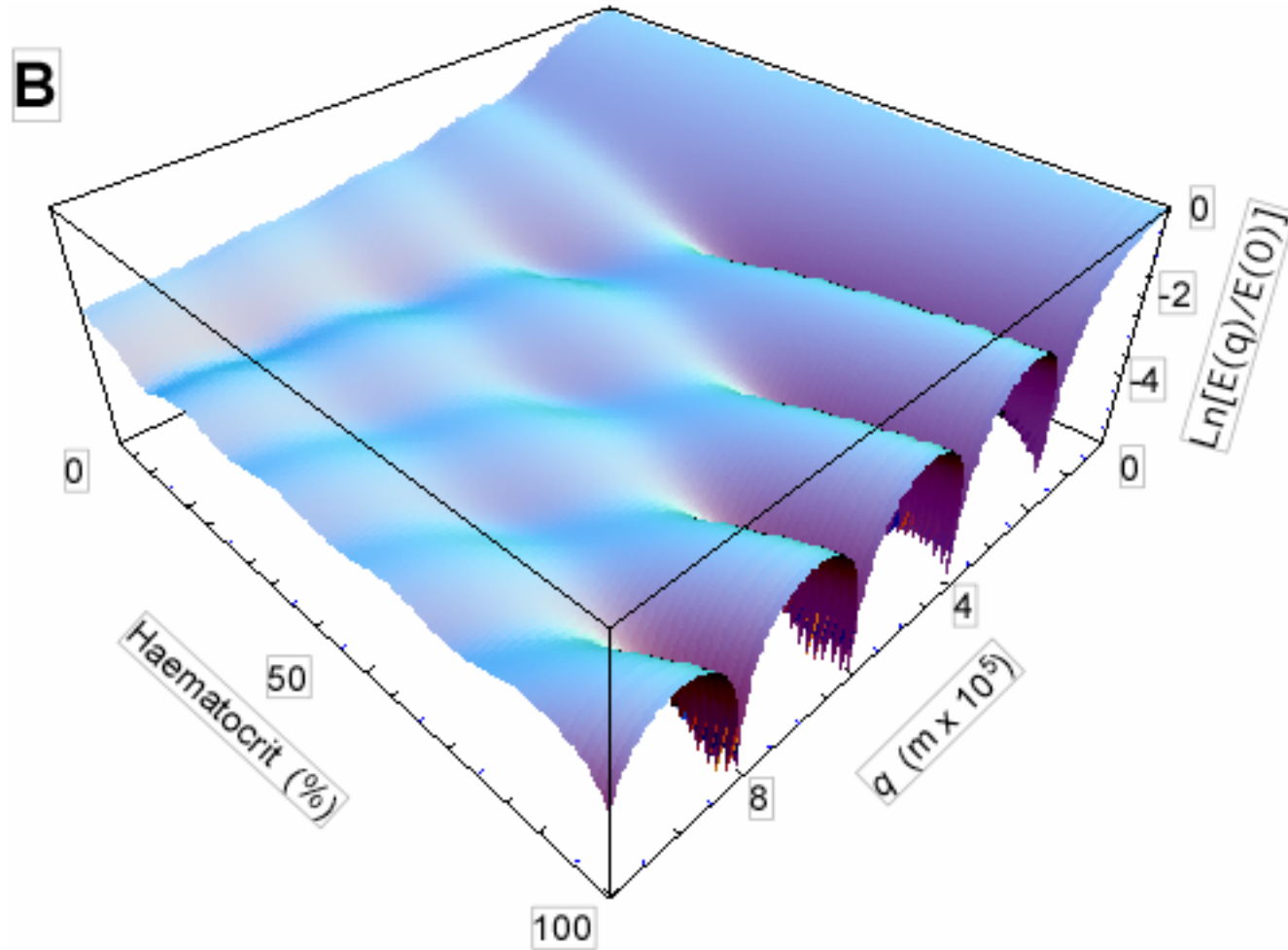
**D**



# $q$ -space plot from stars only



# $q$ -space plot from stars only



Thanks to past and present students...



TIFF (Uncompressed) are needed  
QuickTime™ and a  
TIFF (Uncompressed) decompressor  
are needed to see this picture.

QuickTime™ and a  
TIFF (Uncompressed) decompressor  
are needed to see this picture.

Bill Price is my name!



Bill Bubb	NMR
Bob Chapman	NMR
Tom Eykyn	NMR
David Jacques	DIC
Tim Larkin	<i>Mathematica</i>
Guilhem Pages	NMR & fast $q$ -space
David Regan	NMR & simulation
David Szekely	DIC & <i>Mathematica</i>

Chris Garvey  
Bill Price  
Peter Stilbs

# Grazie!

