Modelos unidimensionais na rede com inspiração em biomembranas: pseudo-transições e quase-fases

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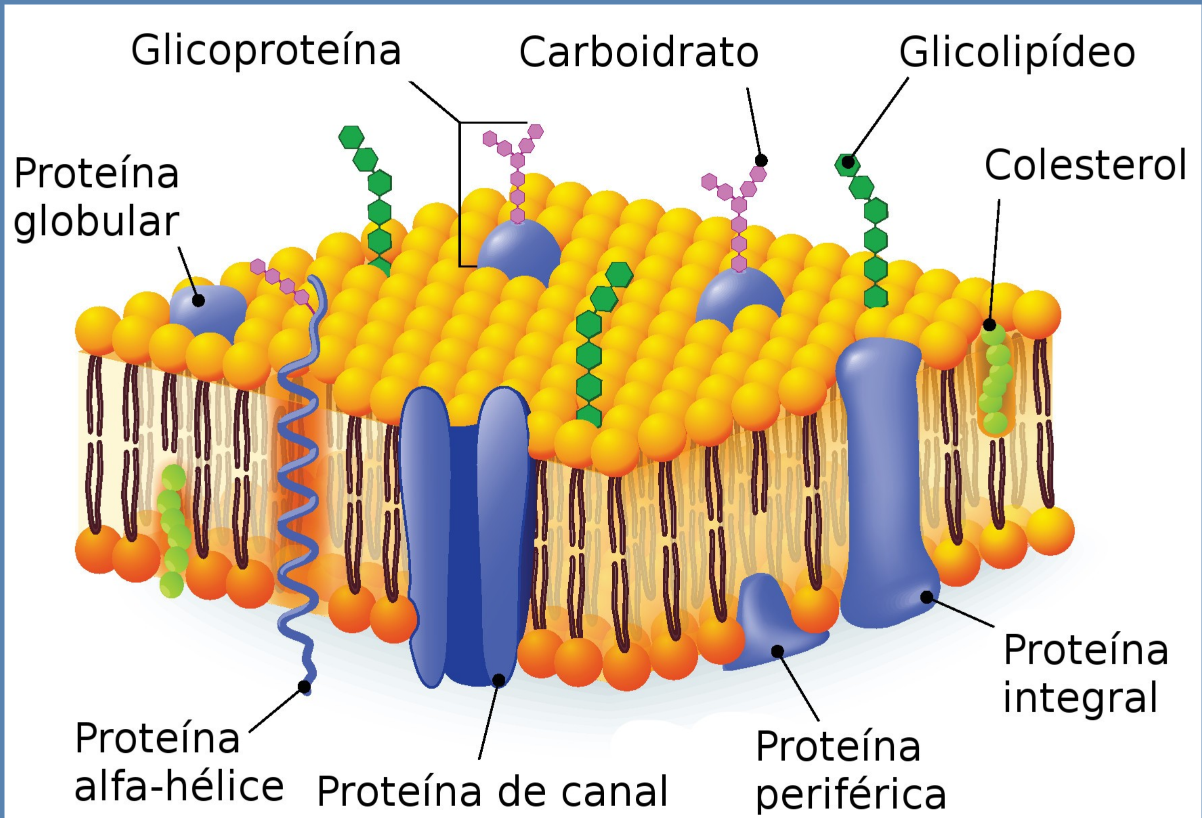
