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N.Angelescu, G.Nenciu, N.S.Tonchev

ON THE THEORY
OF THE EXCITONIC PHASE TRANSITION
IN THE PRESENCE OF A RESERVOIR

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1. INTRODUCTION

This paper is a comment on an approach largely followed when constructing the phase diagram in the $n-\theta$ plane (n is the particle density; θ, the temperature), rather than in the $\mu-\theta$ plane (μ denotes the chemical potential), for a series of mean-field models used to describe the antiferromagnetism of chromium and its alloys ([1,2] and references therein), the metal-insulator transition [3], or the so-called excitonic insulator state of a two-band semimetal [4,5]. The approach consists essentially in soving the self-consistency equation for the order parameter, Δ :

$$\frac{\partial f^{\circ}}{\partial \Delta}(\mu, \theta ; \Delta) = 0 \tag{1}$$

and the fixed-density (or electroneutrality) condition:

$$n = -\frac{\partial f^{\circ}}{\partial \mu}(\mu, \theta; \Delta), \tag{2}$$

as a system in the unknowns Δ and μ . Here, f° denotes the mean-field grand-canonical potential. Among the solutions of the system (1), (2), one chooses that one, $(\Delta(n,\theta), \mu(n, \theta))$, which provides the minimum free energy:

$$\widetilde{F}(n, \theta) = f^{\circ}(\mu(n, \theta), \theta; \Delta(n, \theta)) + n\mu(n, \theta). \tag{3}$$

At first sight, there is nothing wrong here. However, when following this route, it turns out that the phase diagram given by $\widetilde{F}(n, \theta)$ shows only a critical line, in spite of the fact that the $\mu-\theta$ phase diagram shows a critical line changing at a tricritical point into a line of first order phase transitions. This is especially inconvenient in view of the fact that, e.g., experiments of chromium [6] (where n is fixed on physical grounds) show a first order transition in θ . There have been various attempts to explain the origin of the first order transition, either by introducing particle reservoirs of various powers [1] or by taking into account fluctuations [7] , or the contribution of other harmonics [8].

We argue here that the first order transition can be explained without any further sophistication of the original models, simply by solving them correctly. Thereby we clarify also the role of

the reservoir. We point out that the correct free energy, which we denote $F(n, \theta)$, is the convex envelope of $\tilde{F}(n, \theta)$ defined by Eq. (3), and that the phase diagram given by $F(n, \theta)$ has the wanted property: a tricritical point and a region of phase coexistence.

We were in fact led to suspect the correctness of the approach outlined above by the remark that the results obtained in this way present the highly unphysical feature that the free energy, $F(n, \theta)$, is not a convex function of n for sufficiently low temperature. The situation is in close analogy with that encountered in the Van der Waals theory of the liquid-gas transition, with $\tilde{F}$ corresponding to the Van der Waals loop and F presenting a flat spot in analogy with the Maxwell construction. See also the Appendix. We suspect that our considerations apply equally well to the treatment of more elaborated models, like those in Refs. [1,2] or [8].

2. THE MODELS

We shall consider the physical system consisting of two isotropic electron bands, a and b, with equal effective masses:

$$\epsilon_{a,b}(k) = \pm(\frac{k^2}{2m} - \epsilon_F)$$ (4)

and a third band, d, with dispersion law $\epsilon_d(k)$, which will play the role of an electron reservoir [1]. Two types of interactions can lead to the onset of an electron-hole (excitonic) condensate:

a) the interband Coulomb interaction:

$$\mathcal{H}_{e-e} = \sum_{\substack{q,k,k' \\ \mu,\mu'}} v(k,k',q) a^+_{k+q,\mu} a_{k,\mu} b^+_{k'-q,\mu'} b_{k',\mu'}$$ (5)

b) the interband electron-phonon interaction:

$$\mathcal{H}_{e-ph} = \sum_{k,p,\mu} g(k) a^+_{k\mu} b_{p+k,\mu} (c^+_p + c_{-p}) + h.c.$$ (6)

We use the notation $a^+_{k,\mu}$, $b^+_{k,\mu}$, $d^+_{k,\mu}$ for the creation operators for electrons with momentum k and spin μ in bands a, b and d, respectively, and c^+_p for the phonon creation operators.

