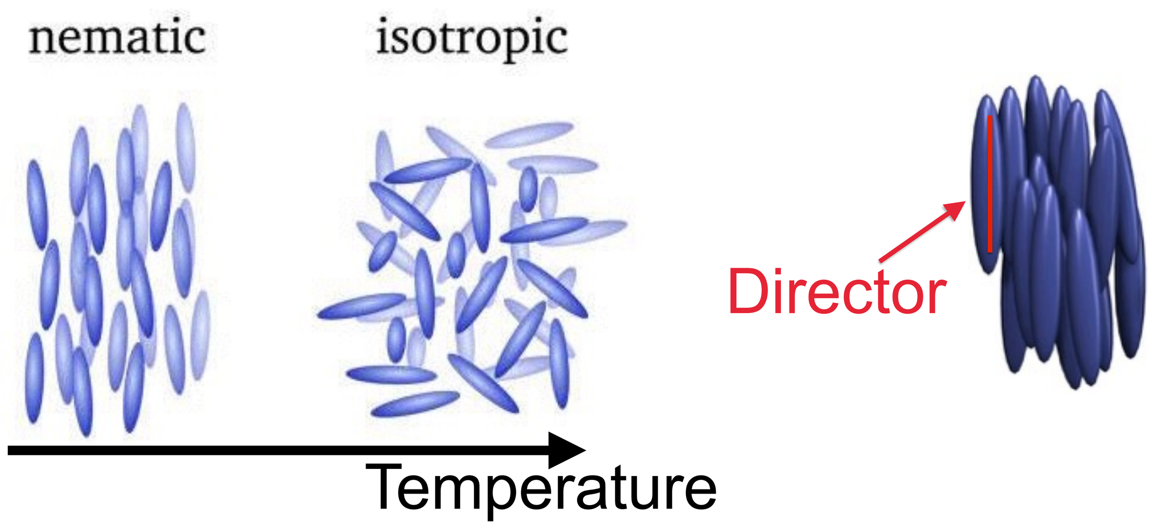
Semi-classical equations of motion for spin nematics

K. Remund[1], R.Pohle[1,2], J. Romhányi[1] and N. Shannon[1]

[1] Theory of Quantum Matter Unit, OIST, Okinawa, Japan
[2] Department of Applied Physics, The University Tokyo, Tokyo, Japan

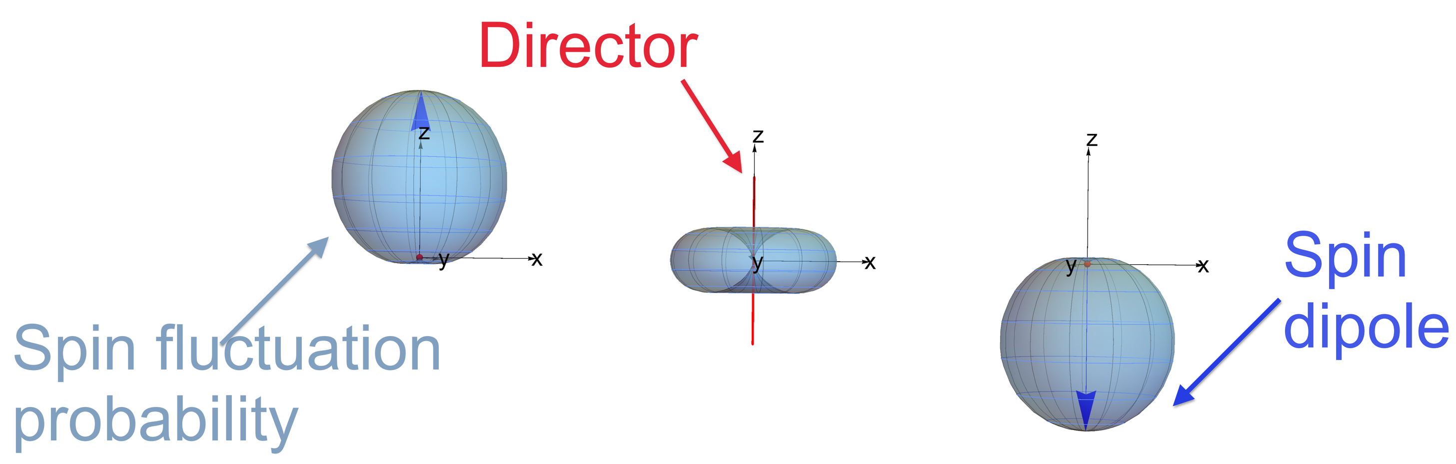
What is a Spin Nematic ?

