BLUME - CAPEL MODEL

TD1 - 1

$$H = -\frac{J_0}{2}\sum_{i\neq j} s_i s_j + \Delta \sum_i s_i^2 \qquad s_i = \pm 1, 0$$

TO GET 1st TERM $\Theta(N)$ $\Rightarrow$ $\boxed{J_0 \to J/N}$

Δ MEASURE THE ENERGY DIFF BTW THE STATE $S_i = +1\ \forall i$ AND THE STATE $S_i = 0\ \forall i$; ie BTW FM AND PM CONF.

- STUDY THE CASE $\Delta = 0$ $\Rightarrow$ CURIE - WEISS FOR FM.
- IF $\Delta \neq 0$ GROUND STATES:

$S_i = \pm 1\ \forall i$ OR $S_i = 0\ \forall i$

$$E_{FM} = -\frac{J}{2N}\sum_{i\neq j} 1 + \Delta N \qquad E_{PM} = 0$$

$$= -\frac{J}{2\cancel{N}}\left(N^2 - \cancel{N}\right) + \Delta \cancel{N}$$

$$E_{FM} = \left(-\frac{J}{2} + \Delta\right)N + \frac{J}{2}$$

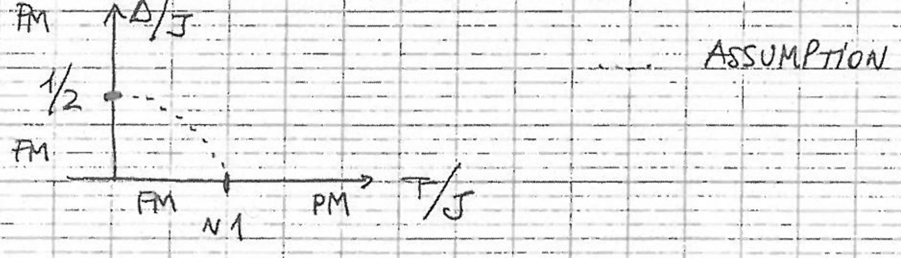
$$\Delta E = E_{FM} - E_{PM} \simeq \left(\Delta - J/2\right)N$$

$\Delta > \frac{J}{2}$: $\Delta E > 0$ PM is GS

$\Delta < \frac{J}{2}$: $\Delta E < 0$ FM is GS

WITH THE ENERGETIC ANALYSIS WE STUDY THE T=0 BEHAVIOUR.

TRANSITION BETWEEN A FM & PM



CANONICAL ENSEMBLE

1- $$Z = \sum_{\{s_i = \pm 1, 0\}} e^{-\beta H[\{s_i\}]}$$ FUNCTION OF (J, Δ, β)

FIRST REMARK : IT DOESN'T DEPEND ON ALL PARAM. INDEP BUT THROUGH

$$(\beta J\ ,\ \beta \Delta)$$

OR, $(\beta J\ ,\ \Delta/J) \Rightarrow$ PHASE DIAGRAM IN TERMS OF THESE, SOMETIMES CALLED

$$k = \beta J \qquad \delta = \Delta/J$$

BUT WE KEEP βJ AND $\beta\Delta$ FOR CLARITY.

2- AUXILIARY VARIABLE

$$x = \frac{1}{N}\sum_i s_i$$ NB: IT'S A GLOBAL VARIABLE

$$+\beta \frac{J}{2N} \underbrace{\sum_{i \neq j} s_i s_j} - \beta\Delta \sum_i s_i^2 = -\beta H[\{s_i\}]$$

$$\hookrightarrow N \frac{1}{N}\sum_i s_i \frac{1}{N}\sum_j s_j - \underbrace{\frac{1}{N}\sum_i s_i^2}$$

1, IF ISING SPINS BUT THEY ARE SPIN 1 VARIABLES HERE ! $\Rightarrow$ AS IN LAST TERM

$$N\left(\frac{1}{N}\sum_i s_i\right)^2$$

$$-\beta H[\{s_i\}] = \frac{\beta J}{2} N \left(\frac{1}{N}\sum_i s_i\right)^2 - \left(\frac{\beta J}{2N} + \beta\Delta\right)\sum_i s_i^2$$

IF THE SPINS WERE ISING VARIABLES $\Rightarrow$

$$x = -N, -N + \frac{2}{N}, -N + \frac{4}{N}, \dots$$ ONE REPLACES $\sum_{\{s_i\}} \to \int dx$

AND ENTROPY WOULD BE EASY TO COMPUTE.

BUT THEY ARE SPIN-1 VARIABLES $\Rightarrow$ ANOTHER METHOD

GAUSSIAN IDENTITY OR HUBBARD-STRATONOVICH TRANSFORM

$$e^{bm^2} = \sqrt{\frac{b}{\pi}} \int_{-\infty}^{\infty} dx \; e^{-bx^2 + 2bmx}$$

APPLIED TO "OPEN" THE SQUARE-TERM IN $\frac{1}{N}\sum_i s_i$
IN THE EXPONENTIAL

$$Z = \sum_{\{s_i = \pm 1, 0\}} e^{-\beta\Delta \sum_{i=1}^{N} s_i^2} \underbrace{\left(e^{+\frac{\beta J}{N}\left(\sum_{i=1}^{N} s_i\right)^2} \right.}$$

REPLACED By ⊛

$$\sqrt{\frac{\beta J N}{2\pi}} \int_{-\infty}^{\infty} dx \; e^{-\frac{\beta J N}{2} \cdot x^2 + 2\frac{\beta J N}{2}\left(\frac{1}{N}\sum_i s_i\right) x}$$

I'VE USED HS FOR $m = \frac{1}{N}\sum_i s_i$ AND $b = \frac{\beta J N}{2}$

- THE "DIAGONAL" TERM GENERATED BY HAVING TRANSFORMED $\sum_{i \neq j}$ INTO $\sum_{ij}$ IS MUCH SMALLER THAN THE $\sum_{ij}$ ONE: $\mathcal{O}(1)$ VS $\mathcal{O}(N)$
$\Rightarrow$ WE DROP IT.

WHAT HAVE WE OBTAINED? WE DECOUPLED THE SPINS IN THE EXPONENTIAL. INDEED, THE SPIN DEPENDENT PART IS

$$-\beta\Delta \sum_i s_i^2 + \frac{\cancel{2}\beta J \cancel{N}}{\cancel{2}} \cancel{\frac{1}{N}} \sum_i s_i \; x \quad \Rightarrow$$

$$= \sum_i \left\{ -\beta\Delta s_i^2 + \frac{\cancel{2}\beta J}{\cancel{2}} s_i x \right\}$$

$$= -\beta \sum_i \left(\Delta s_i^2 - \frac{\cancel{2}}{\cancel{2}} J x s_i \right)$$

NOW, WE CAN COMPUTE THE PARTITION SUM OVER THE $\{S_i\}$ (BEFORE INTEGRATING OVER x $\Longleftrightarrow$ ORDER EXCHANGE) SINCE

$$e^{-\sum_i g_i} = \prod_i e^{-g_i}$$

AND $$\sum_{\{S_i\}} e^{-\sum_i g_i} = \prod_i \left(\sum_{S_i} e^{-g_i} \right)$$

FACTORIZATION OF SUM OVER CONFIG. OF INDIVIDUAL SPINS.

