Heisenberg model

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Contents

Chapter 1

Hessian for $E(\theta_{ij}, \phi_{ij})$

$E = -J1/2 \sum_{ij} \vec{S}_{i,j}\vec{S}_{i+1,j} + \vec{S}_{i,j}\vec{S}_{i,j+1} + J2/2 \sum_{ij} \vec{S}_{i,j}\vec{S}_{i+1,j+1} + J4/2 \sum_{ij} \vec{S}_{i,j}\vec{S}_{i+2,j} + \vec{S}_{i,j}\vec{S}_{i,j+2}$

First element of the Hessian:

$$a_{11} = \begin{pmatrix} \frac{\partial^2 E}{\partial \theta_{11}^2} & \frac{\partial^2 E}{\partial \theta_{11}\partial \phi_{11}} & \frac{\partial^2 E}{\partial \theta_{11}\partial \theta_{12}} & \frac{\partial^2 E}{\partial \theta_{11}\partial \phi_{12}} & \frac{\partial^2 E}{\partial \theta_{11}\partial \theta_{13}} & \frac{\partial^2 E}{\partial \theta_{11}\partial \phi_{13}} & \frac{\partial^2 E}{\partial \theta_{11}\partial \theta_{14}} & \frac{\partial^2 E}{\partial \theta_{11}\partial \phi_{14}} \\ \frac{\partial^2 E}{\partial \phi_{11}\partial \theta_{11}} & \frac{\partial^2 E}{\partial \phi_{11}^2} & \frac{\partial^2 E}{\partial \phi_{11}\partial \theta_{12}} & \frac{\partial^2 E}{\partial \phi_{11}\partial \phi_{12}} & \frac{\partial^2 E}{\partial \phi_{11}\partial \theta_{13}} & \frac{\partial^2 E}{\partial \phi_{11}\partial \phi_{13}} & \frac{\partial^2 E}{\partial \phi_{11}\partial \theta_{14}} & \frac{\partial^2 E}{\partial \phi_{11}\partial \phi_{14}} \\ \frac{\partial^2 E}{\partial \theta_{12}\partial \theta_{11}} & \frac{\partial^2 E}{\partial \theta_{12}\partial \phi_{11}} & \frac{\partial^2 E}{\partial \theta_{12}^2} & \frac{\partial^2 E}{\partial \theta_{12}\partial \phi_{12}} & \frac{\partial^2 E}{\partial \theta_{12}\partial \theta_{13}} & \frac{\partial^2 E}{\partial \theta_{12}\partial \phi_{13}} & \frac{\partial^2 E}{\partial \theta_{12}\partial \theta_{14}} & \frac{\partial^2 E}{\partial \theta_{12}\partial \phi_{14}} \\ \frac{\partial^2 E}{\partial \phi_{12}\partial \theta_{11}} & \frac{\partial^2 E}{\partial \phi_{12}\partial \phi_{11}} & \frac{\partial^2 E}{\partial \phi_{12}\partial \theta_{12}} & \frac{\partial^2 E}{\partial \phi_{12}^2} & \frac{\partial^2 E}{\partial \phi_{12}\partial \theta_{13}} & \frac{\partial^2 E}{\partial \phi_{12}\partial \phi_{13}} & \frac{\partial^2 E}{\partial \phi_{12}\partial \theta_{14}} & \frac{\partial^2 E}{\partial \phi_{12}\partial \phi_{14}} \\ \frac{\partial^2 E}{\partial \theta_{13}\partial \theta_{11}} & \frac{\partial^2 E}{\partial \theta_{13}\partial \phi_{11}} & \frac{\partial^2 E}{\partial \theta_{13}\partial \theta_{12}} & \frac{\partial^2 E}{\partial \theta_{13}\partial \phi_{12}} & \frac{\partial^2 E}{\partial \theta_{13}^2} & \frac{\partial^2 E}{\partial \theta_{13}\partial \phi_{13}} & \frac{\partial^2 E}{\partial \theta_{13}\partial \theta_{14}} & \frac{\partial^2 E}{\partial \theta_{13}\partial \phi_{14}} \\ \frac{\partial^2 E}{\partial \phi_{13}\partial \theta_{11}} & \frac{\partial^2 E}{\partial \phi_{13}\partial \phi_{11}} & \frac{\partial^2 E}{\partial \phi_{13}\partial \theta_{12}} & \frac{\partial^2 E}{\partial \phi_{13}\partial \phi_{12}} & \frac{\partial^2 E}{\partial \phi_{13}\partial \theta_{13}} & \frac{\partial^2 E}{\partial \phi_{13}^2} & \frac{\partial^2 E}{\partial \phi_{13}\partial \theta_{14}} & \frac{\partial^2 E}{\partial \phi_{13}\partial \phi_{14}} \\ \frac{\partial^2 E}{\partial \theta_{14}\partial \theta_{11}} & \frac{\partial^2 E}{\partial \theta_{14}\partial \phi_{11}} & \frac{\partial^2 E}{\partial \theta_{14}\partial \theta_{12}} & \frac{\partial^2 E}{\partial \theta_{14}\partial \phi_{12}} & \frac{\partial^2 E}{\partial \theta_{14}\partial \theta_{13}} & \frac{\partial^2 E}{\partial \theta_{14}\partial \phi_{13}} & \frac{\partial^2 E}{\partial \theta_{14}^2} & \frac{\partial^2 E}{\partial \theta_{14}\partial \phi_{14}} \\ \frac{\partial^2 E}{\partial \phi_{14}\partial \theta_{11}} & \frac{\partial^2 E}{\partial \phi_{14}\partial \phi_{11}} & \frac{\partial^2 E}{\partial \phi_{14}\partial \theta_{12}} & \frac{\partial^2 E}{\partial \phi_{14}\partial \phi_{12}} & \frac{\partial^2 E}{\partial \phi_{14}\partial \theta_{13}} & \frac{\partial^2 E}{\partial \phi_{14}\partial \phi_{13}} & \frac{\partial^2 E}{\partial \phi_{14}\partial \theta_{14}} & \frac{\partial^2 E}{\partial \phi_{14}^2} \end{pmatrix} \tag{1.1}$$