The study of the excitonic phase transition in term of the interactions (5) and/or (6) is usually done within the Hartree-Fock approximation [9,10]. In order to make clear once more the physical assumptions hidden in this approximation, we prefer to replace (5) and (6) by reduced interactions, which on one hand should allow an exact solution, and on the other hand should contain that part of the interaction which is responsible for the excitonic transition:

$$\mathcal{H}^{red.}_{e-e} = -\frac{2\lambda_{e-e}}{V}(\sum_{k,\mu,\nu} a^+_{k,\mu} \gamma_{\mu\nu} b_{k,\nu}) \cdot (\sum_{k,\mu,\nu} b^+_{k,\nu} \gamma_{\nu\mu} a_{k,\mu}),$$ (5')

$$\mathcal{H}^{red}_{e-ph} = \frac{\lambda_{e-ph}}{2\sqrt{V}}(c^+ + c) \sum_{k,\mu} a^+_{k,\mu} b_{k,\mu} + h.c.,$$ (6')

where V is the volume, λ_{e-e} and λ_{e-ph} are effective coupling constants, $\gamma_{\mu\nu} = \delta_{\mu\nu}$ (respectively, $\sigma^z_{\mu\nu}$, where σ^z is the Pauli matrix) for the case of singlet (respectively, triplet) pairing.

In conclusion, we shall work with the models defined by one of the following Hamiltonians:

$$\mathcal{H}_1 = \sum_{k,\mu} (\epsilon_a(k) a^+_{k,\mu} a_{k,\mu} + \epsilon_b(k) b^+_{k,\mu} b_{k,\mu} + \epsilon_d(k) d^+_{k,\mu} d_{k,\mu}) + \mathcal{H}^{red}_{e-e},$$ (7)

$$\mathcal{H}_2 = \omega c^+ c + \sum_{k,\mu} (\epsilon_a(k) a^+_{k,\mu} a_{k,\mu} + \epsilon_b(k) b^+_{k,\mu} b_{k,\mu} +$$

$$+ \epsilon_d(k) d^+_{k,\mu} d_{k,\mu}) + \mathcal{H}^{red}_{e-ph}.$$ (8)

3. CALCULATION OF THE GRAND-CANONICAL POTENTIAL

In the grand-canonical ensemble at given chemical potential μ, one has to add to the model Hamiltonian a term:

$$-\mu \hat{N} = -\mu \sum_{k,\nu} (a^+_{k,\nu} a_{k,\nu} + b^+_{k,\nu} b_{k,\nu} + d^+_{k,\nu} d_{k,\nu})$$ (9)

and evaluate the limit as $V \to \infty$ of the thermodynamical potential:

$$f_V(\mu, \theta) = -\frac{\theta}{V} \ln \text{Tr} \exp[-\frac{1}{\theta}(\mathcal{H} - \mu\hat{N})].$$ (10)

In the cases under consideration, i.e., both for the Hamiltonians (7) and (8) (and even in a more general case, where both interactions $\mathcal{H}^{red}_{e-e}$ and $\mathcal{H}^{red}_{e-ph}$ are present), one can rigorously show [11,12] that:

$$f(\mu, \theta) \equiv \lim_{V \to \infty} f_V(\mu, \theta) = \min_{\Delta \in R(C)} f^o(\mu, \theta; \Delta),$$ (11)

where:

$$f^\circ(\mu, \theta; \Delta) = \lim_{V \to \infty} \left(-\frac{\theta}{V}\right) \cdot \ln \mathrm{Tr} \exp\left[-\frac{1}{\theta}(\mathcal{H}(\Delta) - \mu \hat{N})\right] \tag{12}$$

