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Problem Set 5
The Blume–Emery–Griffiths model

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Reminder

At low temperature, pure ^{4}He changes from a normal fluid to a superfluid phase (the so-called λ transition). When ^{3}He atoms are added, the transition is modified. In this Problem, we shall describe such a ^{3}He-^{4}He mixture. To do so, we will use a lattice model proposed by Blume, Emery, and Griffiths in 1971 [1]. Each of the N sites of the lattice is occupied by a ^{4}He or ^{3}He atom, and has z nearest neighbors. To each site is associated a fictitious spin S_i, taking the values 0 and ±1. A ^{3}He atom at site i corresponds to $S_i = 0$ and a ^4He atom to $S_i = \pm 1$. The spin degree of freedom describes the nature of the system : if $m = \langle S_i \rangle = 0$, the fluid is normal, while if $m \neq 0$, it is a superfluid.

1 Preliminaries

(a) Show that the number of ^{3}He and ^{4}He atoms are given by $N_3 = \sum_{i=1}^{N}(1 - S - i^2)$ and $N_4 = \sum_{i=1}^{N} S_i^2$, respectively, with $N = N_3 + N_4$.

(b) Show that the average fraction x of ^{3}He atoms on the lattice is given by $x = 1 - \langle S_i^2 \rangle$.

$$\begin{aligned} x &= \frac{\langle N_3 \rangle}{N} \\ &= \frac{\sum_{i=1}^{N}(1 - \langle S_i^2 \rangle)}{N} \\ &= \frac{N - \langle S_i^2 \rangle \sum_{i=1}^{N} 1}{N} \\ &= 1 - \langle S_i^2 \rangle \end{aligned}$$

2 Model Hamiltonian

We first introduce an Ising Hamiltonian with an external field H and a coupling constant $-J$ between nearest neighbors which describes the tendency of the system to be superfluid at low temperature,

$$\mathcal{H}_1 = -J\sum_{\langle i,j\rangle} S_i S_j - H\sum_{i=1}^{N} S_i$$

Here, $\langle i,j\rangle$ denotes a sum over nearest neighbor spins.

(a) Briefly justify the use of the above Hamiltonian to describe the ^{3}He-^{4}He mixture. What is the sign of J ?

(b) We then want to describe the interactions between nearest neighbor atoms. Let us denote $-u_{33}$, $-u_{44}$, and $-u_{34} = -u_{43}$ the interaction energy between each type of pairs (^{3}He-^{3}He, ^{4}He-^{4}He, ^{3}He-^{4}He and ^{4}He-^{3}He, respectively). Show that

$$\mathcal{H}_{\text{int}} = -u_{44}\sum_{\langle i,j\rangle} S_i^2 S_j^2 - u_{33}\sum_{\langle i,j\rangle}(1-S_i^2)(1-S_j^2) - 2u_{34}\sum_{\langle i,j\rangle}(1-S_i^2)S_j^2$$

$$\begin{aligned}
\mathcal{H}_{\text{int}} = -u_{44}\sum_{\langle i,j\rangle} S_i^2 S_j^2 \qquad & = 0 \text{ if } S_i^2 \text{ or } S_j^2 = 0 \\
- u_{33}\sum_{\langle i,j\rangle}(1-S_i^2)(1-S_j^2) \qquad & = 0 \text{ if } S_i^2 \text{ or } S_j^2 = 1 \\
- 2u_{34}\sum_{\langle i,j\rangle}(1-S_i^2)S_j^2 \qquad & = 0 \text{ if } S_i^2 = 1 \text{ or } S_j^2 = 0
\end{aligned}$$

There is a 2 in front of u_{34} because $u_{34} = u_{43}$.

(c) Finally, we take into account the chemical potentials μ_3 and μ_4 of the two species (^{3}He and ^{4}He, respectively). The full Hamiltonian then reads $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_{\text{int}} - \mu_3 N_3 - \mu_4 N_4$, where N_3 and N_4 are the number of ^{3}He and ^{4}He atoms, respectively. Show that the above Hamiltonian takes the form

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} S_i S_j - K\sum_{\langle i,j\rangle} S_i^2 S_j^2 - H\sum_{i=1}^{N} S_i - \Delta\sum_{i=1}^{N} S_i^2 + C \tag{1}$$

Give the expressions of the constants K, Δ, and C as a function of the parameters of the problem. In what follows, we set $C = 0$. Why can we do so ?