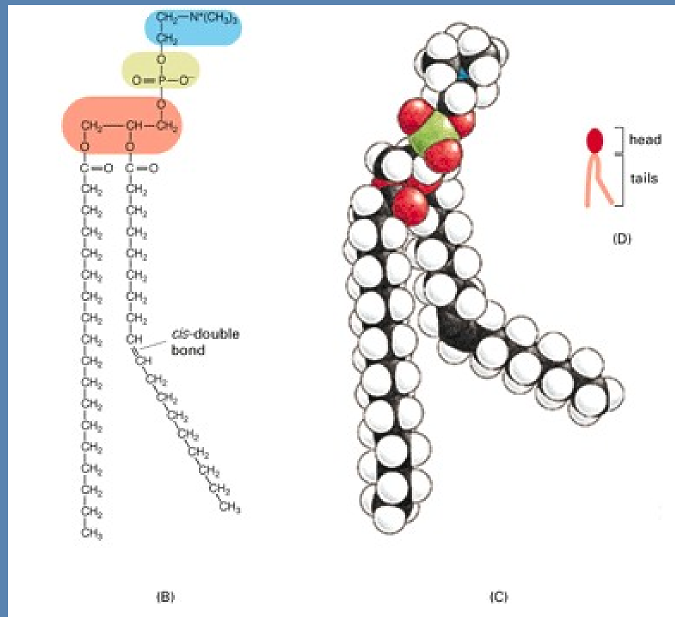
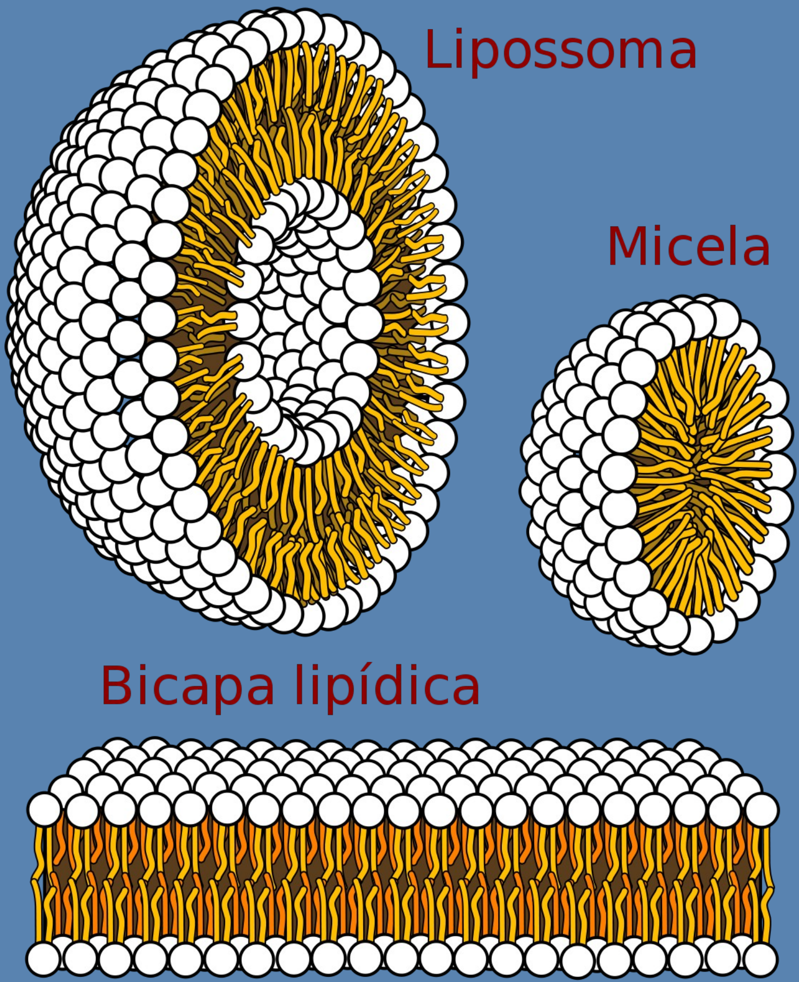
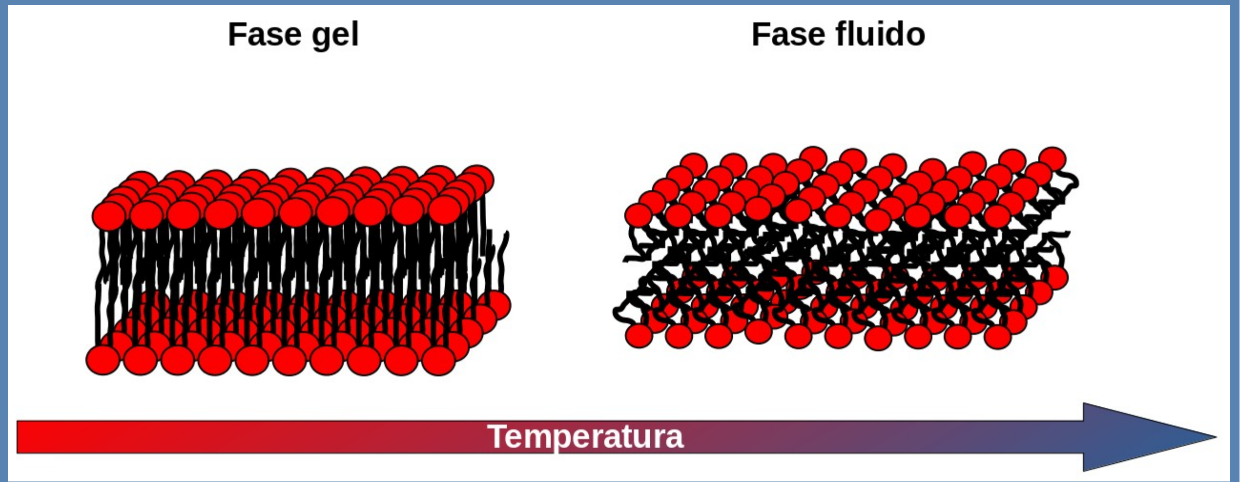
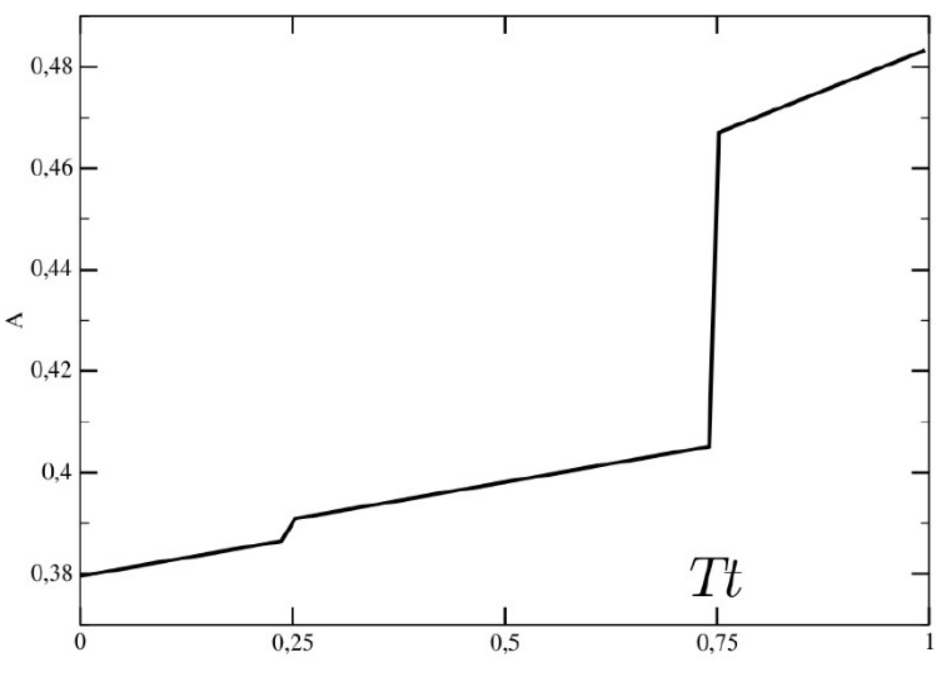
Motivação: Biomembranas