CONCRETELY, FOR EACH i

$$\underbrace{e^{-\left(\Delta - \frac{\cancel{2}Jx}{\cancel{2}}\right)\beta}}_{S_i = 1} + \underbrace{e^{-\left(\Delta + \frac{\cancel{2}Jx}{\cancel{2}}\right)\beta}}_{S_i = -1} + \underbrace{1}_{S_i = 0}$$

THE PARTITION SUM BECOMES

$$Z = \sqrt{\frac{\beta J N}{2\pi}} \int_{-\infty}^{\infty} dx \; e^{-\frac{\beta J N}{2} x^2} \left(1 + e^{-(\Delta - Jx)\beta} + e^{-(\Delta + Jx)\beta} \right)^N \quad ⊛$$

WE CAN REARRANGE THIS EXPRESSION AS

$$Z = \sqrt{\frac{\beta J N}{2\pi}} \int_{-\infty}^{\infty} dx \; e^{-N\beta \tilde{f}(x)}$$

WITH $$\beta \tilde{f}(x) = \frac{\beta J}{2} x^2 - \frac{\cancel{\beta}}{\cancel{\beta}} \ln \left[1 + e^{-\beta\Delta} \left(e^{\beta J x} + e^{-\beta J x} \right) \right] \quad ⊛$$

THIS IS THE GINZBURG-LANDAU FREE-ENERGY DENSITY AS A FUNCTION OF THE VARIABLE x THAT WILL BECOME THE ORDER PARAMETER (PM-FM).

IT IS ACTUALLY A fct OF $(x; \beta J, \beta\Delta)$

OR BETTER STILL $(x; \beta J, \Delta/J)$ ⊛

THE TRICK HAS BEEN TO TRANSFORM THE EVALUATION OF Z INTO AN INTEGRAL THAT CAN BE COMPUTED BY SADDLE-POINT (LAPLACE METHOD) FOR $N \to \infty$.

USING:

$$I(\beta) = \lim_{N \to \infty} \int dx \; e^{-N \tilde{f}(x,\beta)}$$

$$= e^{-N \, \operatorname{Inf}_{x} \tilde{f}(x,\beta)}$$

WITH $\inf_{x}$ THE INFIMUN OF $\tilde{f}(x,\beta)$

IE ONE HAS TO LOOK FOR THE ABSOLUTE MINIMUM x^* AND EVALUATE $\tilde{f}(x,\beta)$ ON IT.

THE ACTUAL FREE-ENERGY OF THE SYST AS A FCT OF THE CONTROL PARAMETERS $(\beta J, \beta\Delta)$ IS THEN

$$-\beta f(\beta J, \beta \Delta) = \frac{\ln Z}{N} \qquad \text{(DENSITY)}$$

$$= \frac{1}{N} \ln e^{-N \operatorname{Inf}_{x} \beta \tilde{f}(x; \beta J, \beta\Delta)}$$

$$= -\beta \operatorname{Inf}_{x} \tilde{f}(x; \beta J, \beta\Delta)$$

$$\boxed{f(\beta J, \beta\Delta) = \operatorname{Inf}_{x} \tilde{f}(x; \beta J, \beta\Delta)}$$

WE NOTE THAT $\tilde{f}(x; \beta J, \beta\Delta) = \tilde{f}(-x; \beta J, \beta\Delta)$

IT'S A SYMM FCT WRT $x=0$.

WHAT IS x^* THAT CORRESPONDS TO $\operatorname{Inf}_{x} \tilde{f}$?

IT'S EQUAL TO $\langle \frac{1}{N} \sum_i s_i \rangle = x^*$

$\Longrightarrow$ YIELD MAGN DENSITY.

THE AVERAGED MAGN DENSITY & THE SADDLE POINT

TD1-4

PROOF

$$\frac{1}{N}\sum_i \langle S_i \rangle = \frac{1}{Z}\sum_{\{S_i\}} e^{-\beta H}\,\frac{1}{N}\sum_i S_i$$

AVERAGED MAGN DENSITY

$$= \frac{1}{\beta N}\frac{\partial}{\partial h}\ln Z(h)\Big|_{h=0}$$

GENERATING FUNCT METHOD (SOURCE h)

WITH $Z(h) = \sum_{\{S_i\}} e^{-\beta H + \beta h \sum_i S_i}$

THAT CORRESPONDS TO $H \to H - h\sum_i S_i$

APPLIED UNIFORM FIELD COUPLED TO MAGN DENSITY

NOW, WE PROCEED AS BEFORE, WE DECOUPLE THE SPINS
THE SPIN-DEP TERMS IN THE EXP IN $Z(h)$ ARE

$$-\beta\Delta\sum_i S_i^2 + \beta J\sum_i S_i x + \beta h\sum_i S_i$$

AND COMPUTING THE PARTITION SUM OVER $\sum_{\{S_i\}}$

$$\Rightarrow \left(1 + e^{-\beta\Delta + \beta J x + \beta h} + e^{-\beta\Delta - \beta J x - \beta h}\right)^N$$

$$= \left(1 + e^{-\beta\Delta}\left(e^{\beta J x + \beta h} + e^{-\beta J x - \beta h}\right)\right)^N$$

THEREFORE

$$Z(h) = \sqrt{\frac{\beta J N}{2\pi}}\int_{-\infty}^{\infty} dx\, e^{-N\beta \tilde{f}_h(x)} \overset{\text{LARGE } N}{\simeq} \sqrt{\frac{\beta J N}{2\pi}}\, e^{-N\beta \tilde{f}_h(x_{SP})}$$

$$\tilde{f}_h(x) = \frac{\beta J x^2}{2} - \ln\left[1 + e^{-\beta\Delta}\left(e^{\beta J x + \beta h} + e^{-\beta J x - \beta h}\right)\right]$$

$$\frac{1}{\beta N}\frac{\partial}{\partial h}\ln Z(h) = -\frac{\cancel{N\beta}}{\cancel{\beta N}}\frac{\partial}{\partial h}\tilde{f}_h(x^h_{SP}) = -\frac{\partial}{\partial h}\tilde{f}_h(x^h_{SP})$$

$$\frac{\partial}{\partial h}\tilde{f}_h(x_{SP}^h) = \underset{\downarrow \text{ EXPLICIT}}{\frac{\partial \tilde{f}_h(x_{SP}^h)}{\partial h}} + \underbrace{\frac{\partial \tilde{f}_h(x_{SP})}{\partial x_{SP}}}_{=0}\Bigg|_{x_{SP}^h} \frac{\partial x_{SP}^h}{\partial h}$$

①

$$= -\frac{e^{-\beta\Delta}\left(e^{\beta h} e^{\beta J x} - e^{-\beta J x - \beta h}\right)}{1+e^{-\beta\Delta}\left(e^{\beta J x+\beta h} + e^{-\beta J x - \beta h}\right)}\Bigg|_{x=x_{SP}^h}$$

STILL TO BE EVALUATED AT $h=0$

ON THE OTHER HAND x_{SP} IS FIXED BY

$$\frac{\partial f_h(x_{SP})}{\partial x_{SP}} \quad \text{OR BETTER WRITTEN} \quad \frac{\partial f_h(x)}{\partial x}\Bigg|_{x=x_{SP}^h} = 0$$

$$0 = \frac{\partial f_h(x)}{\partial x} = \beta J x - \frac{e^{-\beta\Delta}\left(\beta J e^{\beta J x+\beta h} - \beta J e^{-\beta J x - \beta h}\right)}{1+e^{-\beta\Delta}\left(e^{\beta J x+\beta h} + e^{-\beta J x - \beta h}\right)}$$

$$\Longrightarrow \cancel{\beta J} x = \frac{\cancel{\beta J}\, e^{-\beta\Delta}\left(e^{\beta J+\beta h} - e^{-\beta J - \beta h}\right)}{1+e^{-\beta\Delta}\left(e^{\beta J x+\beta h} + e^{-\beta J x - \beta h}\right)}$$

COMPARING WITH ① ABOVE $\Longrightarrow$

$$\frac{\partial \tilde{f}_h(x_{SP}^h)}{\partial h} = -x_{SP}^h$$ NOW BACK TO

$$\boxed{\frac{1}{N}\sum_i \langle S_i\rangle = \frac{1}{\beta N}\frac{\partial}{\partial h}\ln Z(h)\Bigg|_{h=0} = -\frac{\partial}{\partial h}\tilde{f}_h(x_{SP}^h)\Bigg|_{h=0} = x_{SP}}$$

THE EXTREMA OF $\tilde{f}_-$

WHICH ARE THE EXTREMA OF $\tilde{f}(x;\beta J,\beta\Delta)$?

$$\tilde{f}(x;\beta J,\beta\Delta) = \frac{J}{2}x^2 - \frac{1}{\beta}\ln\left[1+e^{-\beta\Delta}\,2\,\mathrm{ch}J\beta x\right]$$

$$\frac{\partial\tilde{f}}{\partial x} = 0 = \frac{J}{\cancel{2}}\cdot\cancel{2}x - \frac{1}{\cancel{\beta}}\,\frac{e^{-\beta\Delta}\,2\,\mathrm{sh}J\beta x\;J\cancel{\beta}}{\left[1+e^{-\beta\Delta}\,2\,\mathrm{ch}J\beta x\right]}$$

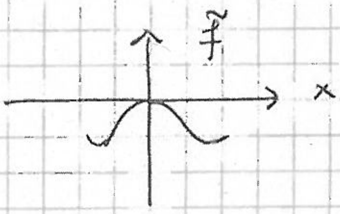
YIELDS x^* AS A SOL.