and $\mathcal{H}(\Delta)$ is a mean-field Hamiltonian given by:

$$\mathcal{H}(\Delta) = \sum_{k,\nu} (\epsilon_a(k) a^+_{k,\nu} a_{k,\nu} + \epsilon_b(k) b^+_{k,\nu} b_{k,\nu} + \epsilon_d(k) d^+_{k,\nu} d_{k,\nu}) - \tag{13}$$

$$- (\Delta \sum_{k,\mu,\nu} a^+_{k,\mu} \gamma_{\mu\nu} b_{k,\nu} + h.c.) + \frac{V}{2\lambda}|\Delta|^2 ,$$

with $\lambda = \lambda_{e-e}$ for $\mathcal{H}_1$, and $\lambda = \dfrac{\lambda^2_{e-ph}}{\omega}$ for $\mathcal{H}_2$. In the former

case, Δ has the meaning of average value of $\lambda V^{-1} \sum_{k,\mu,\nu} a^+_{k,\mu} \gamma_{\mu\nu} b_{k,\nu}$

and is, in principle allowed to take all complex values in Eq. (11); however, as f° does not depend on the phase of Δ, one can restrict consideration to real, positive Δ. In the latter case, Δ has the meaning of average value of $\omega V^{-\frac{1}{2}}(c + c^+)$, so it takes by definitions only real values; the phonon mode is not "thermodynamic", i.e., it does not enter the approximating Hamiltonian $\mathcal{H}(\Delta)$, it only induces an effective electron-electron interaction (for details, see [12,13]).

The r.h.s. of Eq. (12) can be easily calculated and gives:

$$f^\circ(\mu, \theta; \Delta) = -2\theta N(0) \int_{-w}^{w} d\epsilon \{\ln[1 + \exp(\frac{\mu - \mathrm{sign}\,\epsilon \cdot \sqrt{\epsilon^2 + \Delta^2}}{\theta})] +$$

$$\tag{14}$$

$$+ p \cdot \ln[1 + \exp(\frac{\mu - \epsilon}{\theta})]\} + \frac{1}{2\lambda}\Delta^2 ,$$

where $N(0)$ is the density of states [*] at the Fermi level in bands a and b, w is a cut-off parameter, and $2pN(0)$ is the density of states [*] in band d; p is sometimes called the power of the reservoir. We take advantage of the symmetry relation: $f^\circ(-\mu, \theta; \Delta) = 4wN(0)(1 + p)\mu + f^\circ(\mu, \theta; \Delta)$, and henceforth consider only $\mu > 0$. The minimum is attained in Eq. (11) on the set of solutions of the self-consistency equation (gap equation):

$$\frac{\Delta}{N(0)\lambda} = \Delta \int_0^w d\epsilon (\epsilon^2 + \Delta^2)^{-\frac{1}{2}} [\mathrm{th} \frac{\sqrt{\epsilon^2 + \Delta^2} + \mu}{2\theta} + \mathrm{th} \frac{\sqrt{\epsilon^2 + \Delta^2} - \mu}{2\theta}]. \tag{15}$$

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[*] Here the sum over the two spin states is included.

Eq. (15) has been studied in connection with the paramagnetic effect in superconductors [14]. We shall write down the relevant formulae for $\theta = 0$, when all calculations can be performed analytically. The gap equation (15) becomes [*] :

$$\frac{\Delta}{N(0)\lambda} = 2\Delta \int_0^w d\epsilon (\epsilon^2 + \Delta^2)^{-\frac{1}{2}} \theta(\sqrt{\epsilon^2 + \Delta^2} - \mu) \approx \begin{cases} 2\Delta \ln\frac{2w}{\Delta}, & \text{if } \mu \le \Delta \\ \\ 2\Delta \ln\frac{2w}{\mu + \sqrt{\mu^2 - \Delta^2}}, & \text{if } \mu > \Delta \end{cases} \tag{16}$$