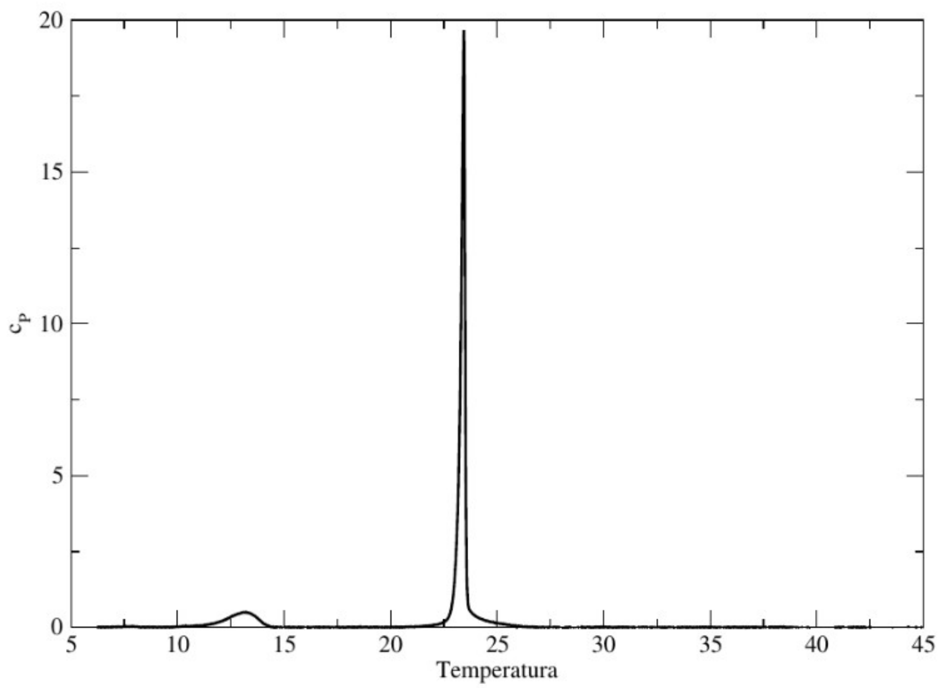





Lipossoma
Micela
Bicapa lipídica


Fase gel
Fase fluido
Temperatura

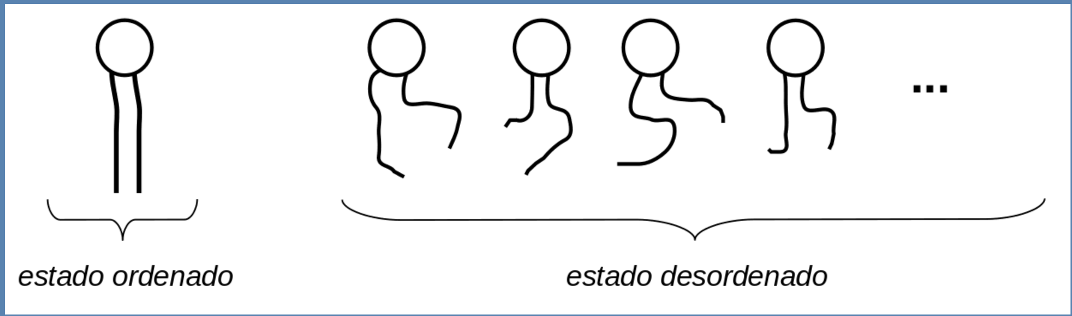




Curva esquemática do aumento de área por’’ cabeça polar. Retirado de Gregor Cevc e Derek Marsh. *Phospholipid B’ilayer.* John Wiley & Sons, 1987

Calor específico a pressão constante, para vesículas construídas com DMPC. Obtido no laboratório de Biofísica do IFUSP.

Modelo de Doniach



η = 0 [desordenado]
η = 1 [ordenado]

$$\mathcal{H}(\{\eta\}) = -\epsilon_o \sum_{(ij)} \eta_i \eta_j - \epsilon_d \sum_{(ij)} (1-\eta_i)(1-\eta_j) - \epsilon_{od} \sum_{(ij)} [\eta_i (1-\eta_j) + (1-\eta_i)\eta_j]$$

$$\Pi A \quad , \quad A = \sum_i [a_o \eta_i + a_d (1-\eta_i)]$$

$$E_{deg} = \frac{\ln \omega}{2\beta} \sum_i (\eta_i - 1) \quad , \quad \beta = 1/k_B T$$

Fluido de rede de Doniach (DLG)

$$\mathcal{H}_{ef}(\{\sigma\}) = -\sum_{i=1}^{L}\Big\{J\sigma_i\sigma_{i+1} + \Delta\sigma_i\sigma_{i+1}(\sigma_i+\sigma_{i+1}) + K\sigma_i^2\sigma_{i+1}^2 + \frac{\mu}{2}(\sigma_i^2+\sigma_{i+1}^2)$$
$$+\frac{\ln\omega}{4\beta}[\sigma_i(\sigma_i-1)+\sigma_{i+1}(\sigma_{i+1}-1)]\Big\}$$

$\sigma = 1$	[ordenado]
$\sigma = -1$	[desordenado]
$\sigma = 0$	[vazio]

