Journal of Statistical Physics, Vol. 15, No. 6, 1976

An Alternative Formulation of Rigorous Mean-Field Theory

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Received July 12, 1976

It is shown how to derive rigorous mean-field theory from a type of many-body interaction.

KEY WORDS: Mean-field theory; many-body interactions.

Since the work of Kac *et al.*[1] in 1963, the classical or mean-field theories of a variety of systems have been derived rigorously. They include the three-dimensional version and extension[2,3] of Ref. 1, quantum mechanical extensions,[4,5] antiferromagnet and melting models,[6] classical correlation functions,[7] and theories of amorphous ferromagnets[8] and metastable states.[9]

The derivations are valuable because of the extensive use of mean-field theories in the literature. One objection to the theories is their inapplicability to the critical region of a phase transition. In particular they yield inaccurate values for critical exponents. On a more theoretical level they lack some appeal (see the introductory comments in Ref. 11) because the transitions are in a sense "forced" by the application of a long-range limit operation on the thermodynamic functions. We outline here how this latter problem may be formally removed by an alternative formulation in terms of a type of many-body interaction.

We take the total potential energy of N particles at points $\mathbf{x}_1, \mathbf{x}_2,\ldots, \mathbf{x}_N$ to be the sum of two-body, three-body, up to N-body interactions:

$$U_N(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \sum_{1\leqslant i<j\leqslant N} [q(\mathbf{x}_i - \mathbf{x}_j) + \Phi_2(\mathbf{x}_i - \mathbf{x}_j)] + \sum_{1\leqslant i<j<k\leqslant N} \Phi_3(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k) + \cdots + \Phi_N(\mathbf{x}_1,\ldots,\mathbf{x}_N) \tag{1}$$

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where

$$\Phi_m(\mathbf{x}_1,\ldots,\mathbf{x}_m) = \sum_{1\leqslant i<j\leqslant m} \psi_m(\mathbf{x}_i - \mathbf{x}_j) \tag{2}$$

$$\psi_m(\mathbf{r}) = \sum_{k=2}^{m} (-1)^{m-k}\binom{m-2}{k-2}\gamma_k{}^\nu\varphi(\gamma_k\mathbf{r}) \tag{3}$$

and

$$\gamma_k = k^{-\eta/\nu} \tag{4}$$

where ν is the dimensionality of the system and η is a constant satisfying

$$0 < \eta < 1 \tag{5}$$

Our main result is that if $q(\mathbf{r})$ and $\varphi(\mathbf{r})$ satisfy the conditions imposed by Lebowitz and Penrose, then the pressure in the thermodynamic limit is given by the Maxwell construction or equal area rule[2] applied to the function

$$p^0(\rho, T) + \tfrac{1}{2}\alpha\rho^2 \tag{6}$$

where ρ is the density, T is the temperature, p^0 is the pressure of a system with two-body potential $q(\mathbf{r})$ alone, and

$$\alpha = \int d\mathbf{r}\, \varphi(\mathbf{r}) \tag{7}$$

the integral being over all of ν-dimensional space. The variational principle of Penrose and Gates holds under the weaker conditions on φ given in Ref. 3.

To establish these results, we substitute (2) and (3) in (1) and obtain

$$U_N(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \sum_{1\leqslant i<j\leqslant N} [q(\mathbf{x}_i - \mathbf{x}_j) + \gamma_N{}^\nu\varphi\{\gamma_N(\mathbf{x}_i - \mathbf{x}_j)\}] \tag{8}$$

We therefore have a genuine two-body interaction through $q(\mathbf{r})$ and an artificial two-body potential $\gamma_N{}^\nu\varphi(\gamma_N\mathbf{r})$ which depends on the total number N of particles in the system. As N increases, the range γ_N^{-1} of interaction also increases.

This may be compared with the model of Lebowitz and Penrose,[2] who use a two-body potential

$$q(\mathbf{r}) + \gamma^\nu\varphi(\gamma\mathbf{r})$$

where γ is an arbitrary positive parameter. They then take the long-range limit $\gamma \to 0$ after the thermodynamic limit $N \to \infty$.