Its solutions are:

$$\Delta_1(\mu, 0) = \Delta_0 \equiv 2w \exp(-1/2N(0)\lambda) \quad \text{for} \quad \mu \le \Delta_0$$

$$\Delta_2(\mu, 0) = \sqrt{\Delta_0(2\mu - \Delta_0)} \quad \text{for} \quad \frac{\Delta_0}{2} \le \mu \le \Delta_0 \tag{17}$$

$$\Delta_3(\mu, 0) = 0 \quad \text{for all } \mu.$$

The values taken by $f^\circ(\mu, 0; \Delta)$ on the set $\Delta_i(\mu, 0)$, $i = 1,2,3$ of solutions of Eq. (16) are represented schematically in the lower part of Fig. 1. The solid line is the graph of $f(\mu,0)$ defined in Eq. (11):

$$f(\mu, 0) = \begin{cases} -2N(0)[\mu w + \frac{1}{2}w^2(1 + \frac{1}{2}\frac{\Delta_0^2}{w^2}) + \frac{1}{2}p(\mu + w)^2] & \text{for } \mu \le \frac{\Delta_0}{\sqrt{2}} \\ \\ -2N(0)(1 + p)\frac{1}{2}(\mu + w)^2 & \text{for } \mu \ge \frac{\Delta_0}{\sqrt{2}} \end{cases} \tag{18}$$

For $\mu \le \Delta_0/\sqrt{2}$, one has the excitonic phase with order parameter Δ_0; for $\Delta_0/\sqrt{2} < \mu < \infty$, one has the normal phase ($\Delta = 0$), and the kink (discontinuous first derivative) at $\mu = \Delta_0/\sqrt{2}$ corresponds to a first order transition in μ.

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[*] For simplicity of formulae, we neglected $O(\Delta/w)$ terms in the r.h.s. of Eq. (16) (weak coupling approximation).
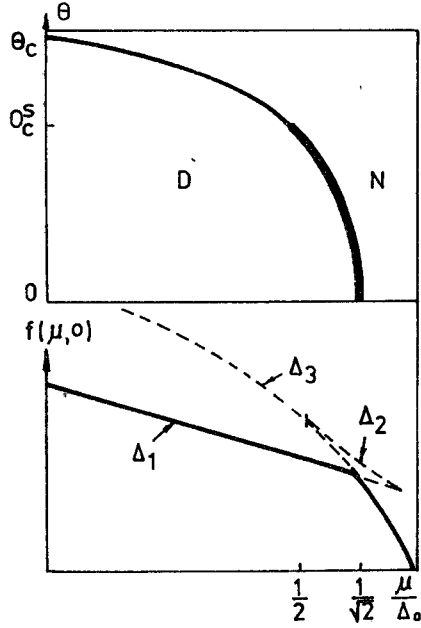
Fig. 1. The grand-canonical potential at zero-temperature and the (μ, θ)-phase diagram (schematical).

Qualitatively the same picture takes place also at fixed $\theta > 0$ up to a certain (tricritical) temperature, θ_c^s. For $\theta > \theta_c^s$, $f(\mu, \theta)$ becomes a differentiable function of μ, and the phase transition will be continuous. The corresponding phase diagram is represented in the upper part of Fig. 1 (with double line meaning a first order transition).

4. THE HELMHOLZ FREE ENERGY

On physical grounds, one is interested in the situation, where the total electron density, n, is kept fixed. The change from the (μ, θ) - to the (n, θ) - variables is to be performed, according thermodynamics, via the Legendre transformation, which expresses the Helmholz free energy, F, in terms of f as [15]:

$$F(n, \theta) = \sup_{\mu} [f(\mu, \theta) + \mu n].$$ (19)

The thremodynamics of the model in the (n, θ)-variables is fully specified by Eqs. (11) and (19).