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_{\text{int}} \underbrace{-\mu_3 N_3 - \mu_4 N_4}_{\text{for conveniance}}$$

So,

$$\begin{aligned}\mathcal{H} = &-J\sum_{\langle i,j\rangle} S_i S_j - H\sum_{i=1}^{N} S_i - u_{44}\sum_{\langle i,j\rangle} S_i^2 S_j^2 - u_{33}\sum_{\langle i,j\rangle}(1-S_i^2)(1-S_j^2) \\ &- 2u_{34}\sum_{\langle i,j\rangle}(1-S_i^2)S_j^2 - \mu_4\sum_{i=1} S_i^2 - \mu_3\sum_{i=1}^{N}(1-S_i^2)\end{aligned}$$

> **Reminder :**
>
> $$\sum_{\langle i,j\rangle} S_i^2 = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\in \mathrm{nn}(i)} S_i^2 = \frac{z}{2}\sum_{i=1}^{N} S_i^2$$
>
> $$\sum_{\langle i,j\rangle} 1 = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\in \mathrm{nn}(i)} 1 = \frac{Nz}{2}$$

So,

$$\begin{aligned}\mathcal{H} = &-J\sum_{\langle i,j\rangle} S_i S_j - \underbrace{[u_{44}+u_{33}-2u_{34}]}_{\equiv K}\sum_{\langle i,j\rangle} S_i^2 S_j^2 - H\sum_{i=1}^{N} S_i - \underbrace{[z(u_{34}-u_{33})+\mu_4-\mu_3]}_{\equiv \Delta}\sum_{i=1}^{N} S_i^2 \\ &\underbrace{-\left(\frac{Nz}{2}u_{33}+\mu_3 N\right)}_{\equiv C}\end{aligned}$$

C is a constant, it just set the zero energy, so we can set it to 0.

3 Mean field approximation

Let us decompose the spin S_i into its average value $\langle S_i \rangle$ and the fluctuations δS_i around the latter : $S_i \langle S_i \rangle + \delta S_i$. Let us further decompose S_i^2 into $\langle S_i^2 \rangle$ and δS_i^2, the fluctuations of S_i^2 around $\langle S_i^2 \rangle$: $S_i^2 = \langle S_i^2 \rangle + \delta S_i^2$.

(a) We define the two correlation functions $C_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$ and $\tilde{C}_{ij} = \langle S_i^2 S_j^2 \rangle - \langle S_i^2 \rangle \langle S_j^2 \rangle$. Show that $C_{ij} = \langle \delta S_i \delta S_j \rangle$ and $\tilde{C}_{ij} = \langle \delta S_i^2 \delta S_j^2 \rangle$. What are the values of C_{ij} and $\tilde{C}_{ij}$ within the mean field approximation (MFA) ?

The idea of the mean-field approximation is to neglect the correlations, so the spin-slin correlation function C_{ij} and $\tilde{C}_{ij}$ are equal to 0,

$$C_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle = \langle \delta S_i \delta S_j \rangle \approx 0$$

$$\tilde{C}_{ij} = \langle S_i^2 S_j^2 \rangle - \langle S_i^2 \rangle \langle S_j^2 \rangle = \langle \delta S_i^2 \delta S_j^2 \rangle \approx 0$$

(b) In the MFA, show that the Hamiltonian (1) reads

$$\mathcal{H} \simeq \frac{Nz}{2}[Jm^2 + K(1-x)^2] - (H + zJm)\sum_{i=1}^{N} S_i - [\Delta + zK(1-x)]\sum_{i=1}^{N} S_i^2$$

$$\begin{aligned}\mathcal{H} = &-J\sum_{\langle i,j \rangle}(m + \delta S_i)(m + \delta S_j)\\ &- K\sum_{\langle i,j \rangle}(1_x + \delta S_i^2)(1 - x + \delta S_j^2)\\ &- H\sum_{i=1}^{N} S_i - \Delta\sum_{i=1}^{N} S_i^2\end{aligned}$$