Liquid Crystals



$$\langle Q^{\alpha\beta}\rangle = \langle d^\alpha d^\beta - \tfrac{1}{3}\delta^{\alpha\beta}\rangle$$

Magnets



$|S^z\rangle = |1\rangle$ $\quad |S^z\rangle = |0\rangle$ $\quad |S^z\rangle = |\bar{1}\rangle$

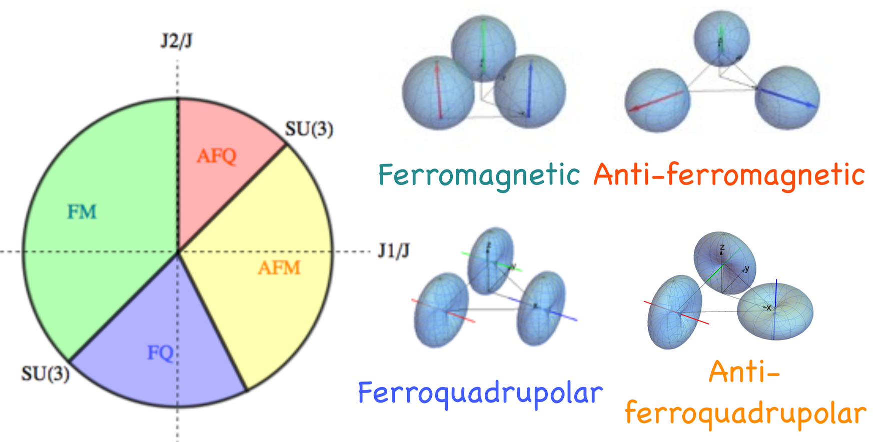
$$\langle Q^{\alpha\beta}\rangle = \langle S^\alpha S^\beta + S^\alpha S^\beta - \tfrac{2S(S+1)}{3}\delta^{\alpha\beta}\rangle$$

Equations of Motions

Model

$$\mathcal{H}_{BBQ} = \sum_{\langle i,j\rangle}\left(J_1 \hat{\mathbf{S}}_i\hat{\mathbf{S}}_j + J_2(\hat{\mathbf{S}}_i\hat{\mathbf{S}}_j)^2\right)$$

$J_1 = J\cos\theta \qquad J_2 = J\sin\theta$



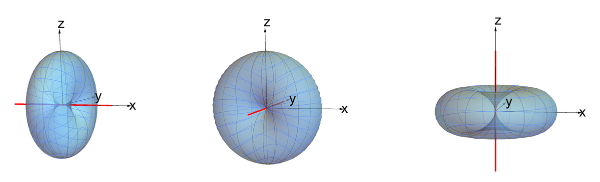
Mean-field diagram for a spin-1 described by the BBQ Hamiltonian on the triangular lattice [1,2,3]

Time-reversal invariant basis

$$|x\rangle = \frac{i}{\sqrt{2}}(|1\rangle - |\bar{1}\rangle)$$

$$|y\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |\bar{1}\rangle)$$

$$|z\rangle = -i|0\rangle$$



$|x\rangle \qquad |y\rangle \qquad |z\rangle$

Method

Introduce quadrupole operators **Q** that respect the symmetries of the nematic state [1,2,3]

$$\hat{Q}_i^{\alpha\beta} = \hat{S}_i^{\beta}\hat{S}_i^{\alpha} + \hat{S}_i^{\beta}\hat{S}_i^{\alpha} - \frac{2}{3}\delta^{\alpha\beta}s(s+1)$$

$$\begin{pmatrix}\hat{Q}_i^{x^2-y^2}\\ \hat{Q}_i^{3r^2-s^2}\\ \hat{Q}_i^{xy}\\ \hat{Q}_i^{yz}\\ \hat{Q}_i^{xz}\end{pmatrix} = \begin{pmatrix}\hat{S}_i^{x2} - \hat{S}_i^{y2}\\ \frac{1}{\sqrt{3}}(2\hat{S}_i^{z2} - \hat{S}_i^{x2} - \hat{S}_i^{y2})\\ \hat{S}_i^x\hat{S}_i^y + \hat{S}_i^y\hat{S}_i^x\\ \hat{S}_i^y\hat{S}_i^z + \hat{S}_i^z\hat{S}_i^y\\ \hat{S}_i^x\hat{S}_i^z + \hat{S}_i^z\hat{S}_i^x\end{pmatrix}$$