Let us mention at once that, while in $f(\mu, \theta)$ the reservoir enters additively, that is, $f(\mu, \theta)$ is a linear function of the reservoir power p, this is not the case for $F(n, \theta)$ due to the Legende transformation, Eq. (19). Following Rice [1], we shall use instead of n the variable:

$$\mu_p = \frac{n}{2N(0)(1+p)} - w$$ (20)

which is linearly related to n and has the meaning of chemical potential in the absence of interactions.

The ground state energy in the new variable, $F(\mu_p, 0)$, calculated from Eqs. (18), (19) is expressed as:

$$F(\mu_p, 0) = \begin{cases} F_c(\mu_p), & \text{for } 0 \le \mu_p \le \frac{p}{p+1} \frac{\Delta_0}{\sqrt{2}} \\[2mm] F_n(\frac{\Delta_0}{\sqrt{2}}) + (\mu_p - \frac{\Delta_0}{\sqrt{2}}) \cdot (\frac{dF_n}{d\mu_p}\big|_{\mu_p = \frac{\Delta_0}{\sqrt{2}}}), & \text{for } \frac{p}{p+1} \frac{\Delta_0}{\sqrt{2}} \le \mu_p \le \frac{\Delta_0}{\sqrt{2}} \\[2mm] F_n(\mu_p), & \text{for } \mu_p \ge \frac{\Delta_0}{\sqrt{2}}, \end{cases}$$ (21)

where the ground state energies for the normal and condensed phases, $F_n(\mu_p)$ and $F_c(\mu_p)$ are:

$$F_n(\mu_p) = 2N(0)(1+p) \frac{\mu_p^2 - w^2}{2},$$ (22)

$$F_c(\mu_p) = 2N(0) [\frac{(1+p)^2}{2p} \mu_p^2 - (1+p)\frac{w^2}{2} - \frac{\Delta_0^2}{4}].$$ (23)

The graph of $F(\mu_p, 0)$ given by Eq. (21) is represented by solid line in the lower part of Figs. 2 and 3 (for $p < 1$ and $p > 1$, respectively). The pure excitonic phase occurs only in the interval

$0 \le \mu_p \le \frac{p}{p+1} \frac{\Delta}{\sqrt{2}}$; for $p = 0$ (i.e. no reservoir) this shrinks

into a point. The kink of f at $\mu = \frac{\Delta_0}{\sqrt{2}}$ leads to the flat spot

over $\frac{p}{p+1} \frac{\Delta_0}{\sqrt{2}} \le \mu \le \frac{\Delta_0}{\sqrt{2}}$, where one has a mixture of the excitonic

and normal phases, while for $\mu > \frac{\Delta_0}{\sqrt{2}}$ only the pure normal phase

persists. On the phase diagram one has mixed states in the whole region denoted DN in the upper parts of Figs. 2 and 3.

Let us remark that one in constrained by calculation difficulties to use the grand-canonical ensemble and then go to the physically relevant parameters (n, θ) via the Legendre transformation. One may think that the most appropriate way of calculating $F(n, \theta)$ should be the use of the canonical ensemble. Though this is justified for systems described by bona fide Hamiltonians, one has to remember that in the case of volume-dependent Hamiltonians (like ours) the use of the canonical ensemble can result in a nonconvex free energy. This is illustrated in the Appendix in the case of the Husimi-Temperley model. On the other hand, the Legendre transformation of the grand-canonical potential always provides a convex free energy.
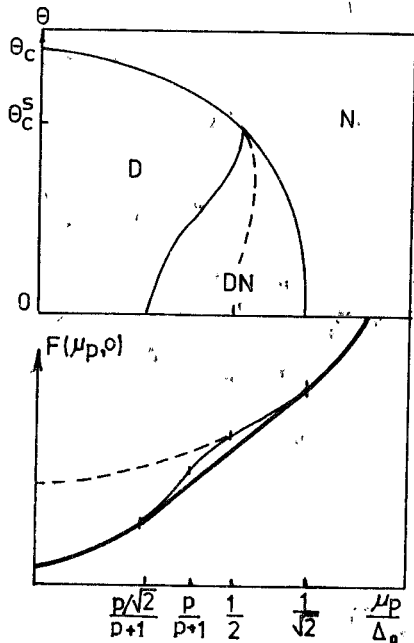
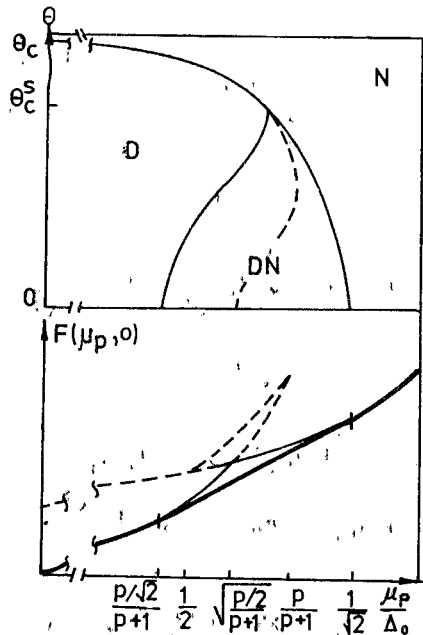Fig. 2. The ground-state energy and the (n, θ)-phase diagram at reservoir power $p < 1$ (schematical).