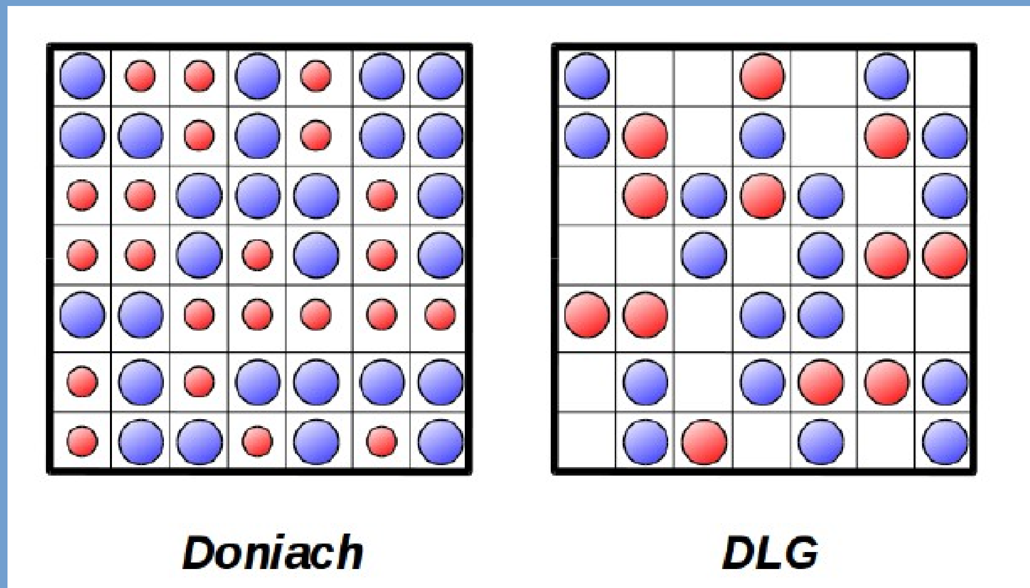


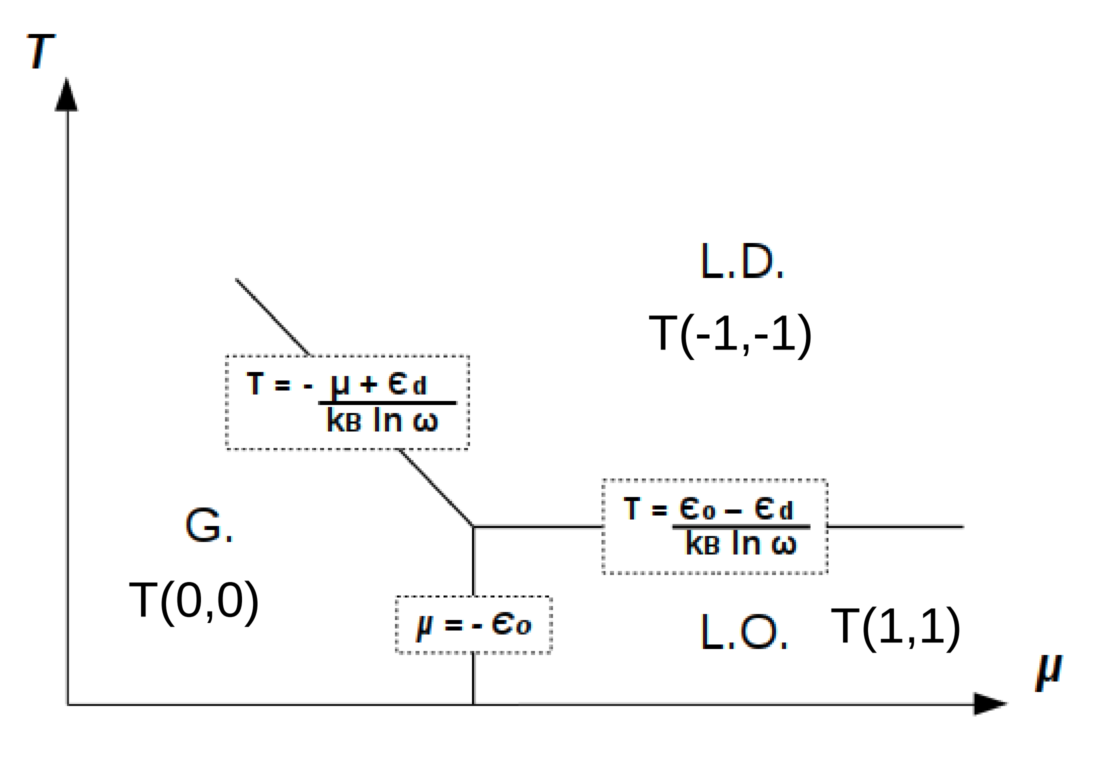
Diagrama de quase-fases

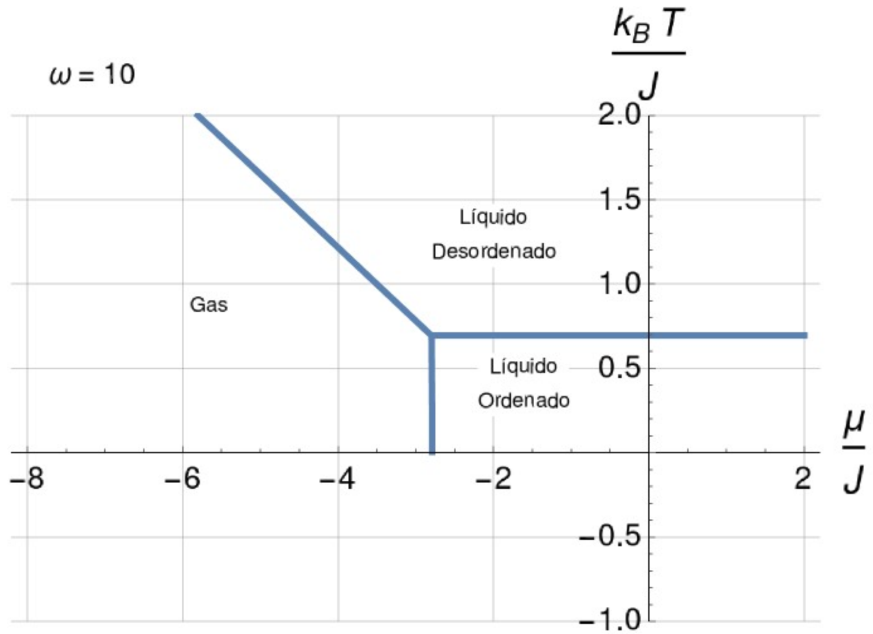
$$\mathbb{T} = \begin{bmatrix} T(-1,-1) & T(-1,0) & T(-1,1) \\ T(0,-1) & T(0,0) & T(0,1) \\ T(1,-1) & T(1,0) & T(1,1) \end{bmatrix} = \begin{bmatrix} \omega z h^{-1} A & \sqrt{\omega z h^{-1}} & \sqrt{\omega} z C \\ \sqrt{\omega z h^{-1}} & 1 & \sqrt{z h} \\ \sqrt{\omega} z C & \sqrt{z h} & z h B \end{bmatrix}$$