5 linearly independent components **Q**

$$\mathcal{H}_{BBQ} = \sum_{\langle i,j\rangle}\left(J_1 - \frac{J_2}{2}\right)\hat{S}_i^\alpha\hat{S}_j^\alpha + \frac{J_2}{4}\left(\hat{Q}_i^{\alpha\beta}\hat{Q}_j^{\beta\alpha}\right)$$

Following ref. [4]

Spin length constraint

8 generators of the algebra su(3): 3 linearly independent components **S**; 5 linearly independent components **Q**

$$\begin{pmatrix}\hat{\mathbf{S}}_i{}^2\\ \hat{S}_i^x\\ \hat{S}_i^y\\ \hat{S}_i^z\\ \hat{Q}_i^{x^2-y^2}\\ \hat{Q}_i^{3r^2-s^2}\\ \hat{Q}_i^{xy}\\ \hat{Q}_i^{yz}\\ \hat{Q}_i^{xz}\end{pmatrix} \rightarrow \begin{pmatrix}\hat{A}_i{}^1{}_1\\ \hat{A}_i{}^1{}_2\\ \hat{A}_i{}^1{}_3\\ \hat{A}_i{}^2{}_1\\ \hat{A}_i{}^2{}_2\\ \hat{A}_i{}^2{}_3\\ \hat{A}_i{}^3{}_1\\ \hat{A}_i{}^3{}_2\\ \hat{A}_i{}^3{}_3\end{pmatrix}$$

9 generators of the algebra u(3)

$$\hat{S}_i^\alpha = -i\epsilon^\alpha{}_\beta{}^\gamma \hat{A}_i{}^\beta{}_\gamma$$

$$\hat{Q}_i^{\alpha\beta} = -\hat{A}_i{}^\alpha{}_\beta - \hat{A}_i{}^\beta{}_\alpha + \frac{2}{3}\delta^{\alpha\beta}\hat{A}_i{}^\gamma{}_\gamma$$

The Hamiltonian is rewritten as $\mathcal{H}_{BBQ} = \sum_{\langle i,j\rangle}\left(J_1\hat{A}_i{}^\alpha{}_\beta\hat{A}_j{}^\beta{}_\alpha + (J_2 - J_1)\hat{A}_i{}^\alpha{}_\beta\hat{A}_j{}^\alpha{}_\beta + \frac{J_2}{4}s^2(s+1)^2\right)$

Sum Rule

$$\hat{A}_i{}^\alpha{}_\beta\hat{A}_j{}^\beta{}_\alpha = \frac{1}{4}\hat{Q}_i^{\alpha\beta}\hat{Q}_j^{\beta\alpha} + \frac{1}{2}\hat{S}_i^\alpha\hat{S}_j^\alpha + \frac{1}{4}s^2(s+1)^2$$

Closure of the Algebra u(3)

$$\left[\hat{A}_i{}^\alpha{}_\beta, \hat{A}_i{}^\gamma{}_\eta\right] = \delta^\gamma{}_\beta\hat{A}_i{}^\alpha{}_\eta - \delta^\alpha{}_\eta\hat{A}_i{}^\gamma{}_\beta$$

Equation of Motion

$$i\hbar\partial_t\hat{A}_i{}^\gamma{}_\eta = \left[\hat{A}_i{}^\gamma{}_\eta, \mathcal{H}_{BBQ}\right]$$

$$= \sum_\delta\Big(J_1(\hat{A}_i{}^\gamma{}_\alpha\hat{A}_{i+\delta}{}^\alpha{}_\eta - \hat{A}_i{}^\alpha{}_\eta\hat{A}_{i+\delta}{}^\gamma{}_\alpha) + (J_2 - J_1)(\hat{A}_i{}^\gamma{}_\alpha\hat{A}_{i+\delta}{}^\eta{}_\alpha - \hat{A}_i{}^\alpha{}_\eta\hat{A}_{i+\delta}{}^\alpha{}_\gamma)\Big)$$