We note from (4) that

$$\begin{aligned} \gamma_N &\to 0 \qquad \text{as} \quad N \to \infty \\ N\gamma_N{}^\nu &\to \infty \qquad \text{as} \quad N \to \infty \end{aligned} \tag{9}$$

Consequently, we have

$$r_0 \ll \gamma_N^{-1} \ll N^{1/\nu} \tag{10}$$

for large N, where r_0 is the hard-core diameter of $q(\mathbf{r})$. Hence we can divide the container into cells of volume ω satisfying

$$r_0 \ll \omega \ll \gamma_N^{-1} \ll N^{1/\nu} \tag{11}$$

for large N. The inequalities of Lebowitz and Penrose therefore apply with γ_N replacing their parameter γ. The result (6) then follows by their method.

Our formulation gives (6), and the consequent van der Waals–Maxwell phase transition, without the use of the additional limiting operation $\gamma \to 0$. The present work is related to the extensive work of Fisher[10] and Fisher and Felderhof,[11] which describes the phase transitions in a class of one-dimensional models with many-body interactions. However, our model does not quite belong to the class considered by these authors, because our potentials Φ_m do not satisfy their tempering conditions.

On the other hand, our results provide an example of a system which violates the usual conditions on interactions, but for which the thermodynamic limit exists and the pressure is a nondecreasing, continuous function of the density ρ. Thus the usual conditions are sufficient, but not necessary.

The same formulation is applicable to other mean-field models. It may be contrasted with the Temperly model, which is a lattice gas (or Ising model) with interaction energy

$$(1/V) \sum_{1 \leqslant i < j \leqslant V} \sigma_i \sigma_j \qquad \text{and} \qquad \sum_{i=1}^{V} \sigma_i = N \tag{12}$$

where $\sigma_i = 0$ or 1. This yields the van der Waals theory *without* the Maxwell construction. As the number of lattice sites V tends to infinity, the interaction decreases at the rate $1/V$, while the thermodynamic limit imposes the condition $N/V \to$ constant, ρ. Consequently it is not possible to divide the system into cells in such a way that the interaction in a single cell is negligible, while each cell contains an arbitrarily large number of particles in the thermodynamic limit. Each cell contributes a factor $\frac{1}{2}\rho^2$. In the new model (and that of Lebowitz and Penrose) the factor $\frac{1}{2}\alpha\rho^2$ in (6) results from interactions between such cells. It is this feature, expressed through (11), which yields the Maxwell construction.

ACKNOWLEDGMENT

I am indebted to Prof. M. E. Fisher for helpful correspondence.

REFERENCES

1. M. Kac, G. E. Uhlenbeck, and P. C. Hemmer, *J. Math. Phys.* **4**:216 (1963).
2. J. L. Lebowitz and O. Penrose, *J. Math. Phys.* **7**:98 (1966).
3. D. J. Gates and O. Penrose, *Comm. Math. Phys.* **15**:225 (1969); **16**:231 (1970); **17**:194 (1970).
4. E. H. Lieb, *J. Math. Phys.* **7**:1016 (1966).
5. P. A. Pearce and C. J. Thompson, *Comm. Math. Phys.* **41**:191 (1975).
6. D. J. Gates, *J. Math. Phys.* **12**:766 (1970).
7. D. J. Gates, *Physica* **81A**:47 (1975).
8. N. E. Frankel and C. J. Thompson, Classical Theory of Amorphous Ferromagnets, Melbourne University research report No. 19 (1975).
9. J. L. Lebowitz and O. Penrose, *J. Stat. Phys.* **3**:211 (1971).
10. M. E. Fisher, *Physics* **3**:255 (1967).
11. M. E. Fisher and B. U. Felderhof, *Ann. Phys.* (*N.Y.*) **58**:176 (1970).