Fig. 3. The ground-state energy and the (n, θ)-phase diagram at reservoir power $p > 1$ (schematical)

5. DISCUSSION OF THE RESULTS

We shall show here that the difference between our approach and the approach in Refs. [1-5,10], which was described in the introduction, consists essentially in that, there, one performs first the Legendre transformation of $f^0(\mu, \theta; \Delta)$ at fixed θ, Δ and only afterwards takes the minimum with respect to Δ, i.e., their definition of the free energy is:

$$\widetilde{F}(n, \theta) = \min_{\Delta} \{ \sup_{\mu} [f^0(\mu, \theta; \Delta) + \mu n] \} \tag{24}$$

instead of (11) and (19).

Indeed, $f^0(\mu, \theta; \Delta)$ is a differentiable function of μ, so the supremum over μ is attained at a stationary point, i.e., on a solution of the electroneutrality equation:

$$n = -\frac{\partial f^0}{\partial \mu}(\mu, \theta; \Delta) \tag{25}$$

which, in our new variable μ_p, Eq. (20), writes explicitly as (compare Ref. [1], Eq. (11)):

$$\mu_p = \frac{1}{2(p+1)} \int_0^w d\epsilon \, [\text{th}\, \frac{\mu - \sqrt{\epsilon^2 + \Delta^2}}{2\theta} + \text{th}\, \frac{\mu + \sqrt{\epsilon^2 + \Delta^2}}{2\theta} + p \cdot \text{th}\, \frac{\mu - \epsilon}{2\theta} + p \cdot \text{th}\, \frac{\mu + \epsilon}{2\theta}]. \tag{25'}$$

The subsequent minimum over Δ provides again the selfconsistency Eq. (15). Let us stress that, irrespective of the particular way of justifying Eqs. (25'), (15), the main point is that these very equations are used and, then, the final result will coincide with (24).

At zero temperature, Eq. (25') gives:

$$\mu_p = \begin{cases} \dfrac{p}{p+1}\mu, & 0 \le \mu \le \Delta \\[3mm] \dfrac{p}{p+1}\mu + \dfrac{1}{p+1}\sqrt{\mu^2 - \Delta^2}, & \mu > \Delta . \end{cases} \tag{26}$$