$$\begin{aligned}\mathcal{H} \approx &-J\frac{m^2 Nz}{2} - Jmz\sum_{i=1}^{N}\delta S_i\\ &- K\frac{(1-x)^2 Nz}{2} - K(1-x)z\sum_{i=1}^{N}\delta S_i^2\\ &- H\sum_{i=1}^{N} S_i - \Delta\sum_{i=1}^{N} S_i^2\end{aligned}$$

$$\mathcal{H} = \frac{Jm^2 Nz}{2} + \frac{K(1-x)^2 Nz}{2} - Jmz\sum_{i=1}^{N} S_i - K(1-x)z\sum_{i=1}^{N} S_i^2 - H\sum_{i=1}^{N} S_i - \Delta\sum_{i=1}^{N} S_i^2$$

$$\mathcal{H}_{\text{MFA}} = \frac{Nz}{2}[Jm^2 + K(1-x)^2] - [H + zJm]\sum_{i=1}^{N} S_i - [\Delta + zK(1-x)]\sum_{i=1}^{N} S_i^2$$

(c) Deduce from the previous question an expression for the grand-canonical partition function Ξ and the grand potential Ω.

$$\begin{aligned}\Xi &= \sum_k e^{-\beta\mathcal{H}}\\ &= \sum_{S_1=-1}^{+1}\cdots\sum_{S_N=-1}^{+1} e^{-\frac{\beta N z}{2}[Jm^2+K(1-x)^2]}\prod_{i=1}^{N} e^{\beta[H+zJm]S_i+\beta[\Delta+zK(1-x)]S_i^2}\\ &= e^{-\frac{\beta N z}{2}[Jm^2+K(1-x)^2]}\times\left\{1+2e^{\beta(\Delta+zK(1-x))}\cosh(\beta(H+zJm))\right\}^N\end{aligned}$$

$$\begin{aligned}\Omega &= -k_BT\ln\Xi\\ &= \frac{Nz}{2}[Jm^2+K(1-x)^2]-Nk_BT\ln[1+2e^{\beta(\Delta+zK(1-x))}\cosh(\beta(H+zJm))]\end{aligned}$$

(d) Show that the two self-consistent equations determining m and x are given by

$$m = \frac{2\exp(\beta[\Delta+zK(1-x)])\sinh(\beta[H+zJm])}{1+2\exp(\beta[\Delta+zK(1-x)])\cosh(\beta[H+zJm])} \tag{2a}$$

$$x = \frac{1}{1+2\exp(\beta[\Delta+zK(1-x)])\cosh(\beta[H+zJm])} \tag{2b}$$

where $\beta = 1/k_BT$.

The numerical solution of Eqs. (2a)(2b), at vanishing external field ($H=0$) and for $K=0$ (which typically corresponds to the experimental situation ; why ?), give the phase diagram of Fig. 1.

$$m = \langle S_i\rangle$$

$$\left\langle\sum_{i=1}^{N} S_i\right\rangle = Nm = \sum_l\left(\sum_i S_i\right)\frac{e^{-\beta\mathcal{H}}}{\Xi} = \frac{1}{\beta}\frac{\partial\ln\Xi}{\partial H} = -\frac{\partial\Omega}{\partial H}$$

Meaning,

$$m = -\frac{1}{N}\frac{\partial\Omega}{\partial H}$$

$$x = 1-\langle S_i^2\rangle$$

$$\left\langle \sum_{i=1}^{N} S_i^2 \right\rangle = N\langle S_i^2\rangle = N(1-x) = \sum_l \left(\sum_i S_i^2\right) \frac{e^{-\beta\mathcal{H}}}{\Xi} = \frac{1}{\beta}\frac{\partial \ln \Xi}{\partial \Delta} = -\frac{\partial \Omega}{\partial \Delta}$$

Meaning,

$$x = 1 + \frac{1}{N}\frac{\partial \Omega}{\partial \Delta}$$

> **Remark :** H is also within m and x, but we know that the true equilibirum for m and x is at the minimum of the energy, meaning that,
>
> $$\frac{\partial \Omega(H, m(H), x(H))}{\partial H} = \frac{\partial \Omega(H, m(H), x(H))}{\partial H} + \underbrace{\frac{\partial \Omega}{\partial m}\frac{\partial m}{\partial H} + \frac{\partial \Omega}{\partial x}\frac{\partial x}{\partial H}}_{=0}$$

