First, some material for rewriting:

Page 20 2.2.6 new first paragraph: The simplest way to represent the results of x-ray data in real space is to Fourier transform the F(q\_z) form factors to obtain electron density profiles rho(z). However, the rho(z) so obtained are on an arbitrary scale, Furthermore, no information is obtained regarding the location of component groups of the lipid or the location of added peptides. Finally, Fourier reconstruction requires knowing the phase factors of individual reflections, although this latter concern is alleviated when diffuse scattering is obtained as the zeros in I(q\_z) locate where the phase factors change sign. Modeling uses the intensities, not the phase factors, it obtains absolute electron densities, and it estimates where the different components of the system are located. Early so-called strip models used constant rho(z) in different z regions. This has been improved by using error functions to smear the artificially sharp edges of the strip model. (Heinrich) When the width of the error function interface is wide enough and the edges are close together, the profile is quite similar to a Gaussian. Models consisting of sums of Gaussians have been used (White). A hybrid model used positive Gaussians for the headgroup and a negative Gaussian for the terminal methyl region superimposed on a modulated baseline for the water and the hydrocarbon (Wiener, Suter and Nagle 1989), which was later replaced by error functions for the hydrocarbons and for water (Klauda et al., 2006). This lab now uses the SDP method which imposes a volumetric constraint to account for the water profile [92].

The SDP method is applicable to joint fitting of neutron and x-ray scattering data when a particular parsing of the component groups is employed. For x-ray scattering data alone, a different parsing similar is more appropriate. (Go to your 2nd paragraph)

p. 76, last sentence: The symmetric ripple phase has only reflection symmetry and not centrosymmetry, so the phase factors are complex, making structure determination much more difficult than for the asymmetric ripple phase which does have centrosymmetry which restricts the phase factors to +/- 1. We therefore focus on the asymmetric ripple phase. We also focus on DMPC over DPPC because it is experimentally difficult to avoid coexistence of the symmetric ripple phase with the asymmetric ripple phase. )go to your paragraph).

p. 176. (Keep 1st sentence) Interestingly, this theory paper [28] states that its results agree with the chain packing reported in PRE2003. However, PRE2003 showed the chains in the major side aligned along the normal as reproduced in Fig. 3.67, in disagreement with Fig. 5 in [28] which agrees with our result in Fig. 3.67. The chains in the minor arm in [28] are portrayed as disordered fluid-like, also in disagreement with PRE2003. We discuss the … next subsection. In view of the successful prediction of [28] of our new result for the major arm, this theory should provide insights into what causes the ripple phase. Unfortunately, there are 18 parameters in this Landau-Ginzburg theory. While many of the terms are understandable, others are difficult to interpret in terms of interactions between lipid molecules.

List pages/issues with major science to do:

Phase factors, including pattern recognition and thinking about how to use diffuse scattering.

p. 135 Area calculations from thickness.

p. 145 Area calculations from integrated headgroup electrons.

p. 178. Need I(q\_r) plots along radials to address tilted interdigitated and/or disordered minor side.

p. 180 WAXS theory for I(q\_r) plots

Think about how curvature and chain orientation (tilt divergence) in the kink region. Make large working figures of Fig. 3.67.