Solving the system (16), (26) results in the following solutions:

$$\Delta^{(1)}(\mu_p) = \Delta_0, \qquad \mu^{(1)}(\mu_p) = \frac{p+1}{p}\mu_p \quad \text{for } 0 \le \mu_p \le \frac{p}{p+1}\Delta_0;$$

$$\Delta^{(2)}(\mu_p) = \sqrt{\frac{(p+1)\Delta_0(2\mu_p - \Delta_0)}{p-1}}, \quad \mu^{(2)}(\mu_p) = \frac{p+1}{p-1}(\mu_p - \frac{\Delta_0}{p+1})$$

and $\frac{p\Delta_0}{p+1}$: $\qquad\qquad\qquad\qquad\qquad\qquad$ for μ_p between $\frac{\Delta_0}{2}$

$$\Delta^{(3)}(\mu_p) = 0, \qquad \mu^{(3)}(\mu_p) = \mu_p \qquad \text{for all } \mu_p.$$

Now, $\widetilde{F}(\mu_p, 0)$ is obtained by taking the minimum among $f^0(\mu^{(i)}(\mu_p), 0; \Delta^{(i)}(\mu_p)) + 2N(0)(1+p)\mu_p\mu^{(i)}(\mu_p)$, $i = 1, 2, 3$. The values taken by the latter (outside the graph of F) are represented (by dotted or by thin line) on Figs. 2 and 3 for $p < 1$ and $p > 1$, respectively. For $p < 1, \Delta$ goes successively through the three solutions on the graph of $\widetilde{F}$, i.e., it goes continuosly to zero. This circumstance is interpreted as a second order transition (see also Refs. [2-5], where $p = 0$ is chosen). For $p > 1$, there is a jump on the graph of $\widetilde{F}$ between Δ_0 and 0 at $\mu_p = \sqrt{\frac{p}{p+1}}\frac{\Delta_0}{\sqrt{2}}$, which is interpreted as a first order transition [1]. In all cases, the

graph of $\tilde{F}$ (the thin line on Figs. 2 and 3) is obviously non-convex of μ_p.

The (mathematically trivial) reason, explaining why Eq. (24) may provide the wrong answer, can be read off from Eqs. (11), (19) and respectively (24), if one remembers that for fixed θ, Δ, f^0 is a concave function of μ, while its Legendre transform is convex of n. Namely: the infimum of a family of convex (respectively, concave) functions may be not convex (respectively, is always concave). It is easy to show that, in fact:

$$F(n, \theta) = C.E. \tilde{F}(n, \theta), \qquad (27)$$

where $C.E.\tilde{F}$ denotes the gratest convex function of n less than or equal to $\tilde{F}$. Eq. (25) determines the chemical potential μ as a function of n only in the pure phase region (see Figs. 2,3).

The following remark about the model is in order. As is seen, when solved correctly, it leads to a first order transition, accompanied by a region of phase coexistence. One may question what form this coexistence may take. If one remembers that the model discards most of the Coulomb interaction, one can expect it to be qualitatively reasonable only if the electron density is constant in space, because otherwise the Coulomb energy cost would be prohibitive. Therefore, one has to imagine the mixed state as a homogeneous fluid of "quasi-particles" with two different energy spectra.

APPENDIX

In order to illustrate the fact that for Hamiltonians with $1/N$-interactions the canonical ensemble can lead to a non-convex Helmholz free energy, we shall consider here the Husimi-Temperley model, in the spin formulation (where the canonical ensemble corresponds to the fixed magnetisation ensemble):

$$\mathcal{H} = - \frac{J}{2N} \sum_{i,j=1}^{N} \sigma_i \sigma_j .$$

The free energy for fixed $m = \frac{1}{N} \sum_{i=1}^{N} \sigma_i$ can be easily calculated (see also [16]):

$$F_{can}(m, \theta) = \lim_{N \to \infty} \frac{\theta}{N} \ln \left[\sum_{\sigma_i = \pm 1 ; \ \Sigma \sigma_i = mN} e^{\frac{N}{2\theta} J m^2} \right]$$

$$= \lim_{N \to \infty} \frac{\theta}{N} \ln \left[\frac{N!}{(N\frac{1+m}{2})! \ (N\frac{1-m}{2})!} e^{\frac{N}{2\theta} J m^2} \right]$$

$$= \frac{J}{2} m^2 - \theta \left[\frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2} \right]$$