Dispersion Relation for the Ferroquadrupolar State

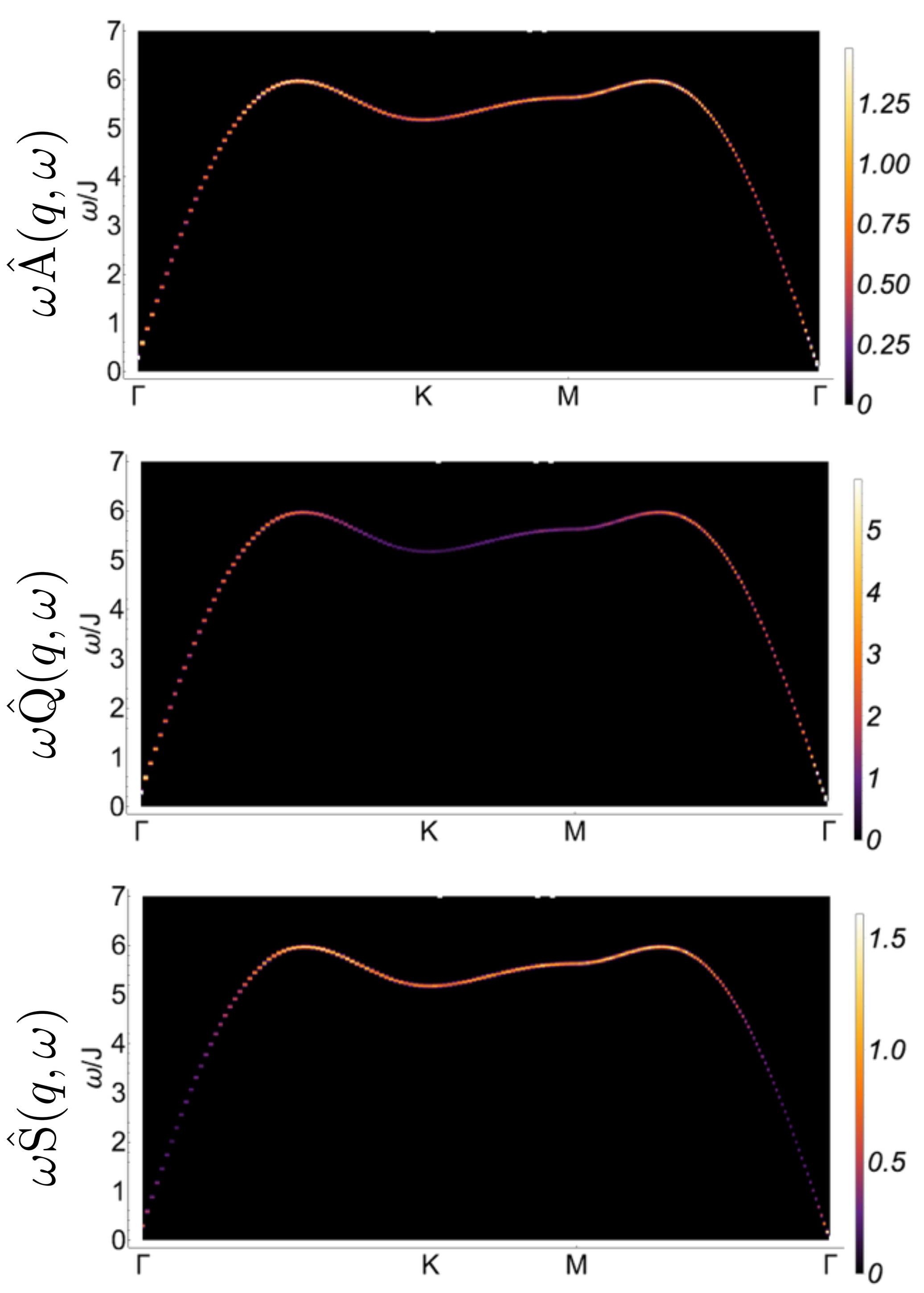
$$\omega_{\mathbf{k}} = +\sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}$$

$$A_{\mathbf{k}} = z(J_1\gamma(\mathbf{k}) - J_2) \qquad B_{\mathbf{k}} = z\gamma(\mathbf{k})(J_2 - J_1)$$