PROBLEM: THIS IS AN IMPLICIT EQ $\Rightarrow$ CAN'T BE SOLVED ANALYTICALLY IN EXPLICIT FORM.

WE NOTE THAT $x^*=0$ IS A SOLUTION $\forall$ PARAM.

BUT THERE MIGHT BE OTHER SOLUTIONS FOR SOME RANGES OF PARAMETERS. $\Rightarrow$ NUMERICS.

LET'S EXPAND $\tilde{f}(x;\beta J,\beta\Delta)$ CLOSE TO $x\simeq 0$ AND LOOK FOR THE PARAMETERS SUCH THAT THE QUADRATIC COEFF IS NEGATIVE:



SIGNATURE OF A 2nd ORDER PHASE TRANS.

$$\tilde{f}(0) = 0$$

$$f'(x\simeq 0) = 0$$

$$f''(x=0) = J - 2e^{-\beta\Delta}\,\frac{\left[\beta J\,\mathrm{ch}J\beta x\left(1+e^{-\beta\Delta}\,2\,\mathrm{ch}J\beta x\right) - \mathrm{sh}\beta Jx\;e^{-\beta\Delta}\,2\,\mathrm{sh}J\beta x\;\beta J\right]}{\left[1+e^{-\beta\Delta}\,2\,\mathrm{ch}J\beta x\right]^2}\Bigg|_{x=0}$$

NOT A VERY GOOD ROAD TO TAKE.

GO BACK TO $f'(x)$ AND EXPAND AROUND $x\simeq 0$.

$$f'(x) = Jx - \frac{2Je^{-\beta\Delta}\ \mathrm{sh} J\beta x}{1+e^{-\beta\Delta}\ 2\mathrm{ch}\, x\beta J} = 0$$

EXPAND AROUND $x \simeq 0$

$$\cancel{J}x - \frac{2\cancel{J}e^{-\beta\Delta}\ J\beta x}{1+e^{-\beta\Delta}\ 2} = 0$$

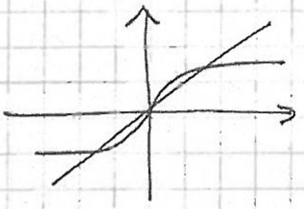
$$\Longrightarrow \quad 1 - \frac{2e^{-\beta\Delta}\ \beta J}{1+e^{-\beta\Delta}\ 2} = 0$$

$$1 + 2e^{-\beta\Delta} - 2\beta J e^{-\beta\Delta} = 0$$

$$\boxed{\frac{1}{2}e^{\beta\Delta} + 1 - \beta J = 0}$$

CRITICAL 2nd ORDER LINE.

IT'S LIKE $x = \mathrm{th}\,\beta x$



FOR NORMAL ISING CASE

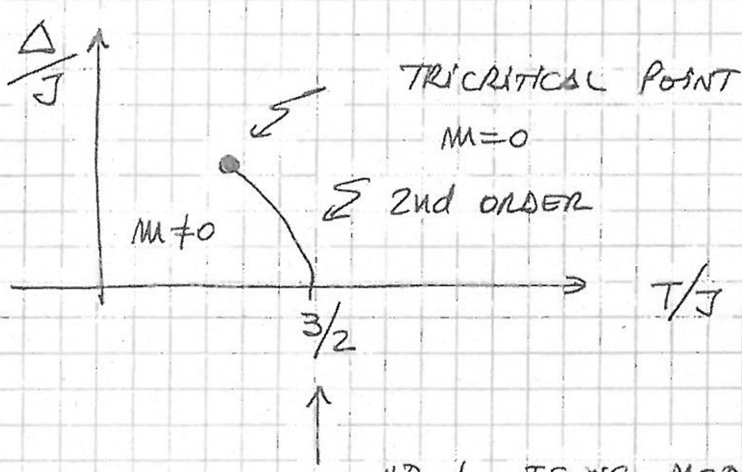
THE FUNCT HERE IS MORE "COMPLEX" BUT THE IDEA IS THE SAME.

CRITICAL β FROM
$x \simeq \beta x \Longrightarrow \beta = 1$
$(J=1)$.

$$\frac{2e^{-\beta\Delta}\ \mathrm{sh}\,\beta x}{1+e^{-\beta\Delta}\ 2\mathrm{ch}\, x}$$ PLAYS THE ROLE of $\mathrm{th}\,\beta x$

INDEED, if $\Delta = 0 \Longrightarrow \dfrac{2\,\mathrm{sh}\,\beta x}{1+2\mathrm{ch}\, x}$

BUT THIS IS NOT THE ISING FORM SINCE WE HAVE SUMMED OVER $S=1$ SPINS $\{1,-1,0\}$.



TRICRITICAL POINT $(\Delta/J \simeq 0.4621,$ $J/\beta \simeq 3)$.

NB ≠ ISING MODEL VALUE

IF WE INCREASE Δ, say $\Delta \ll 1 \Rightarrow$

$$0 = \frac{1}{2}\beta\Delta + 1 - \beta J \Rightarrow \beta J = 1 + \frac{1}{2}\beta\Delta$$

BUT I WANT TO LOOK AT PHASE DIAGRAM AS A FCT OF $(\Delta/J) \Rightarrow$

$$\beta J = 1 + \frac{1}{2}\beta J\left(\frac{\Delta}{J}\right)$$

$$\beta J = \frac{1}{1 - \frac{1}{2}\left(\frac{\Delta}{J}\right)}$$

is THIS is WRONG SINCE I EXPANDED $e^{\beta\Delta}$ ASSUMING $\beta\Delta \ll 1$? IS THIS TRUE? No, IT'S OK, SINCE β is FINITE CLOSE TO T_c

$$\Downarrow$$

$$\boxed{T/J = 1 - \frac{1}{2}\frac{\Delta}{J}}$$

BACK TO EQ.

$$\frac{1}{2}e^{\beta\Delta} + 1 - \beta J = 0$$

$$\frac{1}{2}e^{\beta J\left(\frac{\Delta}{J}\right)} + 1 - \beta J = 0$$

(NOT NEEDED ↑)

THE COEFF OF x^4 HAS TO BE POSITIVE

$\Rightarrow$ CONDITION

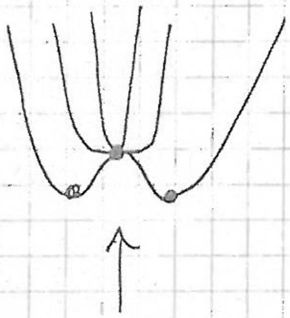
$$\boxed{4 - e^{\beta\Delta} > 0} \Longrightarrow \text{TRICRITICAL POINT}$$

$$\frac{\Delta}{J} = \frac{\ln 4}{3} \simeq 0.4621 \qquad J\beta = 3$$

TO FIND A 1st ORDER PHASE TRANS ONE NEEDS TO COMPARE

$$\tilde{f}(x^* \neq 0 ; \beta J, \Delta/J) = \tilde{f}(0 ; \beta J, \Delta/J)$$

CAN ONLY BE DONE NUMERICALLY.