and is obviously non-convex as a function of m. On the other hand, the grand-canonical potential (corresponding to fixed external magnetic field, h):

$$f(h, \theta) = \lim_{N \to \infty} (-\frac{\theta}{N}) \ln \left[\sum_{\{\sigma_i = \pm 1\}} e^{\frac{1}{2\theta} \frac{J}{N} (\sum_{i=1}^{N} \sigma_i)^2 + \frac{h}{\theta} \sum_{i=1}^{N} \sigma_i} \right]$$

$$= \lim_{N \to \infty} (-\frac{\theta}{N}) \ln \left[(\frac{NJ}{2\pi\theta})^{1/2} \int_{-\infty}^{\infty} dy \ e^{- \frac{N}{\theta} (\frac{J}{2} y^2 - \theta \ln ch \frac{Jy+h}{\theta} - \theta \ln 2)} \right]$$

$$= \max_{y \in R} \left[\frac{J}{2} y^2 - \theta \ln ch \frac{Jy+h}{\theta} - \theta \ln 2 \right]$$

gives, after the Legendre transformation:

$$F(m, \theta) = C.E. F_{can}(m, \theta) .$$

As is well known [17], the origin of this pathology is the $1/N$-interaction; when one considers $N \to \infty$ for a fixed short-range interaction and only afterwards takes the Van der Waals limit, one obtains the correct results $F(m, \theta)$.

It is interesting to note that for the (classical or quantum) Heisenberg model with $1/N$-interaction:

$$\mathcal{H} = - \frac{J}{2N} \vec{S}^2 , \qquad \vec{S} = \sum_{i=1}^{N} \vec{s}_i$$

the canonical ensemble ($m^z = \frac{1}{N} S^z$) calculation gives the correct free energy. The simple calculation (in the quantum spin 1/2 case) is as follows:

$$F_{can}(m^z, \theta) = \lim_{N \to \infty} \frac{\theta}{N} \ln \left[Tr_{\{S^z = Nm^z\}} e^{\frac{J}{2\theta N} \vec{S}^2} \right]$$

$$= \lim_{N \to \infty} \frac{\theta}{N} \ln \left[\sum_{S = Nm^z}^{N/2} \frac{N! (2S+1)}{(\frac{N}{2} + S + 1)! (\frac{N}{2} - S)!} e^{\frac{J}{2\theta N} S(S+1)} \right]$$

$$= \max_{m^z \leq x \leq \frac{1}{2}} \left\{ \frac{J}{2} x^2 - \theta \left[\left(\frac{1}{2} + x \right) \ln \left(\frac{1}{2} + x \right) + \left(\frac{1}{2} - x \right) \ln \left(\frac{1}{2} - x \right) \right] \right\},$$

which is nothing but the Legendre transform of the grand-canonical $f(h, \theta)$ [18].

As the models we consider in the body of the paper better resemble the Heisenberg model, we believe that, for them, the canonical ensemble provides the correct result, but up to now we were not able to verify this.

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Ангелеску Н., Ненчу Г., Тончев Н.С.   E17-82-798
О теории экситонного фазового перехода при наличии
резервуара

Для некоторого класса среднеполевых моделей, часто встречающихся при описании экситонного фазового перехода, получена фазовая диаграмма в переменных плотность-температура. Попутно выяснена роль резервуара. Показано, что обычный подход, основанный на уравнении электронейтральности, приводит к неправильному результату для таких значений плотности и температуры, при которых имеет место смесь фаз.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Angelescu N., Nenciu G., Tonchev N.S.   E17-82-798
On the Theory of the Excitonic Phase Transition
in the Presence of a Reservoir

The phase diagram in the density-temperature variables is obtained for a class of mean-field models currently used in describing the excitonic phase transition. Thereby the role of the reservoir is clarified. It is pointed out that the usual approach employing the electroneutrality equation leads to incorrect results for those values of density and temperature at which phase coexistence takes place.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.