$\frac{\partial^2 E}{\partial \theta_{ij}^2} = 0,\ \frac{\partial^2 E}{\partial \phi_{ij}^2} = 0,\ \frac{\partial^2 E}{\partial \theta_{ij}\partial \phi_{ij}} = 0, \quad when\ i = j$

$$\begin{aligned}
\frac{\partial^2 E}{\partial \theta_{ij}\partial \theta_{ij+1}} &= -J1/2[\cos\theta_{ij}\cos\theta_{ij+1} + \sin\theta_{ij}\sin\theta_{ij+1}\cos(\phi_{ij} - \phi_{ij+1})], \\
\frac{\partial^2 E}{\partial \phi_{ij}\partial \phi_{ij+1}} &= -J1/2[\cos\theta_{ij}\cos\theta_{ij+1}\cos(\phi_{ij} - \phi_{ij+1})], \\
\frac{\partial^2 E}{\partial \theta_{ij}\partial \phi_{ij+1}} &= -J1/2[\cos\theta_{ij}\sin\theta_{ij+1} + \sin\theta_{ij+1}\cos\theta_{ij+1}\sin(\phi_{ij} - \phi_{ij+1})], \\
\frac{\partial^2 E}{\partial \theta_{11}\partial \theta_{12}} &= -J1/2[\cos\theta_{11}\cos\theta_{12} + \sin\theta_{11}\sin\theta_{12}\cos(\phi_{11} - \phi_{12})], \\
\frac{\partial^2 E}{\partial \phi_{11}\partial \phi_{12}} &= -J1/2[\cos\theta_{11}\cos\theta_{12}\cos(\phi_{11} - \phi_{12})], \\
\frac{\partial^2 E}{\partial \theta_{11}\partial \phi_{12}} &= -J1/2[-\sin\theta_{11}\cos\theta_{12}\sin(\phi_{11} - \phi_{12})], \\
\frac{\partial^2 E}{\partial \theta_{12}\partial \phi_{11}} &= -J1/2[\sin\theta_{11}\cos\theta_{12}\sin(\phi_{11} - \phi_{12})].
\end{aligned}$$

Then, matrix (1.1) has following form:

$$a_{11} = -J1/2 \begin{pmatrix} 0 & 0 & \cos\theta_{11}\cos\theta_{12} + \sin\theta_{11}\sin\theta_{12}\cos(\phi_{11} - \phi_{12}) \\ 0 & 0 & \cos\theta_{11}\sin\theta_{12}\sin(\phi_{11} - \phi_{12}) \\ \cos\theta_{11}\cos\theta_{12} + \sin\theta_{11}\sin\theta_{12}\cos(\phi_{11} - \phi_{12}) & \cos\theta_{11}\sin\theta_{12}\sin(\phi_{12} - \phi_{11}) & 0 \\ -\sin\theta_{11}\cos\theta_{12}\sin(\phi_{11} - \phi_{12}) & \cos\theta_{12}\cos\theta_{11}\cos(\phi_{12} - \phi_{11}) & 0 \end{pmatrix} \tag{1.2}$$

$$Hess_{m,n} = \begin{pmatrix} a_{1,1} & 0 & 0 & 0 & \cdots & 0 \\ 0 & a_{2,2} & 0 & 0 & \cdots & 0 \\ 0 & 0 & a_{3,3} & 0 & \cdots & 0 \\ 0 & 0 & 0 & a_{4,4} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & a_{m,n} \end{pmatrix}$$