$X^*=0$ BECOMES A MAX

X^* REMAINS A MIN UNTIL SPINODAL.

$$\frac{1}{T} = \frac{\partial S}{\partial \varepsilon} = \frac{\partial S_0}{\partial \varepsilon} \Rightarrow \frac{1}{k_B T} = \frac{\cancel{2}}{\cancel{2}\Delta} \ln\left[\frac{1-\varepsilon/\Delta}{\varepsilon/2\Delta}\right]$$

USING $A_m = 0$ $\Rightarrow$

THIS YIELDS THE CRITICAL MICRO-CANONIC TEMPERATURE

$$\boxed{\beta_c J = \frac{\exp(\beta/\Delta)}{2} + 1}$$

OR, IN TERMS OF ε:

$$\boxed{\beta J = \frac{\Delta}{\varepsilon}}$$

THE SAME CRITICAL 2nd ORDER CURVE AS WITH THE CANONICAL APPROACH.

TRICRITICAL POINT $A_m = B_m = 0$

$$\frac{\left(\frac{1}{2\Delta}\right)^2}{2(J\beta)^2}\left[1 + 2\exp\left(-\frac{\beta J}{\Delta}\right)\right] - \frac{1}{4\Delta\beta} + \frac{1}{12} = 0$$

SOME J's MISSING IN THIS EXPRESSION

$$\frac{1}{2\Delta} = 1{,}0813 \quad J\beta = \underbrace{3{,}0272}_{} \neq 0 \quad \text{IN CANONICAL} \ !$$

SMALL DIFF BUT A DIFFERENCE

MICROCANONICAL ENSEMBLE

LET'S COUNT THE NUMBER OF CONFIGURATIONS WITH

N_+ SPINS 1
N_- SPINS -1
N_0 SPINS 0

CONSTRAINT ON N_+, N_-, N_0: $N = N_+ + N_- + N_0$ (1)

THE MAGNETIZATION is $M = N_+ - N_-$ (2)

THE QUADRUPOLE MOMENT is $\varphi = N_+ + N_-$ (3)

$$\varphi = \sum_i s_i^2$$

FROM THESE THREE CONDITIONS ONE COULD EXTRACT N_+, N_- AND N_0 AS FUNCTIONS OF N, M, φ.

THE ENERGY, OR THE HAMILTONIAN

$$H = -\frac{J}{2N} \sum_{i \neq j} s_i s_j + \Delta \sum_i s_i^2$$

$$= -\frac{J}{2N} \left(\sum_i s_i \right)^2 + \frac{J}{2N} N + \Delta \sum_i s_i^2$$

CAN BE WRITTEN IN TERMS OF $\{M, \varphi\}$

$$H = -\frac{J}{2N} M^2 + \frac{J}{2} + \Delta \varphi$$

AND AS A FUNCTION OF $\{N_+, N_-, N_0\}$

$$H = -\frac{J}{2N} (N_+ - N_-)^2 + \frac{J}{2} + \Delta (N_+ + N_-)$$

AS BEFORE WE CAN DROP THE TERM $O(1)$ WRT THE TWO MACROSCOPIC TERMS (1st & 3rd) ↙

$$H \simeq -\frac{J}{2N} M^2 + \Delta \varphi$$

$\ln \Omega$

THE "ENTROPY" OR, MORE PRECISELY, THE NUMBER OF MICROSCOPIC CONFIGURATIONS Ω COMPATIBLE WITH THE MICROSCOPIC OCCUPATION NUMBERS N_+, N_-, N_0 IS

$$\Omega = \frac{N!}{N_+!\,N_-!\,N_0!}$$

STIRLING $\ln N! \simeq N \ln N - N$

$$\ln \Omega = \ln N! - \ln N_+! - \ln N_-! - \ln N_0!$$

LET'S WRITE N_+, N_-, N_0 INTERMS OF N, M, Q FROM (1)-(3):

$N_0 = N - N_+ - N_-$ FROM (1) → (4)

IN (2) & (3)

$M + Q = 2N_+$ $\quad M - Q = -2N_-$

$\Longrightarrow$

$N_+ = \frac{M+Q}{2} = \frac{N(m+q)}{2}$ FROM EXTENSIVE TO INTENSIVE ORDER PARAMETERS

$N_- = \frac{Q-M}{2} = \frac{N(q-m)}{2}$

BACK IN (4) $N_0 = N - \frac{N(m+q)}{2} - \frac{N(q-m)}{2}$

$= \frac{N}{2}\left[2 - m - q - q + m\right]$

$= \frac{N}{\cancel{2}}\,\cancel{2}(1-q)$

$N_0 = N(1-q)$

USING THE FORMS JUST DERIVED FOR $\{N_+, N_-, N_0\}$

$$\ln \Omega = \ln N! - \ln \frac{N(m+q)}{2}! - \ln \frac{N(q-m)}{2}! - \ln N(1-q)!$$

WE CAN USE STIRLING IN EACH TERM

$$\ln \Omega \simeq N \ln N - N - \frac{N(m+q)}{2} \ln \frac{N(m+q)}{2} + \frac{N(m+q)}{2}$$

$$- \frac{N(q-m)}{2} \ln \frac{N(q-m)}{2} + \frac{N(q-m)}{2}$$

$$- N(1-q) \ln N(1-q) + N(1-q)$$

AND NOW SIMPLIFY. THE "LINEAR" TERMS ARE

$$-N + \frac{N(\cancel{m}+\cancel{q})}{2} + \frac{N(\cancel{q}-\cancel{m})}{2} + N(1-\cancel{q}) = \cancel{-2N}\ 0$$

$$\ln \Omega \simeq N \ln N - \cancel{2N} - \frac{N(m+q)}{2} \ln \frac{N(m+q)}{2}$$

$$- N\left(\frac{q-m}{2}\right) \ln N\left(\frac{q-m}{2}\right) - N(1-q) \ln N(1-q)$$

FIRST TERM is a CONST, ie INDEP of $\{m, q\}$ THE ORDER PARAMETERS

LOOK AT TERMS $\propto N \ln N$:

$$N \ln N - \frac{N}{2}(m+q) \ln \frac{N}{2} - \frac{N}{2}(q-m) \ln \frac{N}{2} - N(1-q) \ln N$$

$$= N \ln N - \frac{N}{2}(\cancel{m}+\cancel{q}) \ln N - \frac{N}{2}(\cancel{q}-\cancel{m}) \ln N - N(1-\cancel{q}) \ln N$$

$$+ \frac{N}{2}(\cancel{m}+q) \ln 2 + \frac{N}{2}(q-\cancel{m}) \ln 2$$

$$= \cancel{N \ln N} - N \cancel{\ln N} + N q \ln 2 = N q \ln 2$$

$$\ln\Omega \simeq \cancel{2N} - \frac{N}{2}(m+q)\ln(m+q) - \frac{N}{2}(q-m)\ln(q-m)$$
$$- N(1-q)\ln(1-q) + Nq\ln 2$$

CALL IT ENTROPY S :

$$S = k_B \ln\Omega \simeq \cancel{2N} - N\left\{ \frac{(m+q)}{2}\ln(m+q) + \frac{(q-m)}{2}\ln(q-m) + (1-q)\ln(1-q) - q\ln 2 \right\} k_B$$

WE HAVE WRITTEN THE ENTROPY AS A FUNCTION OF m AND q.
BUT WE PREFER TO WRITE IT AS A FUNCTION OF m AND ε.
BACK TO EXPRESSION OF HAMILTONIAN

$$H = \frac{-J}{2N}M^2 + \Delta Q$$

TERM $O(1)$ IN N ALREADY DROPPED

$$\frac{H}{N} = \varepsilon = \left\{ \frac{-J}{2N}(Nm)^2 + \Delta Nq \right\}\frac{1}{N}$$

$$\varepsilon = \frac{-J}{2}m^2 + \Delta q$$

$$\Longrightarrow \quad q = \left(\varepsilon + \frac{J}{2}m^2\right)\frac{1}{\Delta}$$

$$S(m,\varepsilon) = k_B\ln\Omega$$

$$= -k_B N \left\{ \frac{1}{2\Delta}\left(m + \varepsilon + \frac{J}{2}m^2\right)\ln\frac{1}{\Delta}\left(m + \varepsilon + \frac{Jm^2}{2}\right)\right.$$

$$+ \frac{1}{2\Delta}\left(\varepsilon + \frac{Jm^2}{2} - m\right)\ln\frac{1}{\Delta}\left(\varepsilon + \frac{Jm^2}{2} - m\right)$$

$$+ \left[1 - \frac{1}{\Delta}\left(\varepsilon + \frac{J}{2}m^2\right)\right]\ln\left[1 - \frac{1}{\Delta}\left(\varepsilon + \frac{Jm^2}{2}\right)\right]$$

$$\left. - \left(\varepsilon + \frac{J}{2}m^2\right)\frac{1}{\Delta}\ln 2 \right\}$$

FROM HERE WE HAVE $S(\varepsilon, m)$.

