Phase transitions in systems with coupled order parameters

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The properties of one-dimensional systems with coupled order parameters are investigated. Mean-field results are reviewed, and some essentially exact results, including fluctuations, are obtained numerically. Our results show the possibility of mixed phases and pseudo-first-order transitions.

A variety of physical systems exhibit properties which depend upon the interplay of two order parameters. Some examples which have been discussed are ferromagnetic-antiferromagnetic,[1] ferroelectric-ferromagnetic,[2] and ferroelectric-piezoelectric crystals: crystalline-superfluid[3]; and orientation-position[4] ordering in molecular and liquid crystals. The coexistence and interaction of two order parameters appears particularly interesting in nearly-one-dimensional systems where fluctuations broaden the region over which ordering occurs. Here, for example, recent work on organic charge-transfer salts raises questions concerning the interplay of the Peierls distortion and the Hubbard correlations,[5] or the Peierls distortion and the BCS pairing.[6–8] Another closely related problem is that of intensities and correlations in a two-mode laser near threshold.[9] Here we investigate the properties of one-dimensional systems with coupled order parameters. After formulating the problem, the mean-field properties are reviewed, and then some essentially exact results are given, including fluctuation effects.[10,11]

We consider, for simplicity, a system with two scalar order parameters $x(l)$ and $y(l)$. The coordinate l measures the position along a sample of length L. For a given spatial configuration of the fields, $x(l)$ and $y(l)$, the effective free energy of the system is assumed to be given by the functional[12]

$$\beta F[x,y]=\int_0^L dl\left[\frac{1}{2}\left(\frac{dx}{dl}\right)^2+\frac{1}{2}\left(\frac{dy}{dl}\right)^2+V(x,y)\right] , \qquad (1)$$

with

$$V(x,y)=a_1x^2+\tfrac{1}{2}b_1x^4+a_2y^2+\tfrac{1}{2}b_2y^4+\lambda x^2y^2 . \qquad (2)$$

Here $\beta=1/kT$, $a_1=[(T-T_1)/T_1]\,\overline{a}_1$, $a_2=[(T-T_2)/T_2]\,\overline{a}_2$, where $T_1>T_2$,[13] and $\overline{a}_1$, $\overline{a}_2$, b_1, b_2, and λ are positive constants. The choice of a positive coupling constant λ implies a competition between the two ordering parameters.

The statistical mechanics of this system[10,11] are obtained by averaging the quantities of interest over all possible configurations of the x and y fields. For example, the partition function is given by the functional integral

$$Z=\int \delta x\delta y\, E^{-\beta F[x,y]} \qquad (3)$$

and the intensity of the x field is given by

$$\langle x^2\rangle=\int \delta x\delta y\, e^{-\beta F[x,y]}x^2(i)/Z \qquad (4)$$

which is clearly independent of position in the large-L limit. In the usual way, the functional integrations can be expressed in terms of the eigenstates of a particle of mass $m=1$ ($\hbar=1$) moving in a potential field $V(x,y)$. The free energy per unit length in units of kT is given by the ground-state eigenvalue E_0, and the intensity $\langle x^2\rangle$ is given by the ground-state expectation value of x^2.

In this approach, mean-field theory corresponds to the classical approximation in which the particle rests at the absolute minimum of the potential energy $V(x,y)$. Before discussing the results obtained from a numerical solution of the quantum-mechanical problem, it is useful to review the mean-field theory[3] predictions. For a given set of parameters $(\overline{a}_1,\overline{a}_2,b_1,b_2,\lambda)$, the positions of the minima (x_0,y_0) of $V(x,y)$ depend upon T. For $T>T_1$, V has only a single minimum at the origin. As T decreases below T_1, the origin of the xy plane becomes a saddle point with two minima moving symmetrically out along the $\pm x$ axis to $x_0=\pm(-a_1/b_1)^{1/2}$. When T decreases below T_2, the structure of V depends upon whether the coupling is weak, $\lambda^2<b_1b_2$, or strong, $\lambda^2>b_1b_2$.[13] In the weak-coupling case, provided that $\overline{a}_1\lambda/\overline{a}_2b_1<1$, there will be a temperature $T_A<T_2$ given by