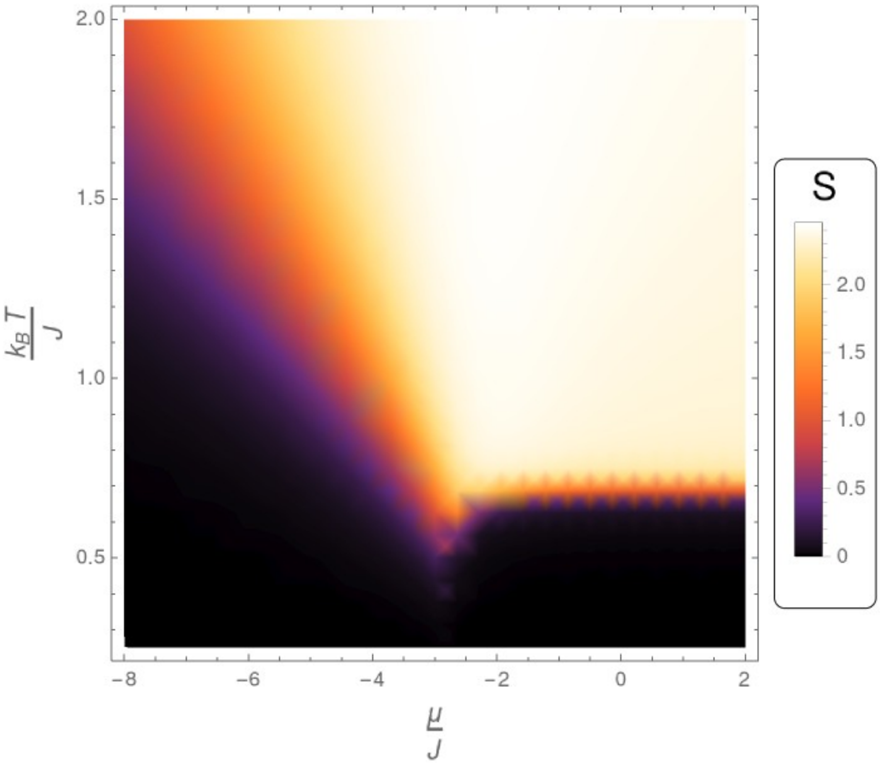
T(-1,-1) = T(0,0) : $T = -\dfrac{\mu + \epsilon_d}{k_B \ln \omega}$