And so, using the formulas found for m and x we get

$$\begin{cases} m = \dfrac{2\exp(\beta[\Delta + zK(1-x)])\sinh(\beta[H + zJm])}{1 + 2\exp(\beta[\Delta + zK(1-x)])\cosh(\beta[H + zJm])} \\ x = \dfrac{1}{1 + 2\exp(\beta[\Delta + zK(1-x)])\cosh(\beta[H + zJm])} \end{cases}$$

4 Description of the phase transition

In the following, we aim at better understanding the phase diagram displayed in Fig. 1. We therefore look at the properties of the system close to the phase transition, *i.e.*, the order parameter m is close to zero. From now on, we consider the case where $K = 0$.

(a) Let us introduce the potential $G(m) = \Omega(H) + Hm$. Justify the use of such a potential in order to study the phase transition at vanishing external field ($H = 0$).

$$\Omega(H) = \frac{NzJm^2}{2} - Nk_BT\ln\big(1 + 2e^{\beta\Delta}\cosh(\beta[H - zKm])\big)$$

But m is a function of H,
we need to perform a Legendre transformation,

$$G(m) = \Omega(H) + Hm$$

Meaning,

$$\frac{\partial G}{\partial m} = H$$

For $H = 0$, m is a minimum of G, meaning it motivate a $G(m)$ expansion.

(b) We now aim at expanding $G(m)$ in powers of the order parameter m as

$$G(m) = G(0) + \frac{1}{2}am^2 + \frac{1}{4}bm^4 + \frac{1}{6}cm^6 + \mathcal{O}(m^8)$$

Limiting the expansion above to second order in m, show that $a = \delta k_BT - zJ$, where we set $\delta = 1 + e^{-\beta\Delta}/2$.
Hint : Expand Eq. (2a) for both $\beta H \ll 1$ and $m \ll 1$ in order to obtain H as a series expansion in m.
In what follows, we will admit that $b = \frac{k_BT}{8}\delta^2\left(1 - \frac{\delta}{3}\right)$ and $c = \frac{k_BT}{12}\delta^3(1 - \frac{3\delta}{4} + \frac{3\delta^2}{20})$.

$$\frac{\partial G(m)}{\partial m} = am \longrightarrow H$$

We can link them through the self-consistent equation, (2a),

$$m = \frac{2e^{\beta\Delta}\sinh(\beta[H + zJm])}{1 + 2e^{\beta\Delta}\cosh(\beta[H + zJm])}$$

Meaning,

$$m \approx \frac{2e^{\beta\Delta}\beta[H+zJm]}{1+2e^{\beta\Delta}}$$
$$= \frac{\beta[H+zJm]}{1+\frac{e^{-\beta\Delta}}{2}}$$

Which can we wrote,

$$\frac{\delta}{\beta}m = H + zJm$$

$$(k_B T\delta - zJ)\, m = H \equiv am$$

So we get

$$a = (k_B T\delta - zJ)$$

(First Landau Coefficient)

(c) Let us assume that $c > 0$. Sketch $\Delta G(m) = G(m) - G(0)$ as a function of m when $b > 0$. Then show that there exists a second-order phase transition at the critical temperature $T_c(x) = T_c(0)(1-x)$, with $k_B T_c(0) = zJ$.

We assume $c > 0$,

$$G(m) = G(0) + \frac{am^2}{2} + \frac{bm^4}{4} + \frac{cm^6}{6} + \mathcal{O}(m^8)$$

We know that

$$b \propto 1 - \frac{\delta}{3}$$

Meaning it can be either positive or negative. From (2b),

$$x = \frac{1}{1+2e^{\beta\Delta}\cosh(\beta[H+zJm])} \simeq \frac{1}{1+2e^{\beta\Delta}}$$

