Application of the Blume-Emery-Griffiths Model to Cold-Atom Mixtures

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The Blume-Emery-Griffiths (BEG) model is a simple lattice model that exhibits both first-order and second-order phase transitions. Since its introduction in 1971 as an Ising-type model that captures the phase diagram of $He^3 - He^4$ mixture, the model has been extensively studied and generalized. A recent generalization of the model by Loois et al. is proposed to be of interest to studies of cold-atom mixtures. The original BEG model and the proposed generalization are reviewed.

Lattice models have played a critical role in expanding the frontiers of statistical mechanics and mathematical physics [1]. Techniques such as renormalization group, series expansion, and duality transformations have been developed to study the richness of the phase diagrams modeled by such relatively simple models. The discreteness of the lattice models also facilitates numerical simulations by techniques such as Monte Carlo algorithms. It would be interesting to test the results obtained from such studies of the lattice models by simulating the models with trapped ultracold atoms, as they are virtually free from experimental complications arising from defects and phonons present in solid state systems. Also, interatomic interactions can be easily tuned using Feshbach resonance [2] and chemical potentials by adjusting the trap depth, so various parts of a phase diagram of interest can be quickly probed. Study of multi-component mixtures (Bose-Fermi, Fermi-Fermi) has been an active area of research in the field of ultracold atoms (see [3] for references); a simple lattice model that may mimic the behaviors of such mixtures is the Blume-Emery-Griffiths (BEG) model.

The BEG model is a spin-1 lattice model that describes a mixture of non-magnetic ($s = 0$) and magnetic ($s = 1$) components [4]. The model was originally inspired by the experimental observation that the continuous superfluid transition in He^4 with He^3 impurity becomes a first order transition into normal (He^3) and superfluid (He^4) phase separation above some critical He^3 concentration [5]. Despite the fact that the physical order parameter of the superfluid is continuous (whereas the order parameter in the model is two-valued), the phase diagram obtained by mean-field approximation of the model is in qualitative agreement with experimental data.

We first review the original BEG mean-field solution obtained in 1971, in the context of modeling $He^4 - He^3$ mixture. A He^3 atom at site i corresponds to $s_i = 0$, and a He^4 atom corresponds to $s_i = \pm 1$; the model assumes unit filling at each site and no vacancies. Then the number of He^3 and He^4 are given by

$$N_3 = \sum_i^N (1 - s_i^2) \tag{1}$$

$$N_4 = \sum_i^N s_i^2 \tag{2}$$

There are two order parameters in the model. The first is the superfluid order parameter, which is provided by

$$M = \frac{1}{N} \sum_{i=1}^N \langle s_i \rangle \tag{3}$$

The second is the He^3 impurity concentration, which is given by

$$x = \frac{\langle N_3 \rangle}{N}$$

The effective Hamiltonian in the BEG model is defined as

$$\beta \mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - K \sum_{\langle i,j \rangle} s_i^2 s_j^2 + \Delta \sum_i s_i^2 \tag{4}$$

where the first term is responsible for superfluid ordering (creating kinetic energy cost for "phase slip" in superfluid) and the last two terms represent the combined effects of intra- and inter-species interactions and chemical potentials [4]. It is clear that increasing Δ favors higher impurity concentration. We note that one can also "discover" the BEG Hamiltonian by performing renormalization group procedure on spin-1 Ising model $-J \sum_{\langle i,j \rangle} s_i s_j$ [1]. Under discrete translation symmetry, the most general spin-1 Ising interaction between two spins s and s' closed under renormalization procedure is

$$g - \frac{h}{2}(s + s') - Jss' + \frac{\Delta}{2}(s^2 + s'^2) + \frac{v}{2}\left(s^2 s' + s'^2 s\right) - K s^2 s'^2 \tag{5}$$

By symmetry consideration, $\{g, J, K, \Delta, h = v = 0\}$ is the minimal set of coupling parameters closed under

renormalization group for $J \neq 0$, and this set describes the BEG Hamiltonian.