AT FIXED ε WE CAN LOOK FOR THE VALUE OF m THAT MAXIMIZES THE ENTROPY

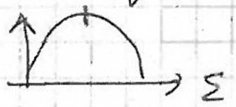
$$\frac{\partial S(\varepsilon, m)}{\partial m} = 0 \Longrightarrow m^* \qquad \text{EXTREMA}$$

$$\frac{\partial^2 S(\varepsilon, m)}{\partial m^2} \begin{cases} > 0 & \text{MINIMUM} \\ < 0 & \text{MAXIMUM.} \Longleftarrow \end{cases}$$

REPLACING IN S:

$$S(\varepsilon, m^*) = \sup_m S(\varepsilon, m) = S(\varepsilon)$$

NB THIS MODEL HAS ENERGY BOUNDED FROM ABOVE AND ONE EXPECTS $S(\varepsilon)$ TO BE FORMED BY TWO PARTS, WITH POSITIVE & NEGATIVE SLOPE



HERE BELOW ε FIXED AND DEPENDENCE ON m STUDIED.
ONE FINDS, TAYLOR EXPANSION AROUND m^* (maximum of $S(\varepsilon, m)$):

$$\frac{S(\varepsilon, m)}{N} = s_0 + A_m m^2 + B_m m^4 + O(m^6)$$

HERE m^* ASSUMED TO BE $m^* = 0$

$$s_0 = s(\varepsilon, m=0) = -\left(1 - \frac{1}{\Delta}\varepsilon\right) \ln\left(1 - \frac{1}{\Delta}\varepsilon\right) - \frac{\;}{\Delta}\varepsilon \ln\left(\frac{\varepsilon}{2\Delta}\right)$$

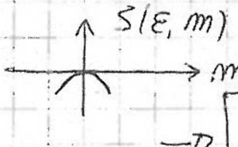
$$A_m = -\frac{J}{2\Delta} \ln \frac{\varepsilon/2\Delta}{1 - \varepsilon/\Delta} - \frac{\Delta}{2\varepsilon}$$

$$B_m = \frac{-\,1/2\Delta}{4\varepsilon\,(1 - \varepsilon/\Delta)} + \frac{\Delta}{4\varepsilon^2} - \frac{8}{96\,\Delta^3 \varepsilon^3}$$

SOME J'S ARE MISSING HERE

IN PM $A_m < 0$, $B_m < 0$ $\Longrightarrow$ $m^* = 0$ MAXIMIZES S

2nd TRANS AT $A_m = 0$, $B_m < 0$



→ AS FOR GINZBURG-LANDAU FREE-ENERGY QUADRATIC TERM DISAPPEARS AT TRANSITION. $\Longrightarrow \boxed{A_m^{CRIT}(\varepsilon)}$

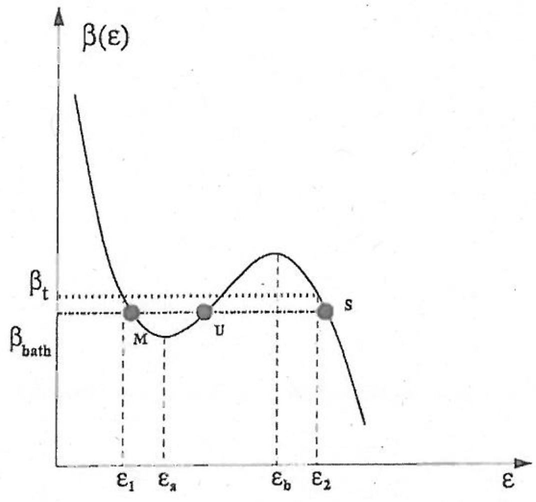


Fig. 9. Inverse temperature β as a function of energy ε. The Maxwell's construction is shown by the dotted line, while the dash-dotted line indicates the inverse temperature of the bath β_{bath}. U denotes an unstable macroscopic state with negative specific heat, while M and S are metastable and stable, respectively.

The fact that the presence of a canonical first order phase transition is necessary to obtain ensemble inequivalence was conjectured in Ref. [14]. This statement has been put on a more rigorous basis in Refs. [20,42], analyzing the convexity properties of the entropy $s(\varepsilon)$. In fact, it has been shown [20] that if the rescaled free energy $\phi(\beta)$ is differentiable, then the entropy $s(\varepsilon)$ can be obtained by its Legendre–Fenchel transform. This applies also for second order phase transitions, when the second derivative of $\phi(\beta)$ is discontinuous. Therefore, in the presence of a second order phase transition in the canonical ensemble, the microcanonical and canonical ensembles are equivalent.

In this subsection we have discussed in detail the case where no singularity is present in the entropy. Although already showing all the features of ensemble inequivalence, this case is not generic and we will discuss in the next subsection a model that has a second order phase transition in the microcanonical ensemble and still a first order transition in the canonical ensemble.

Let us conclude this subsection with a remark. We have remarked that energies between ε_1 and ε_2 correspond to the same value of β in the canonical ensemble. It is interesting to figure out what happens if an initially isolated system with negative specific heat and with an energy between ε_1 and ε_2, is put in contact with a heat bath that has its inverse temperature β_{bath}. Looking at Fig. 9 can be of help to understand the argument. We consider the case where the energy of the system lies in the range in which the specific heat is negative $[\varepsilon_a, \varepsilon_b]$ when the system is put in contact with the bath. Let us take for instance point U in Fig. 9 as an initial point. We are interested to study the behavior of the system subjected to small perturbations, so that it can still be considered to be initially close to a microcanonical system. We see immediately that the system becomes unstable. In fact, if it gets a small amount of energy from the bath, its temperature lowers (negative specific heat!), and therefore further energy will flow from the bath to the system, inducing a lowering of the system's temperature and then creating instability. If, on the contrary, the initial energy fluctuation decreases the system's energy, its temperature rises, inducing a further energy flow towards the bath, and, hence, an increase of system's temperature. Thus, in contact with a heat bath, the system does not maintain an energy in which its microcanonical specific heat is negative. The flow of energy started by the initial energy fluctuations stops when the system reaches the same temperature of the bath again, but at an energy for which its specific heat is positive. Looking at Fig. 9, it is clear that this could be either outside the range $[\varepsilon_1, \varepsilon_2]$, i.e. point S, or inside this range, point M. This feature is valid for all points U inside $]\varepsilon_a, \varepsilon_b]$. Once in M, the system will be in a thermodynamically metastable state and a sufficiently large fluctuation in the energy exchange with the bath will make it leave this metastable state, ending up again in a state with energy outside $[\varepsilon_1, \varepsilon_2]$, i.e. point S, which has the same inverse temperature of the bath β_{bath}. If the system instead jumps directly from U to S, it will stay there because this point lies on a thermodynamically stable branch.