$$\frac{T_A}{T_2}=\left(1-\frac{\overline{a}_1\lambda}{\overline{a}_2b_1}\right)\Big/\left(1-\frac{\overline{a}_1\lambda}{\overline{a}_2b_1}\,\frac{T_2}{T_1}\right) ,$$

below which the minima along the x axis branch out into the x–y plane:

$$x_0=\pm\left(\frac{a_2\lambda-a_1b_2}{b_1b_2-\lambda^2}\right)^{1/2} , \quad y_0=\pm\left(\frac{a_1\lambda-a_2b_1}{b_1b_2-\lambda^2}\right)^{1/2} . \qquad (5)$$

As T is lowered further, the minima move away from the x axis. Finally, if $(\bar{a}_2\lambda/\bar{a}_1 b_2) > 1$, there will exist a temperature $T_B < T_A$ given by

$$\frac{T_B}{T_2} = \left(1 - \frac{\bar{a}_1 b_2}{\bar{a}_2\lambda}\right)\Big/\left(1 - \frac{\bar{a}_1 b_2}{\bar{a}_2\lambda}\frac{T_2}{T_1}\right),$$

where the minima are on the y axis. Then for $T < T_B$, the minima move out along the y axis at $y_0 = \pm(-a_2/b_2)^{1/2}$. In mean-field theory, second-order phase transitions occur at T_A and T_B when the system goes from a pure x state to a mixed state, and from a mixed state to a pure y state, respectively.

In the strong coupling case, where $\lambda^2 > b_1 b_2$, we have $T_B > T_A$, so that for $T < T_B$ there are minima along both the x and y axes, at $x = \pm(-a_1/b_1)^{1/2}$ and $y = \pm(-a_2/b_2)^{1/2}$, respectively. For T near T_B, the lower absolute minima lie along the x axis, but as T is decreased below a temperature T_0 ($T_B > T_0 > T_A$) given by

$$\frac{T_0}{T_2} = \left[1 - \left(\frac{b_2}{b_1}\right)^{1/2}\frac{\bar{a}_1}{\bar{a}_2}\right]\Big/\left[1 - \left(\frac{b_2}{b_1}\right)^{1/2}\frac{\bar{a}_1}{\bar{a}_2}\frac{T_2}{T_1}\right];$$

the minima along the y axis become the points of lowest potential energy. Thus, in the strong coupling case, mean-field theory predicts a first-order phase transition at T_0 from an x-ordered to a y-ordered system. The condition for the existence of T_0 is $\bar{a}_2^2/b_2 > \bar{a}_1^2/b_1$, which also implies the existence of T_B. The condition for the existence of T_A is $\bar{a}_1\lambda/\bar{a}_2 b_1 < 1$.

For one-dimensional systems, one knows that the first-order[14] and second-order[10,11] transitions predicted by mean-field theory are broadened by fluctuations. The effect of fluctuations is represented in the quantum-mechanical problem by the spread of the wave function around the potential

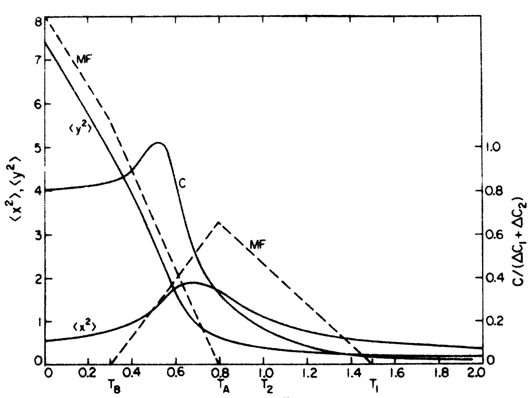

FIG. 1. Intensities $\langle x^2\rangle$, $\langle y^2\rangle$, and the specific heat C are plotted vs T for the weak coupling case ($b_1b_2 > \lambda^2$). MF denotes mean-field theory. The parameters: $\bar{a} = 1.75$, $\bar{a}_2 = 4$, $b_1 = 0.25$, $b_2 = 0.5$, $\lambda = 0.25$, $T_1 = 1.5$, $T_2 = 1$. Note the broadened transitions at T_A and T_B. All temperatures are measured in units of units of T_2.