The mean-field solution is obtained by minimizing the expectation value of the free energy with respect to a trial probability distribution in the form $\rho = (\rho_1)^N$ (where $\rho_1 \propto \exp(-\beta h)$). The mean field energy βh is

$$\beta h = -zJMs + [\Delta - zK(1-x)]s^2 \tag{6}$$

where z is the number of nearest neighbors. From the mean field distribution one can calculate the order parameters of the system:

$$1 - x = \frac{2\cosh zJM}{\exp(\Delta - zK(1-x)) + 2\cosh(zJM)} \tag{7}$$

$$M = \frac{2\sinh zJM}{\exp(\Delta - zK(1-x)) + 2\cosh(zJM)} \tag{8}$$

Experimentally, the impurity concentration x is the fixed variable and K, Δ are self-consistently defined from x using Eq. (7),(8). However, it is simpler to fix Δ and numerically solve for M and x. There will be multiple solutions for (M, x) in general, and one has to check that it minimizes the free energy. One can find an analytical description of the phase boundaries by expanding the free energy as a power series of M (i.e. Landau-Ginzburg theory of phase transition):

$$\beta f = \beta f_0 + aM^2 + bM^4 + cM^6 + \dots \tag{9}$$

Only even powers occur because of symmetry. See Appendix for derivation of a, b, c. For $K = 0$, the expressions are

$$a = \frac{1}{2}(\delta - zJ) \tag{10}$$

$$b = \frac{1}{8}\left(\delta^2 - \frac{\delta^3}{3}\right) \tag{11}$$

$$c = \frac{1}{6}\left(\frac{\delta^3}{2} - \frac{3}{8}\delta^4 + \frac{3}{40}\delta^5\right) \tag{12}$$

$$\delta = 1 + \frac{1}{2}e^{\Delta} = (1-x)^{-1}|_{M=0} \tag{13}$$

Second-order transition occurs for $a < 0, b, c > 0$, while first-order transition occurs for $b < 0, a, c > 0$. From Eq. (10) since $J = \hat{J}(k_B T)^{-1}$ it is clear that the superfluid transition temperature T_s goes as

$$\frac{k_B T_s}{z\hat{J}} = 1 - x \tag{14}$$

The second order phase boundary continues until the tricritical point A, which occurs when $a = b = 0$. This corresponds to $T_c/T_s(0) = 1 - x_c = \frac{1}{3}$, which is reasonably close to the experimental value reported in [5] ($T_c/T_s(0) = 0.4, 1 - x_c = 0.331$). See Figure 1 for the phase diagram at $K = 0$. The $K = 0$ case is also known in the literature as the Blume-Capel model [6, 7], which was developed to model first-order phase transitions in magnetic systems. It is shown in [4] that the phase diagram becomes qualitatively different at high K/J ratio, and low K/J ratio resembles experimental findings.

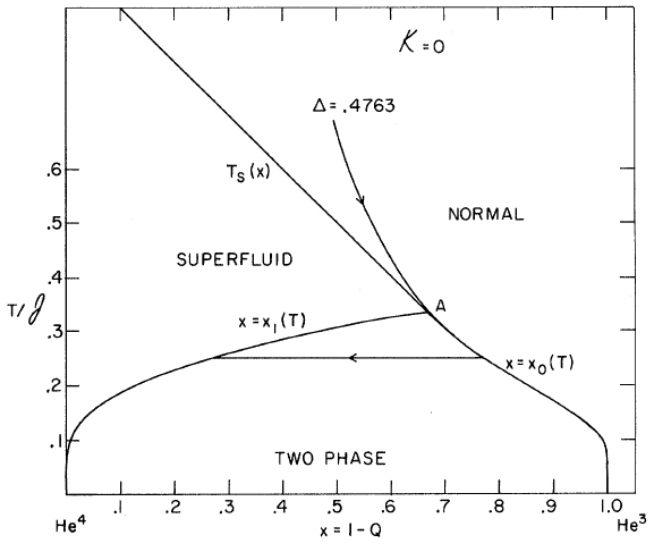

FIG. 1. Reproduced from [4]. Mean-field phase diagram of BEG model for $K = 0$. The tricritical point A separates the second-order transition from first-order transition.

We conclude the review of the mean-field solution by noting some qualitative differences between the model and the physical systems [4]. First, the mean-field solution predicts $\frac{\partial T_s}{\partial x}$ is continuous at the tricritical point, whereas experiment shows otherwise [5]. Also, it is found that because of Fermi statistics He^3 becomes miscible with He^4 at small concentration ($< 6\%$) and at very low temperature [8].