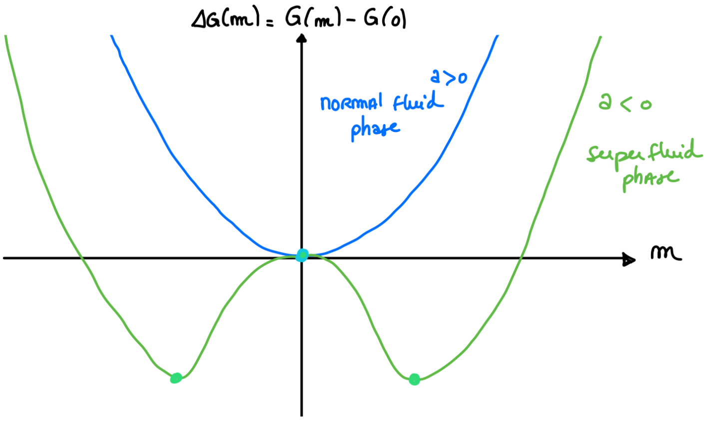
So,

$$1 - x = \frac{2e^{\beta\Delta}}{1+2e^{\beta\Delta}} = \frac{1}{\delta} \iff \delta = \frac{1}{1-x}$$

Meaning it's somehow a measure of the fraction of ^{3}He.

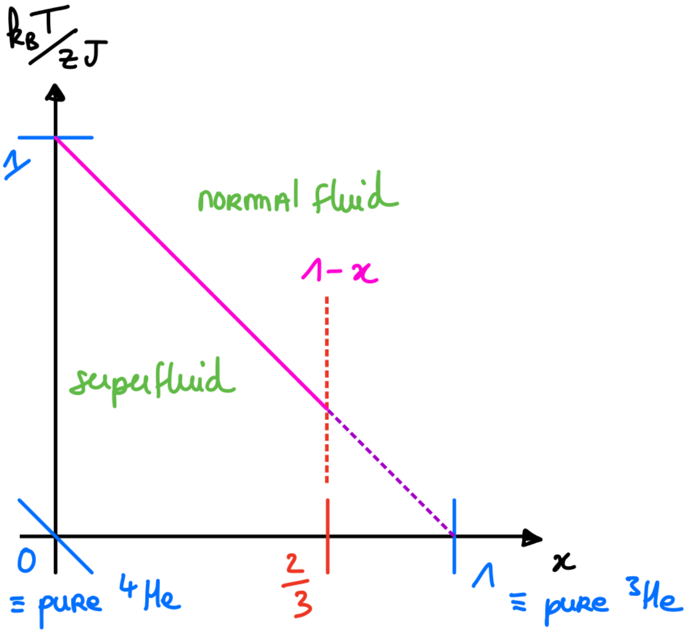
- If we assume $b > 0$, it means that $\delta < 3$,