$$\gamma(\mathbf{k}) = \frac{1}{z}\sum_\delta e^{-i\mathbf{k}\delta}$$

Application to the Ferroquadrupolar State

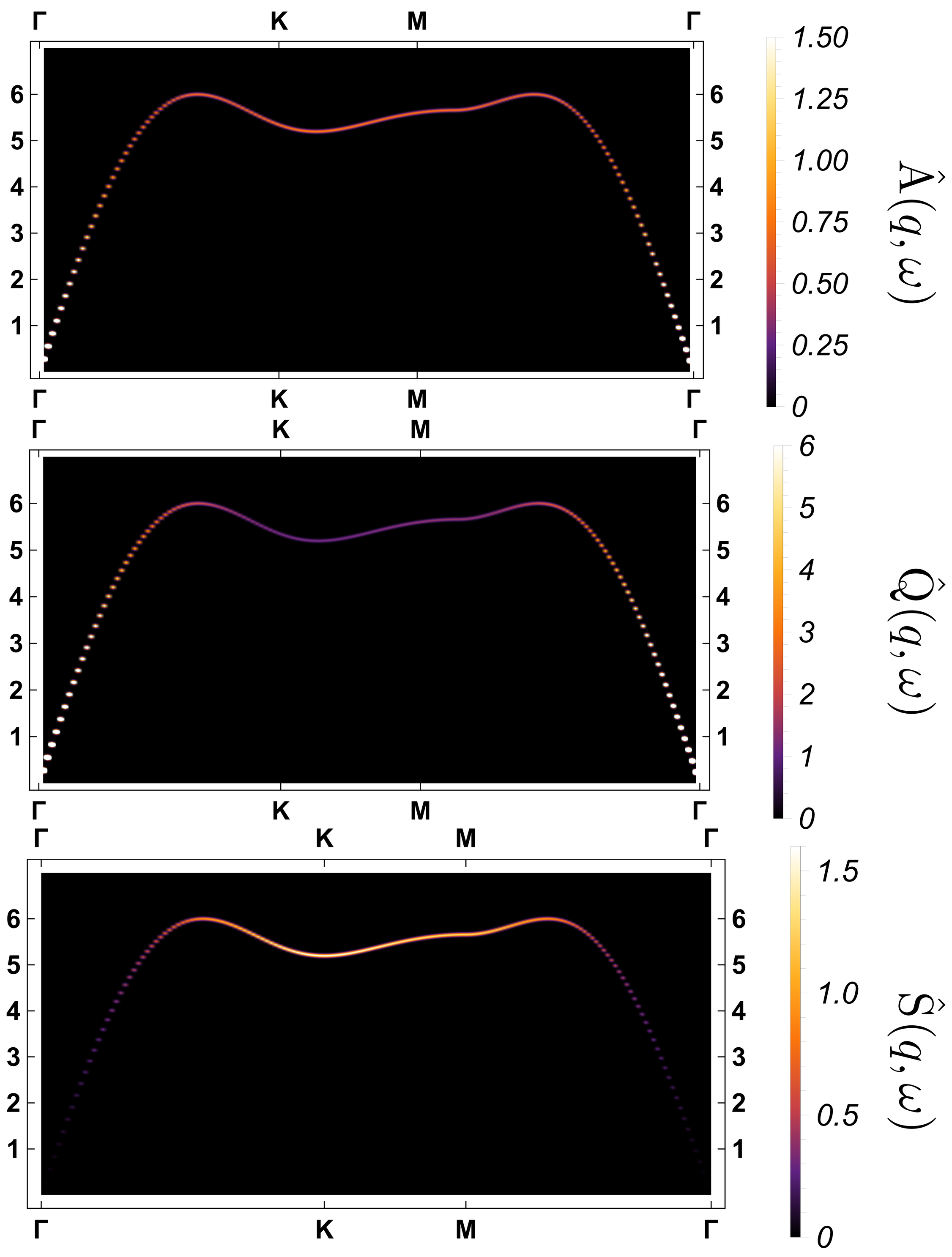
Molecular Dynamics using the Equations of Motion



Molecular dynamics simulations from numerical integration of EoM for U(3) matrices, $\hat{A}_i{}^\alpha{}_\beta$. Initial configurations of $\hat{A}_i{}^\alpha{}_\beta$ are drawn from classical Monte Carlo simulations of $\mathcal{H}_{BBQ}$ at temperature $T = 0.01J$

Results for spin dynamics compare well with QMC [5].