T(-1,-1) = T(1,1) : $T = \dfrac{\epsilon_o - \epsilon_d}{k_B \ln \omega}$

T(0,0) = T(1,1) : $\dfrac{\mu + \epsilon_o}{k_B T} = 0$







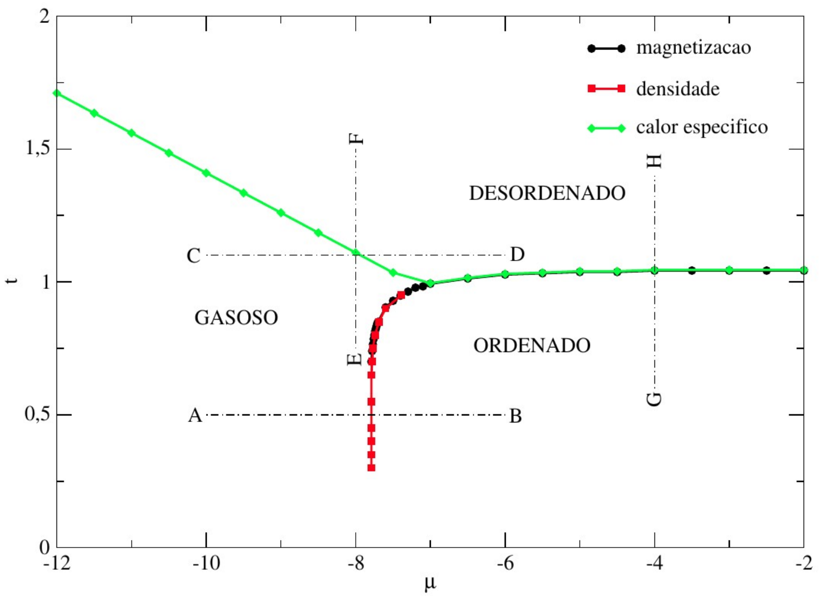
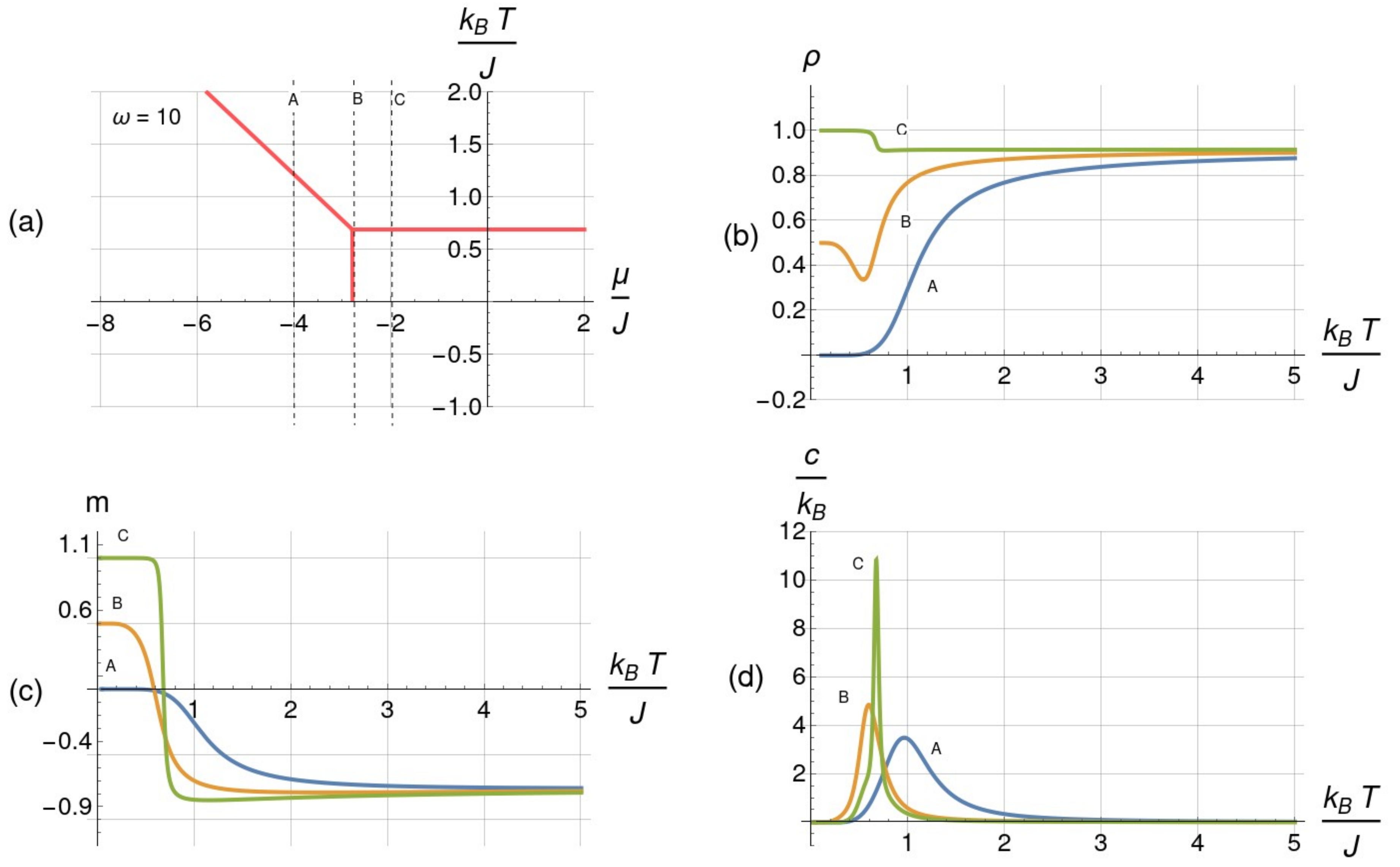
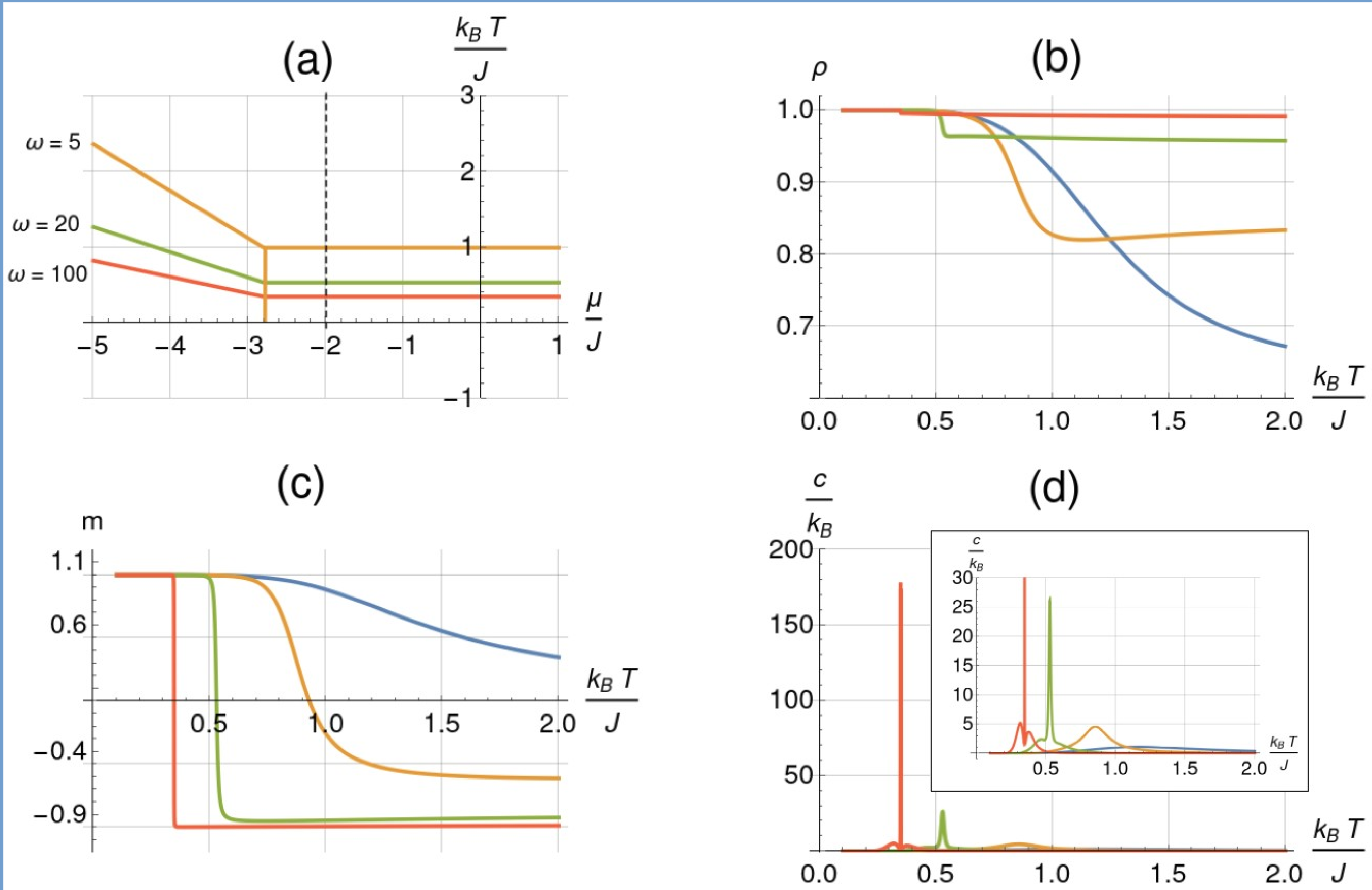