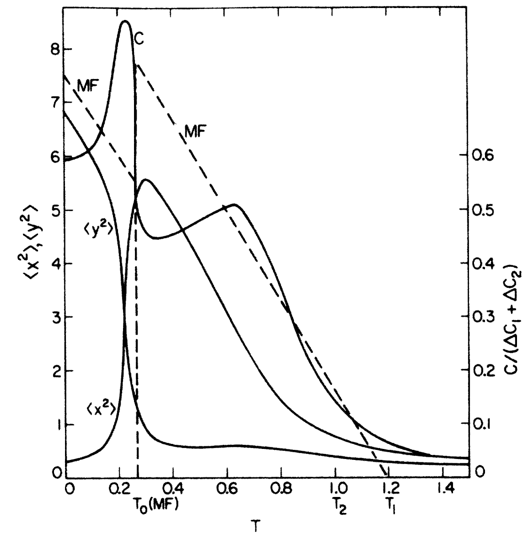

FIG. 2. Same as Fig. 1, for the strong coupling case ($b_1b_2 < \lambda^2$). The parameters: $\bar{a}_1 = 2.5$, $\bar{a}_2 = 3$, $b_1 = 0.25$, $b_2 = 0.5$, $\lambda = 0.5$, $T_1 = 1.2$, $T_2 = 1$. Note the pseudo-first-order transition at T_0 and the broadened transition at T_1.

minimum, and its penetration by tunneling to classically forbidden regions. The Hamiltonian for a particle moving in the potential $V(x, y)$, Eq. (2), was represented in a basis composed of products of harmonic oscillator wave functions depending on x and y. This matrix was then diagonalized to obtain the eigenvalues and eigenstates.[15]

Typical results for the order-parameter intensities $\langle x^2\rangle$, $\langle y^2\rangle$, and the specific heat are plotted versus T in Figs. 1 and 2. The mean-field results for $\langle x^2\rangle$ and $\langle y^2\rangle$ are shown as the dashed lines labeled MF. Figure 1 represents the weak coupling case, and one sees that the plot of the mean-field results, Eq. (5), shows $\langle x^2\rangle$ decreasing from its peak value at T_A to zero at T_B as $\langle y^2\rangle$ grows. The effect of the fluctuations is to smooth this behavior out.

Figure 2 shows a strong coupling case in which mean-field theory predicts a first-order transition at T_0. Here, while the fluctuations remove the discontinuity, one sees that the change from x to y ordering occurs over a narrow temperature region. This behavior is evident in the specific heat. The first broad maximum in C arises from the smeared second-order transition associated with x ordering; the narrow peak at lower temperatures reflects the pseudo-first-order transition near T_0.[16] A common qualitative feature of these two examples is that the weaker ordering (which eventually, at low temperatures, is overcome by the competing type of ordering) shows an interesting temperature dependence, developing a peak whose structure depends on the details of the model.

This peaking of the intensity of the weaker order parameter can also occur in the strong coupling case, even when the parameters are such that the absolute minima always remain along the x axis. In this case, the existence of secondary minima along the y axis, even though they lie higher than the minima along the x axis, can lead to enhancement of $\langle y^2 \rangle$ over the limited temperature region. The intensities then are typically more slowly varying functions of temperature than those for the pseudo-first-order transition shown in Fig. 2.

Finally, it is important to remember[17] that in the systems of experimental interest, there is always some interchain coupling which may lead to three-dimensional ordering at some lower temperature.

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[12]In applying this to certain one-dimensional systems, one must recognize that these systems may have very large critical regions. Thus, a careful treatment of the temperature dependence of the coefficients in Eq. (2) may be necessary. Moreover, related to the large size of the critical region, there are questions concerning the applicability and convergence of the field-theoretic model [Eqs. (1), (2), and (3)]. Here we ignore these difficulties and investigate the problem of two coupled order parameters within the framework of this model.

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