Problema 1: Modelo de Blume-Capel - Aproximación variacional

$$H = -J \sum_{\langle i,j \rangle} s_i s_j + D \sum_i s_i^2 \tag{1}$$

$$H_0 = -\eta \sum_i s_i + D \sum_i s_i^2 \tag{2}$$

Desigualdad de Bogoliuvob-Peierls:

$$f \leq f_\rho = f_0 + \frac{1}{N} \langle H - H_0 \rangle_0. \tag{3}$$

Función de partición para el hamiltoniano de prueba:

$$\begin{aligned}
\mathcal{Z}_0 &= \sum_{\{s_i\}} e^{-\beta H_0} \\
&= \sum_{\{s_i\}} \exp \left[\beta\eta \sum_i s_i - \beta D \sum_i s_i^2 \right] \\
&= \sum_{\{s_i\}} \prod_i \exp \left[\beta\eta s_i - \beta D s_i^2 \right] \\
&= \prod_i \sum_{s_i = 0, \pm 1} \exp \left[\beta\eta s_i - \beta D s_i^2 \right] \\
&= \left[1 + e^{-\beta\eta - \beta D} + e^{\beta\eta - \beta D} \right]^N \\
&= \left[1 + 2e^{-\beta D} \cosh(\beta\eta) \right]^N, \\
&= \mathcal{Z}_{01}^N,
\end{aligned} \tag{4}$$

donde

$$\mathcal{Z}_{01} = 1 + 2e^{-\beta D} \cosh(\beta\eta). \tag{5}$$

Energía libre:

$$\begin{aligned}
f_0 &= -\frac{1}{\beta N} \ln \mathcal{Z}_0 \\
&= -\frac{1}{\beta} \ln \left[1 + 2e^{-\beta D} \cosh(\beta\eta) \right]
\end{aligned} \tag{6}$$

Magnetización:

$$
\begin{aligned}
m_0 &= \langle s_i \rangle_0 \\
&= \frac{1}{\mathcal{Z}_{01}} \sum_{s_i=0,\pm 1} s_i e^{\beta \eta s_i - \beta D s_i^2} \\
&= \frac{1}{\mathcal{Z}_{01}} \left[-e^{-\beta\eta - \beta D} + e^{\beta\eta - \beta D} \right] \\
&= \frac{2e^{-\beta\eta} \sinh(\beta\eta)}{1 + 2e^{-\beta\eta} \cosh(\beta\eta)}
\end{aligned}
\tag{7}
$$

Segundo momento:

$$
\begin{aligned}
\langle s_i^2 \rangle_0 &= \frac{1}{\mathcal{Z}_{01}} \sum_{s_i=0,\pm 1} s_i^2 e^{\beta \eta s_i - \beta D s_i^2} \\
&= \frac{1}{\mathcal{Z}_{01}} \left[e^{-\beta\eta - \beta D} + e^{\beta\eta - \beta D} \right] \\
&= \frac{2e^{-\beta\eta} \cosh(\beta\eta)}{1 + 2e^{-\beta\eta} \cosh(\beta\eta)}
\end{aligned}
\tag{8}
$$

Valores medios de los hamiltonianos respecto del hamiltoniano de prueba:

$$
\begin{aligned}
\langle H_0 \rangle_0 &= -\eta \sum_i \langle _0 s_i \rangle + D \sum_i \langle s_i^2 \rangle_0 \\
&= -\eta N m_0 + DN \langle s_i^2 \rangle_0
\end{aligned}
$$

$$
\begin{aligned}
\langle H \rangle_0 &= -J \sum_{\langle i,j \rangle} \langle s_i s_j \rangle_0 + D \sum_i \langle s_i^2 \rangle_0 \\
&= -J \sum_{\langle i,j \rangle} \langle s_i \rangle_0 \langle s_j \rangle_0 + D \sum_i \langle s_i^2 \rangle_0 \\
&= -J \frac{Nz}{2} m_0^2 + DN \langle s_i^2 \rangle_0
\end{aligned}
$$

Proponemos la función variacional

$$
\begin{aligned}
\Phi(\eta) &= f_0 + \frac{1}{N} \langle H - H_0 \rangle_0 \\
&= -\frac{1}{\beta} \ln \left[1 + 2e^{-\beta D} \cosh(\beta\eta) \right] - J \frac{z}{2} m_0^2 + \eta m_0
\end{aligned}
\tag{9}
$$

Derivamos con respecto a η e igualamos a cero para hallar el mínimo

$$
\begin{aligned}
\frac{\partial \Phi}{\partial \eta} &= -\frac{2e^{-\beta\eta}\sinh(\beta\eta)}{1+2e^{-\beta\eta}\cosh(\beta\eta)} - Jzm_0\frac{\partial m_0}{\partial \eta} + m_0 + \eta\frac{\partial m_0}{\partial \eta} \\
&= (\eta - Jzm_0)\,\frac{\partial m_0}{\partial \eta},
\end{aligned} \tag{10}
$$

donde usamos la igualdad 7.
La expresión anterior implica que la solución al problema variacional es

$$\eta = Jzm_0. \tag{11}$$

Reemplazando en 9, tenemos

$$\Phi(\eta) = -\frac{1}{\beta}\ln\left[1+2e^{-\beta D}\cosh(\beta\eta)\right] + \frac{1}{2Jz}\eta^2 \tag{12}$$

Realizamos un desarrollo de Taylor de orden 4 de la expresión anterior, teniendo en cuenta la siguiente relación:

$$\ln\left[1+c\cosh(x)\right] = \ln(c+1) + \frac{c}{2c+1}x^2 + \frac{c(1-2c)}{24(c+1)^2}x^4 \tag{13}$$