Theoretically, the BEG model has played an important role in the position-space renormalization group (PSGR) analysis of the Potts model. In PSRG steps, a Hamiltonian is mapped to another Hamitonian with fewer number of spin variables, which is related to a cluster of original spins in the lattice. If a cluster contains spins of different states, assigning a common weight factor, the procedure overestimates the tendency to order. Nienhuis et al. suggested that since a completely disordered cell should have little influence on aligning neighboring spins, it should be treated as a vacant state. Thus, they proposed to generalize the weight factor so that a simple Potts model is mapped under PSRG to a dilute Potts lattice gas, where, besides the Potts spin variable ($s = 1, \dots, q$), a lattice variable ($t = 0, 1$) keeps track of vacancies:

$$\beta\mathcal{H} = -\sum_{\langle i,j \rangle} t_i t_j (K + J\delta_{s_i,s_j}) + \Delta \sum_i t_i \tag{15}$$

where one can see that the $q = 2$ case corresponds to the BEG model. Nienhuis et al. note that previous nu-

merical RG methods before their analysis have failed to detect first-order transitions in the Potts model for $q > 4$ which was an exact result obtained by Baxter. Using their technique for mapping to a dilute gas model they were able to obtain the changeover from second-order to first-order transition.

Since its introduction, the BEG model has been extensively studied with many different realizations, such as repulsive biquadratic couplings ($K < 0$) [9] and random-bond configurations [10], exhibiting a variety of phase diagrams with distinct topologies. It is natural to ask whether the BEG model can be applied to studies of ultracold-atom mixtures, where the system naturally displays both $U(1)$ symmetry breaking (corresponding to $s = \pm 1$) and density fluctuations ($|s| = 0, 1$). Loois et al. proposed a two-component version of the BEG model for $K = 0$, in order to describe systems with two order parameters, such as magnetic ordering and superconductivity ordering, both of which can be cast as an Ising variable in the original spirit of BEG. [11]. Naturally this model can also describe Bose-Bose mixtures of ultracold atoms. The proposed generalization is

$$\beta\mathcal{H} = -J_1 \sum_{\langle i,j \rangle} \sigma_i \sigma_j - J_2 \sum_{\langle i,j \rangle} s_i s_j + \Delta \sum_i \sigma_i^2 + h \sum_i \sigma_i \tag{16}$$

In this generalization, the spins (s_i, σ_i) can take the values $(\pm 1, 0), (0, \pm 1)$. Hence every site is occupied by one type of boson or the other, but not both. The order parameters in the system are defined as

$$c = \frac{1}{N} \sum_i \sigma_i^2$$

$$m_{FM,\sigma} = \frac{1}{N} \sum_i \sigma_i$$

$$m_{AFM,\sigma} = \frac{1}{N} \sum_i (-1)^i \sigma_i$$

$$m_s = \frac{1}{N} \sum_i s_i$$

Loois et al. performed Monte Carlo simulations for a variety of parameter sets. Each iteration allowed local flips of s and σ as well as same-site replacement of σ by s and vice versa. The zero magnetic field case is of interest for cold atom experiments, and we review their simulation results. They identify four phases in general: a S phase, where m_s is nonzero; a FM phase, where $m_{FM,\sigma}$ is nonzero; a phase separation (PS) regime, and lastly the N phase where there is neither order nor phase separation. See Figure 2 for the phase diagram for $J_2/J_1 = 0.1$. Because of the weakness of J_2, the S phase does not set until at very low temperature. The phase diagram for the magnetic part (σ) is similar to the original BEG phase diagram. For non-zero concentration of magnetic dopants the system enters the phase separation regime. The superfluid part (s) is not diluted by the magnetic dopants so the critical temperature stays relatively flat throughout the variation of concentration. An interesting observation made by the authors is that there is no critical ratio $(J_2/J_1)_c$ for which the superfluidity complete disappears. Also, there is no true coexistence of the two different order parameters.

It would be interesting to experimentally observe this lack of coexistence of two orders and the failure to completely suppress one order parameter, but so far there has been relatively little effort on Bose-Bose mixtures compared to Bose-Fermi and Fermi-Fermi mixtures, the latter receiving much attention due to interest in pairing in the presence of mass and/or spin imbalance. One notable experiment is the $^{87}\mathrm{Rb} - {}^{41}\mathrm{K}$ double-species BEC carried out in the group of Massimo Inguscio, where a small, delocalized concentration of ^{41}K enhanced the loss of coherence of ^{87}Rb superfluid loaded in optical lattice, as the lattice depth was raised [12]. The experiment did not probe into a possible Mott insulator structure, so the loss of coherence cannot be simply interpreted as enhanced phase transition into a Mott insulator. Experimentally, for a faithful realization of the two-component BEG model, the constraint $\sigma_i^2 + s_i^2 = 1$ per site seems to be a peculiar and challenging requirement. A very large, positive interspecies scattering length would be necessary, perhaps aided by a possible interspecies Feshbach resonance. A recent popular two-species bosonic system is $^{87}\mathrm{Rb} - {}^{133}\mathrm{Cs}$ for the creation of polar molecules, and the system does possess a rich interspecies Feshbach resonances structure. [13]. Since such system are proposed to be prepared in optical lattice, test of the two-component BEG model may be accessible.