$$\frac{1}{1-x} < 3 \longrightarrow x < \frac{2}{3}$$

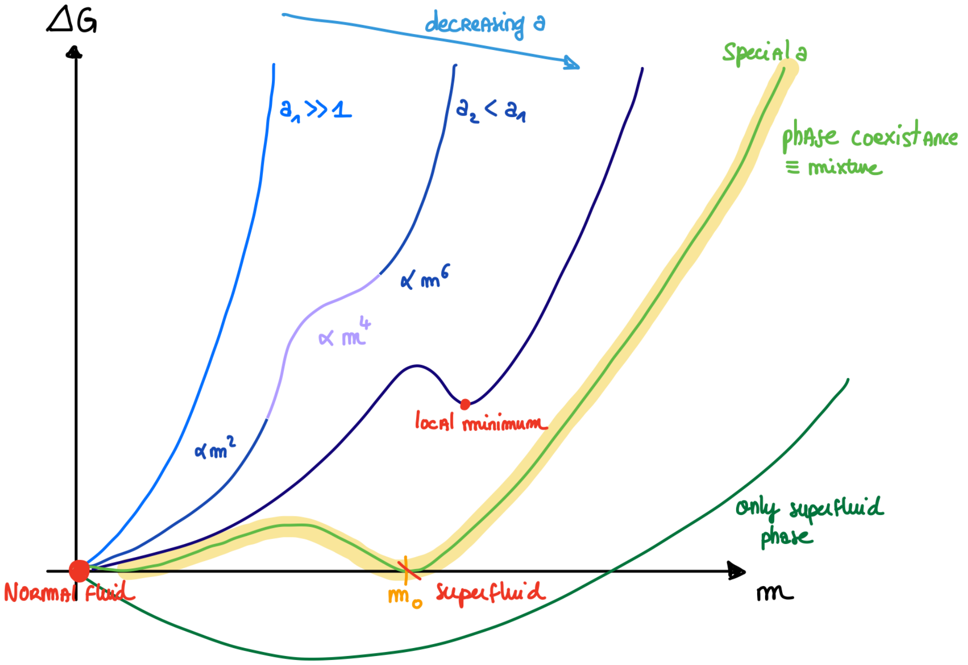


So we get a continuous phase transition for $a = 0$,

$$k_B T_c = (1 - x) z J$$



(d) Sketch $\Delta G(m)$ for $b < 0$. What happens in this case? Show that the equation for the first-order phase transition line is given by $a = 3b^2/16c$.



Let's determine the special a,

$$\Delta G = \frac{c}{6} m^2 (m^2 - m_0^2)^2$$

and it is equal to 0 for $m = 0$ or $m = \pm m_0$.
We need to have the same behavior as

$$\frac{am^2}{2} + \frac{bm^4}{4} + \frac{cm^6}{6}$$

from

$$\frac{cm^6}{6} - \frac{1}{3} c m_0^2 m^4 + \frac{c}{6} m_0^4 m^2$$

And so we get,

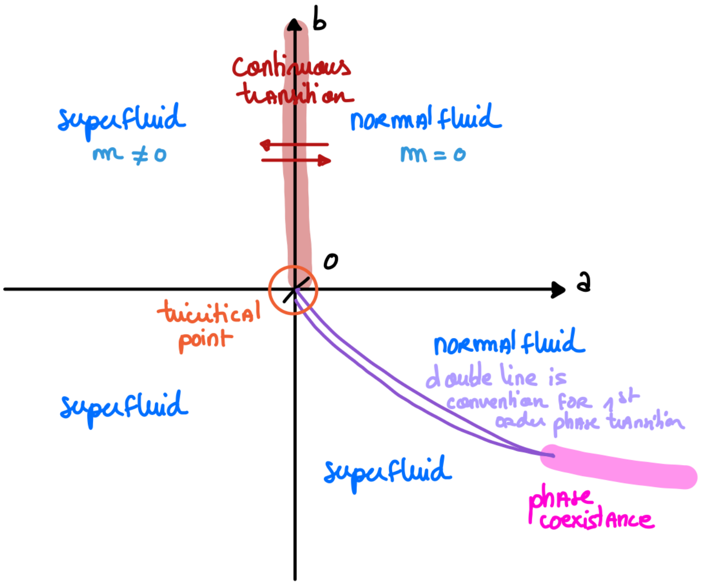
$$\begin{cases} -\dfrac{c}{3} m_0^2 = \dfrac{b}{4} \\ \dfrac{cm_0^4}{6} = \dfrac{a}{2} \end{cases} \implies m_0 = \pm \sqrt{\frac{3b}{4c}}$$

And we get

$$\begin{aligned} a &= \frac{cm_0^4}{3} \\ &= \frac{c9b^2}{3 \times 16c^2} \\ &= \frac{3b^2}{16c} \end{aligned}$$

it defines the condition for phase coexistence.

(e) Show that there exists a tricritical point (T_t, x_t). Calculate T_t and x_t.



$$b^2 = \frac{16ca}{3} \longrightarrow b = -\sqrt{\frac{16ca}{3}}$$

At tricritical point, $a = b = 0$,

$$\begin{cases} a = k_B T\delta - zJ = \dfrac{k_B T}{1-x} - zJ \\ b = \dfrac{k_B T}{8}\delta^2\left(1 - \dfrac{\delta}{3}\right) \end{cases} = 0$$

Meaning,

$$1 - \frac{\delta}{3} = 0 \longrightarrow \delta = 3 \longrightarrow x_t = \frac{2}{3}$$

And we get,

$$k_B T_t = \frac{zJ}{3}$$

(f) Compare your theoretical predictions with the experimental results in Fig. 2.

Too good to be true, yet it is true.