4.2. An analytical solvable example: The mean-field Blume–Emery–Griffiths model

We have presented above the main physical and mathematical aspects related to ensemble equivalence or inequivalence in the study of long-range systems. Other mathematical approaches and tools, that exist, will be presented in connection with concrete examples. Actually, this subsection is dedicated to a toy model that exhibits all the features that have been discussed so far, in particular ensemble inequivalence and negative specific heat in the microcanonical ensemble. Historically, the relation between first order phase transition and negative specific heat for long-range systems in the thermodynamic limit was first pointed out in Refs. [104,105]. The phenomenology we are going to discuss in this section has been heuristically described in Ref. [106].

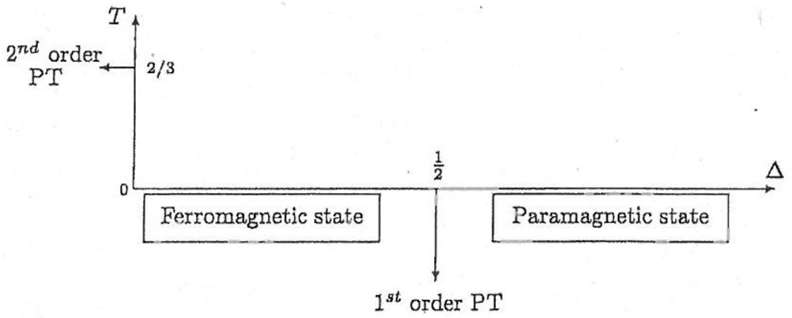


Fig. 10. Elementary features of the phase diagram of the Blume–Emery–Griffiths model, showing the phase transitions on the temperature T and local coupling Δ axis, respectively.

4.2.1. *Qualitative remarks*

The Blume–Emery–Griffiths (BEG) model is a lattice spin model with infinite range, mean-field like interactions whose phase diagram can be obtained analytically both within the canonical and the microcanonical ensembles. This study enables one to compare the two resulting phase diagrams and get a better understanding of the effect of the non-additivity on the thermodynamic behavior of the model.

The model we consider is a simplified version of the Blume–Emery–Griffiths model [107], known as the Blume–Capel model, where the quadrupole–quadrupole interaction is absent. The model is intended to reproduce the relevant features of superfluidity in He^3–He^4 mixtures. Recently, it has also been proposed as a realistic model for metallic ferromagnetism [108]. It is a lattice system (5), and each lattice point i is occupied by a spin-1 variable, i.e., a variable S_i assuming the values $S_i = 0, \pm 1$. We will consider the mean-field version of this model, for which all lattice points are coupled with the same strength. The Hamiltonian is given by

$$H = \Delta \sum_{i=1}^{N} S_i^2 - \frac{J}{2N}\left(\sum_{i=1}^{N} S_i\right)^2, \tag{73}$$

where $J > 0$ is a ferromagnetic coupling constant and $\Delta > 0$ controls the energy difference between the ferromagnetic $S_i = 1, \forall i$, or $S_i = -1, \forall i$, and the paramagnetic, $S_i = 0, \forall i$, states. In the following we will set $J = 1$, without loss of generality since we consider only ferromagnetic couplings. The paramagnetic configuration has zero energy, while the uniform ferromagnetic configurations have an energy $(\Delta - 1/2)N$. In the canonical ensemble, the minimization of the free energy $F = E - TS$ at zero temperature is equivalent to the minimization of the energy. One thus finds that the paramagnetic state is the more favorable from the thermodynamic point of view if $E(\{\pm 1\}) > E(\{0\})$, which corresponds to $\Delta > 1/2$. At the point $\Delta = 1/2$, there is therefore a phase transition; it is a *first* order phase transition since, it corresponds to a sudden jump of magnetization from the ferromagnetic state to the paramagnetic state.

For vanishingly small ratio Δ, the first term of Hamiltonian (73) can be safely neglected so that one recovers the Curie–Weiss Hamiltonian (1) with spin 1, usually introduced to solve the Ising model within the mean-field approximation. It is well known that such a system has a *second* order phase transition when $T = 2/3$ (we recall that we are adopting units for which $J = 1$, $k_B = 1$). Since one has phase transitions of different orders on the T and Δ axis (see Fig. 10), one expects that the (T, Δ) phase diagram displays a *transition line* separating the low temperature ferromagnetic phase from the high temperature paramagnetic phase. The transition line is indeed found to be first order at large Δ values, while it is second order at small Δ's.

4.2.2. *The solution in the canonical ensemble*

The canonical phase diagram of this model in the (T, Δ) is known since long time [107,109,110]. The partition function reads

$$Z(\beta, N) = \sum_{\{S_1,\ldots,S_N\}} \exp\left(-\beta\Delta \sum_{i=1}^{N} S_i^2 + \frac{\beta J}{2N}\left(\sum_{i=1}^{N} S_i\right)^2\right). \tag{74}$$

Using the Gaussian identity

$$\exp(bm^2) = \sqrt{\frac{b}{\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x \exp(-bx^2 + 2mbx), \tag{75}$$

(often called the Hubbard–Stratonovich transformation) with $m = \sum_i S_i/N$ and $b = N\beta J/2$, one obtains

$$Z(\beta, N) = \sum_{\{S_1,\ldots,S_N\}} \exp\left(-\beta\Delta \sum_{i=1}^{N} S_i^2\right) \sqrt{\frac{N\beta}{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x \exp\left(-\frac{N\beta}{2}x^2 + mN\beta x\right). \tag{76}$$

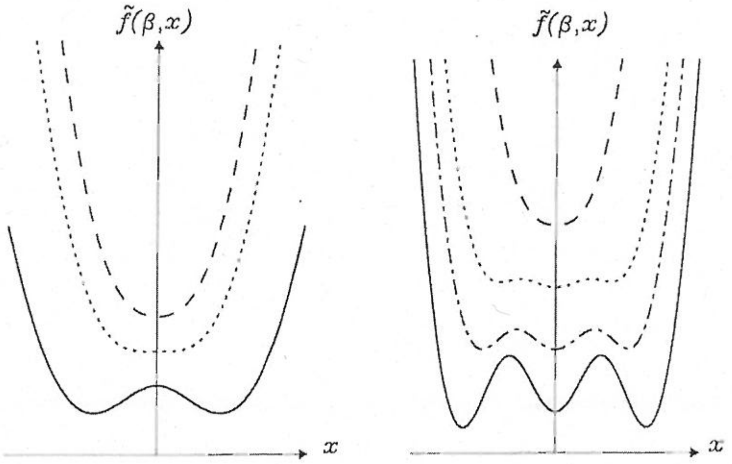


Fig. 11. Free energy $\tilde{f}(\beta, x)$ vs. x for different values of the inverse temperature $\beta = 1/T$. Left panel shows the case of a *second* order phase transition, temperature values $T = 0.8$ (dashed line), 0.63 (dotted), 0.4 (solid) when $\Delta = 0.1$ are displayed. Right panel shows the case of a *first* order phase transition with $\Delta = 0.485$ when $T = 0.5$ (dashed), 0.24 (dotted), 0.21 (dash-dotted), 0.18 (solid).

One then easily gets

$$Z(\beta, N) = \sqrt{\frac{N\beta}{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x \exp(-N\beta\tilde{f}(\beta, x)) \tag{77}$$

where

$$\tilde{f}(\beta, x) = \frac{1}{2}x^2 - \frac{1}{\beta}\ln[1 + \mathrm{e}^{-\beta\Delta}(\mathrm{e}^{\beta x} + \mathrm{e}^{-\beta x})]. \tag{78}$$

The integral in (77) can be computed using the saddle point method where N is the large parameter. The free energy is thus

$$f(\beta) = \inf_x \tilde{f}(\beta, x). \tag{79}$$

It is not difficult to see that the spontaneous magnetization $\langle m \rangle$ is equal to the value of x at the extremum which appears in Eq. (79). We should also note that $\tilde{f}(\beta, x)$ is even in x; therefore, if there is a value of x different from 0 realizing the extremum, the opposite value also realizes it. This means that if the minimum $\bar{x}$ is equal to 0 the system is in the paramagnetic phase, while if $\bar{x} \neq 0$ the system is in the ferromagnetic phase, where it can assume a positive or a negative magnetization. The phase diagram, in the (T, Δ) plane, is then divided into a paramagnetic region ($\bar{x} = 0$) and a ferromagnetic one ($\bar{x} \neq 0$).