It seems striking that the original BEG model has been able to largely capture the phase diagram $\mathrm{He}^3 - \mathrm{He}^4$, which possess highly quantum behaviors at low temperature, in the broad approximation of projecting order parameter phase to two discrete values. It will be equally fascinating if this rough approximation holds for two-component BEG model as well.

Derivation of Landau-Ginzburg parameters

The coefficients a, b, c in the analytic expression for $\beta f(M)$ can be found by considering the response of the system to a fictitious "magnetic field" H (which has no physical meaning) [4]. The introduction of $H \sum s_i$ basically replaces zJM by $zJM - H$ in the mean field energy and thus in the expressions for x and M. The thermodynamic potential is described by the Gibbs potential $\Phi = \beta f - MH$, so $H = -\frac{\partial \Phi}{\partial M}$, since Φ is at minimum at zero field. Then one can use Eq. (8) to write H implicitly as a series in M and thus obtain a, b, c. Following from

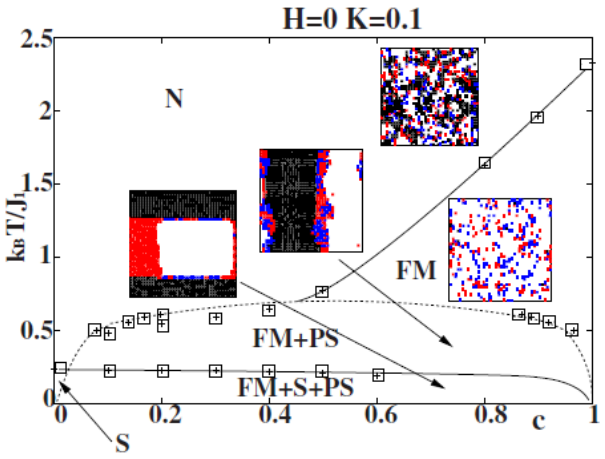

FIG. 2. Reproduced from [11]. Solid lines represent second-order transition; dashed lines represent first-order transition. Black (white) represents $\sigma = 1\,(-1)$; red (blue) represents $s = 1\,(-1)$.

Eq. (9), we have

$$H(M) = -2aM - 4bM^3 - 6cM^5 + \dots$$

Eq. (8) with $zJM \to zJM - H$ implicitly defines H as a function of M. If we take a partial derivative with respect to M on both sides, we get, after simplification using hyperbolic trigonometry,

$$1 = -\frac{(2e^{\Delta}\cosh(zJM - H) + 4)}{\left(e^{\Delta} + 2\cosh(zJM - H)\right)^2}\left(zJ - \frac{\partial H}{\partial M}\right)$$

Since $\frac{\partial H}{\partial M} = -2a$ at $H = M = 0$, the above expression gives

$$a + \frac{zJ}{2} = \frac{e^{\Delta} + 2}{4}$$

One can obtain b and c by taking higher order partial derivatives of both sides of Eq. (8) with respect to M.

[1] M. Kardar, *Statistical physics of fields* (Cambridge University Press, 2007).
[2] S. Inouye, M. Andrews, J. Stenger, H.-J. Miesner, D. Stamper-Kurn, and W. Ketterle, Nature **392**, 151 (1998).
[3] M. Inguscio and L. Fallani, *Atomic physics: precise measurements and ultracold matter* (Oxford University Press, 2013).
[4] M. Blume, V. J. Emery, and R. B. Griffiths, Phys. Rev. A **4**, 1071 (1971).
[5] E. H. Graf, D. M. Lee, and J. D. Reppy, Phys. Rev. Lett. **19**, 417 (1967).
[6] M. Blume, Phys. Rev. **141**, 517 (1966).
[7] H. Capel, Physica **32**, 966 (1966).
[8] J. Bardeen, G. Baym, and D. Pines, Phys. Rev. **156**, 207 (1967).
[9] W. Hoston and A. N. Berker, Phys. Rev. Lett. **67**, 1027 (1991).
[10] K. Hui and A. N. Berker, Phys. Rev. Lett. **62**, 2507 (1989).
[11] C. Loois, G. Barkema, and C. M. Smith, Physical Review B **78**, 184519 (2008).
[12] J. Catani, L. De Sarlo, G. Barontini, F. Minardi, and M. Inguscio, Phys. Rev. A **77**, 011603 (2008).
[13] K. Pilch, A. D. Lange, A. Prantner, G. Kerner, F. Ferlaino, H.-C. Nägerl, and R. Grimm, Phys. Rev. A **79**, 042718 (2009).