Diagrama obtido por aproximação de Campo médio (da tese do Henrique Guidi)



(a)
ω = 10
A
B
C
$\frac{k_B T}{J}$
$\frac{\mu}{J}$
(b)
ρ
(c)
m
(d)
$\frac{c}{k_B}$



(a)
$\frac{k_B T}{J}$
3
2
1
−1
ω = 5
ω = 20
ω = 100
$\frac{\mu}{J}$
−5
−4
−3
−2
−1
1
(b)
ρ
1.0
0.9
0.8
0.7
0.0
0.5
1.0
1.5
2.0
$\frac{k_B T}{J}$
(c)
m
1.1
0.6
−0.4
−0.9
0.5
1.0
1.5
2.0
$\frac{k_B T}{J}$
(d)
$\frac{c}{k_B}$
200
150
100
50
0.0
0.5
1.0
1.5
2.0
$\frac{k_B T}{J}$
$\frac{c}{k_B}$
30
25
20
15
10
5
0.5
1.0
1.5
2.0
$\frac{k_B T}{J}$

Considerações finais

- A importância dos modelos unidimensionais na busca por pistas sobre o comportamento dos sistemas em dimensões maiores;

- o papel da temperatura sobre a intensidade da pseudo-transição;

- a análise dos elementos da matriz de transferência para a obtenção do diagrama de fases.

- Entropia residual