Let us now show that the two regions are divided by a second order phase transition line and a first order phase transition line, which meet at a tricritical point. As in the Landau theory of phase transitions, we find a second order transition line by a power series expansion in x of the function $\tilde{f}(\beta, x)$ in Eq. (78). The second order line is obtained by equating to zero the coefficient of x^2, i.e., by the relation

$$A_c \equiv \beta - \frac{1}{2}\mathrm{e}^{\beta\Delta} - 1 = 0, \tag{80}$$

provided that the coefficient of x^4 is positive, i.e., provided that

$$B_c \equiv 4 - \mathrm{e}^{\beta\Delta} > 0. \tag{81}$$

The tricritical point is obtained when $A_c = B_c = 0$. This gives $\Delta = \ln(4)/3 \simeq 0.4621$ and $\beta = 3$. The continuation of the critical line after the tricritical point is the first order phase transition line, which can be obtained by finding numerically the local maximum value $\bar{x} \neq 0$ (magnetic phase) for which $\tilde{f}(\beta, x)$ is equal to $\tilde{f}(\beta, 0)$ (paramagnetic phase), i.e., by equating the free energies of the ferromagnetic and the paramagnetic phases. The behavior of the function $\tilde{f}(\beta, x)$ as β varies is shown in Fig. 11: panel (a) represents the case of a second order phase transition ($\Delta = 0.1$) and panel (b) the case of a first order phase transition ($\Delta = 0.485$).

A picture of the phase diagram is shown in Fig. 12.

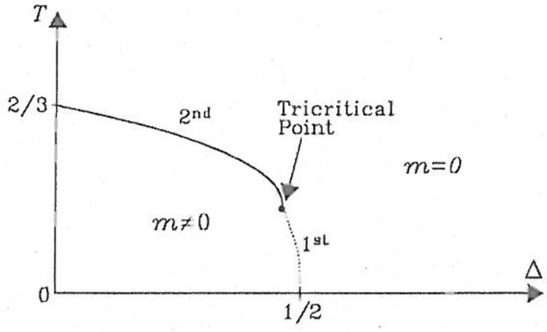


Fig. 12. Phase diagram of the Blume–Emery–Griffiths model in the canonical ensemble. The second order transition line (solid) ends at the tricritical point (•), where the transition becomes first order (dotted).

4.2.3. *The solution in the microcanonical ensemble*

The derivation of the phase diagram of the BEG model (73) in the *microcanonical ensemble* relies on a simple counting problem [14], since all spins interact with equal strength, independently of their mutual distance. A given macroscopic configuration is characterized by the numbers N_+, N_-, N_0 of up, down and zero spins, with $N_+ + N_- + N_0 = N$. The energy E of this configuration is only a function of N_+, N_- and N_0 and is given by

$$E = \Delta Q - \frac{1}{2N}M^2, \tag{82}$$

where $Q = \sum_{i=1}^{N} S_i^2 = N_+ + N_-$ (the quadrupole moment) and $M = \sum_{i=1}^{N} S_i = N_+ - N_-$ (the magnetization) are the two order parameters. The number of microscopic configurations Ω compatible with the macroscopic occupation numbers N_+, N_- and N_0 is

$$\Omega = \frac{N!}{N_+!N_-!N_0!}. \tag{83}$$

Using Stirling's approximation in the large N limit, the entropy, $S = \ln \Omega$, is given by

$$S = -N\left[(1-q)\ln(1-q) + \frac{1}{2}(q+m)\ln(q+m) + \frac{1}{2}(q-m)\ln(q-m) - q\ln 2\right], \tag{84}$$

where $q = Q/N$ and $m = M/N$ are the quadrupole moment and the magnetization per site, respectively. Eq. (82) may be written as

$$q = 2K\varepsilon + Km^2, \tag{85}$$

where $K = 1/(2\Delta)$. Using this relation, the entropy per site $\tilde{s} = S/N$ can be expressed in terms of m and ε, as follows

$$\begin{aligned}\tilde{s}(\varepsilon, m) = {} & -(1 - 2K\varepsilon - Km^2)\ln(1 - 2K\varepsilon - Km^2) - \frac{1}{2}(2K\varepsilon + Km^2 + m)\ln(2K\varepsilon + Km^2 + m) \\ & - \frac{1}{2}(2K\varepsilon + Km^2 - m)\ln(2K\varepsilon + Km^2 - m) + (2K\varepsilon + Km^2)\ln 2.\end{aligned} \tag{86}$$

At fixed ε, the value of m which maximizes the entropy corresponds to the equilibrium magnetization. The corresponding equilibrium entropy

$$s(\varepsilon) = \sup_m \tilde{s}(\varepsilon, m) \tag{87}$$

contains all the relevant information about the thermodynamics of the system in the microcanonical ensemble. As usual in systems where the energy per particle is bounded from above, the model has both a positive and a negative temperature region: entropy is a one humped function of the energy. In order to locate the continuous transition line, one develops $\tilde{s}(\varepsilon, m)$ in powers of m, in analogy with what has been done above for the canonical free energy

$$\tilde{s} = \tilde{s}_0 + A_{mc}\, m^2 + B_{mc}\, m^4 + O(m^6), \tag{88}$$

where

$$\tilde{s}_0 = \tilde{s}(\varepsilon, m = 0) = -(1 - 2K\varepsilon)\ln(1 - 2K\varepsilon) - 2K\varepsilon\ln(K\varepsilon), \tag{89}$$

and

$$A_{mc} = -K \ln \frac{K\varepsilon}{(1-2K\varepsilon)} - \frac{1}{4K\varepsilon}, \tag{90}$$

$$B_{mc} = -\frac{K}{4\varepsilon(1-2K\varepsilon)} + \frac{1}{8K\varepsilon^2} - \frac{1}{96K^3\varepsilon^3}. \tag{91}$$

In the paramagnetic phase both A_{mc} and B_{mc} are negative, and the entropy is maximized by $m = 0$. The continuous transition to the ferromagnetic phase takes place at $A_{mc} = 0$ for $B_{mc} < 0$. In order to obtain the critical line in the (T, Δ) plane, we first observe that temperature is calculable on the critical line ($m = 0$) using (53) and (89). One gets

$$\frac{1}{T} = 2K \ln \frac{1-2K\varepsilon}{K\varepsilon}. \tag{92}$$

Requiring now that $A_{mc} = 0$, one gets the following expression for the critical line

$$\beta = \frac{\exp[\beta/(2K)]}{2} + 1. \tag{93}$$

Equivalently, this expression may be written as $\beta = 1/(2K\varepsilon)$. The microcanonical critical line thus coincides with the critical line (80) obtained for the canonical ensemble. The tricritical point of the microcanonical ensemble is obtained at $A_{mc} = B_{mc} = 0$. Combining these equations with Eq. (92), one finds that, at the tricritical point, β satisfies the equation

$$\frac{K^2}{2\beta^2}\left[1 + 2\exp\left(-\frac{\beta}{2K}\right)\right] - \frac{K}{2\beta} + \frac{1}{12} = 0. \tag{94}$$

Eqs. (93) and (94) yield a tricritical point at $K \simeq 1.0813$, $\beta = 3.0272$. This has to be compared with the canonical tricritical point located at $K = 1/(2\Delta) = 3/\ln(16) \simeq 1.0820$, $\beta = 3$. The two points, although very close to each other, do not coincide. The microcanonical critical line extends beyond the canonical one. This feature, which is a clear indication of ensemble inequivalence, was first found analytically for the BEG model [14] and later confirmed for gravitational models [4,34]. The non-coincidence of microcanonical and canonical tricritical points is a generic feature, as proven in Ref. [42].