Flavor-wave Theory



Dynamical Structure Factors

$$\hat{\xi}(\mathbf{q},\omega) = \left|\langle gs|\hat{\xi}^{\alpha\beta}|ex\rangle\right|^2\delta(\omega - \omega_{\mathbf{q}}))$$

$$\hat{A}\ (\mathbf{q},\omega) = 2\frac{A_{\mathbf{q}}}{\sqrt{A_{\mathbf{q}}^2 - B_{\mathbf{q}}^2}} \qquad \hat{S}(\mathbf{q},\omega) = 2\frac{\sqrt{A_{\mathbf{q}} + B_{\mathbf{q}}}}{\sqrt{A_{\mathbf{q}} - B_{\mathbf{q}}}}$$

$$\hat{Q}(\mathbf{q},\omega) = 4\frac{\sqrt{A_{\mathbf{q}} - B_{\mathbf{q}}}}{\sqrt{A_{\mathbf{q}} + B_{\mathbf{q}}}}$$

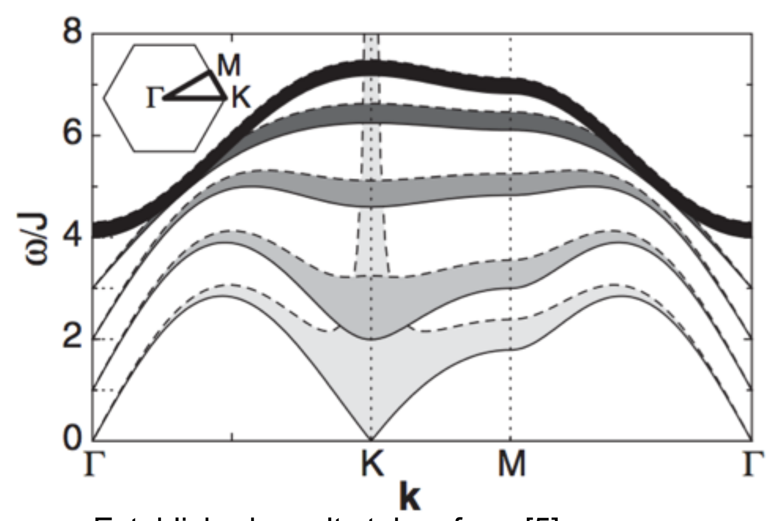
The sum rule is satisfied

The parameter for the Ferroquadrupolar state were chosen to be

$$\theta = \frac{3\pi}{2}$$

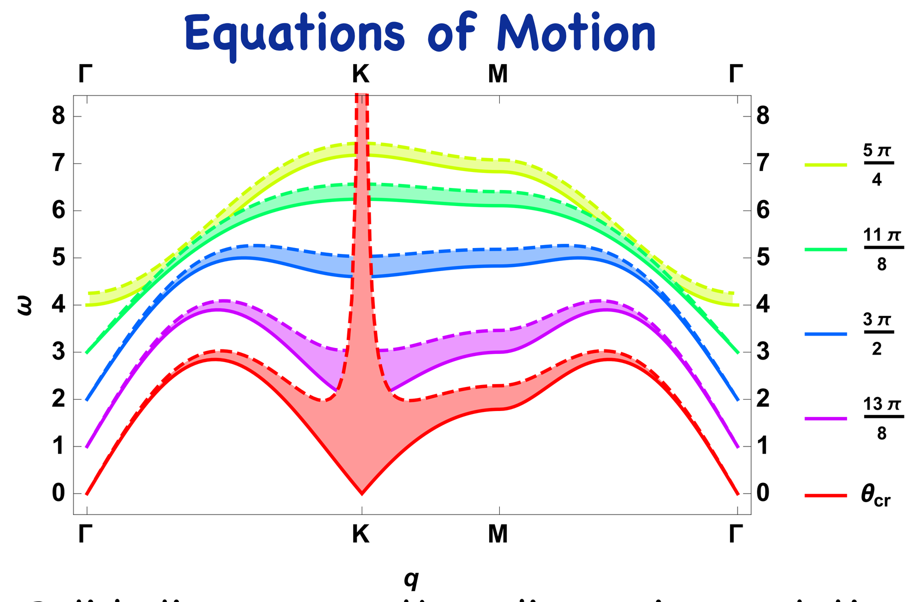
$$J = 1$$

Flavor-wave Theory



Established results taken from [5].

Equations of Motion



Solid lines are the dispersion relations and dashed lines are the intensities of the spin-dipole dynamical structure factor.

Different curves represent different value of θ within the FQ state.

References

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[3] Lauchli et al., Phys. Rev. Lett. **97**, 087205 (2006)
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