4.2.4. *Inequivalence of ensembles*

We have already discussed in general terms the question of ensemble equivalence or inequivalence in Sections 4.1.1 and 4.1.3. Inequivalence is associated to the existence of a convex region of the entropy as a function of energy. This is exactly what happens for the BEG model in the region of parameters $1 < K < 3\ln(16)$. Since the interesting region is extremely narrow for this model [14], it is more convenient to plot a schematic representation of the entropy and of the free energy (see Fig. 13). We show what happens in a region of K where both a *negative specific heat* and a *temperature jump* are present. The entropy curve consists of two branches: the high energy branch is obtained for $m = 0$ (dotted line), while the low energy one is for $m \neq 0$ (full line). The $m = 0$ branch has been extended also in a region where it corresponds to metastable states, just to emphasize that these correspond to a smaller entropy and that it remains a concave function overall the energy range. We have not extended the $m \neq 0$ branch in the high energy region not to make the plot confusing: it would also correspond to a metastable state. The two branches merge at an energy value ε_t where the left and right derivatives do not coincide; hence microcanonical temperature is different on the two sides, leading to a *temperature jump*. It has been proven in Ref. [42], that for all types of bifurcation the temperature jump is always negative. In the low energy branch, there is a region where entropy is locally convex (thick line in Fig. 13), giving a *negative specific heat* according to formula (70). The convex envelope, with constant slope β_t is also indicated by the dash-dotted line. In the same figure, we plot the rescaled free energy $\phi(\beta)$, which is a concave function, with a point β_t where left and right derivatives (given by ε_1 and ε_2 respectively) are different. This is the first order phase transition point in the canonical ensemble.

A schematic phase diagram near the canonical tricritical point (CTP) and the microcanonical one (MTP) is given in Fig. 14. In the region between the two tricritical points, the canonical ensemble yields a first order phase transition at a higher temperature, while in the microcanonical ensemble the transition is still continuous. It is in this region that negative specific heat appears. Beyond the microcanonical tricritical point, temperature has a jump at the transition energy in the microcanonical ensemble. The two lines emerging on the right side from the MTP correspond to the two limiting temperatures which are reached when approaching the transition energy from below and from above (see Fig. 15c and d). The two microcanonical temperature lines and the canonical first order phase transition line all merge on the $T = 0$ line at $\Delta = 1/2$.

To get a better understanding of the microcanonical phase diagram and also in order to compare our results with those obtained for self-gravitating systems [4,34] and for finite systems [9,19,31,87], we consider the temperature–energy relation $T(\varepsilon)$ (also called in the literature the "caloric curve"). Also this curve has two branches: a high energy branch (92) corresponding to $m = 0$, and a low energy branch obtained from (53) using the spontaneous magnetization $m_s(\varepsilon) \neq 0$. At the intersection point of the two branches, the two entropies become equal. However, their first derivatives at the crossing point can be different, resulting in a jump in the temperature, i.e. *a microcanonical first order transition*. When the transition is

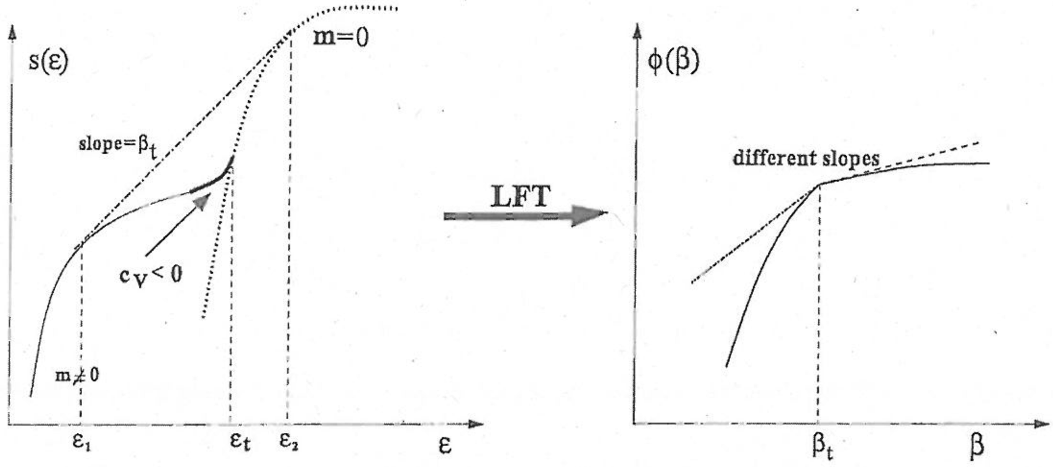


Fig. 13. Left graph: schematic plot of the entropy $s(\varepsilon)$ as a function of energy density ε for the BEG model in a case where negative specific heat coexists with a temperature jump. The dash-dotted line is the concave envelope of $s(\varepsilon)$ and the region with negative specific heat $c_V < 0$ is explicitly indicated by the thick line. Right graph: Rescaled free energy $\phi(\beta)$: the first order phase transition point β_t is shown.

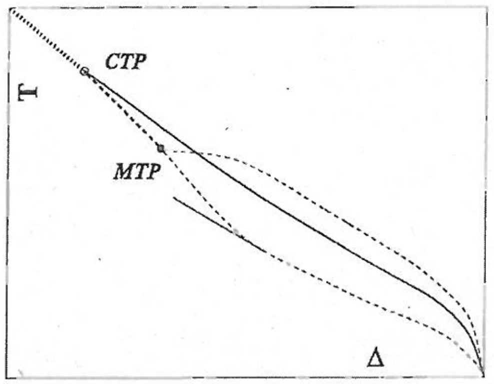


Fig. 14. A schematic representation of the phase diagram, where we expand the region around the canonical (CTP) and the microcanonical (MTP) tricritical points. The second order line, common to both ensembles, is dotted, the first order canonical transition line is solid and the microcanonical transition lines are dashed (with the bold dashed line representing a continuous transition).

continuous in the microcanonical ensemble, i.e. the first derivative of the entropy branches at the crossing point are equal, the BEG model always displays, at variance with what happens for gravitational systems, a discontinuity in the second derivative of the entropy. This is due to the fact that here we have a true symmetry breaking transition [42]. Fig. 15 displays the $T(\varepsilon)$ curves for decreasing values of K. For $K = 3/\ln(16)$, corresponding to the canonical tricritical point, the lower branch of the curve has a zero slope at the intersection point (Fig. 15a). Thus, the specific heat of the ordered phase diverges at this point. This effect signals the canonical tricritical point through a property of the microcanonical ensemble. Decreasing K, down to the region between the two tricritical points, a *negative specific heat* in the microcanonical ensemble first arises ($\partial T/\partial\varepsilon < 0$), see Fig. 15b. At the microcanonical tricritical point, the derivative $\partial T/\partial\varepsilon$ of the lower branch diverges at the transition point, yielding a vanishing specific heat. For smaller values of K, a jump in the temperature appears at the transition energy (Fig. 15c). The lower temperature corresponds to the $m = 0$ solution (92) and the upper one is given by $\exp(\beta/2K) = 2(1-q^*)/\sqrt{(q^*)^2 - (m^*)^2}$, where m^*, q^* are the values of the order parameters of the ferromagnetic state at the transition energy. The negative specific heat branch disappears at even smaller values of K, leaving just a temperature jump (see Fig. 15d). In the $K \to 1$ limit the low temperature branch, corresponding to $q = m = 1$ in the limit, shrinks to zero and the $m = 0$ branch (92) occupies the full energy range.

4.3. Entropy and free energy dependence on the order parameter

In this section, we will discuss in detail the dependence of both the canonical free energy and the microcanonical entropy on the order parameter. This will allow to understand more deeply the relation between the two ensembles by revisiting Maxwell constructions. Besides that, we will also discover an interesting physical effect, *negative susceptibility*, of which we will give an explicit example, see Section 4.5.4.