Phase transitions in exactly soluble models

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(Received 20 April 1982)

A linearized version of the Hartree-Fock method is reinvestigated in order to develop a new technique for the study of phase transitions. This is studied with reference to an exactly soluble model, yielding excellent results.

[NUCLEAR STRUCTURE Phase transitions. Approximate many body methods applied to a soluble model.]

When a given property of some physical system undergoes a qualitative change, one speaks of *phase transitions.* These are more or less sharply defined, and are usually associated with the thermodynamic limit. Gilmore, Feng, and others[1–5] have shown, in recent studies, that the concept of phase transition is both valid and useful even for a (relatively) small number of particles, within the context of exactly soluble models of the Lipkin[6] type. In the case of these models, the order of the transition is the degree of the derivative of the (variational) physical quantity [usually the ground state (g.s.) energy] that first experiences a noticeable (and more or less "abrupt") change.

Theoretical descriptions of the properties of a many-fermion system usually "start" with a Slater determinant which is either varied or perturbed in some (rather involved) way and most people would agree in considering that the best such determinant is the one provided by the Hartree-Fock (HF) approach. It is well-known that this "best starting determinant" may, in some circumstances, display rapid changes as a function of some suitable parameter. Consequently, one speaks, in the sense referred to above, of "phase transitions."

Kümmel[7] has recently suggested that the HF approximation may not always be the most convenient route to follow in order to investigate these phase transitions within the framework of a single-determinant description and proposed, instead, a "maximum overlap" approximation. An alternative way of implementing Kümmel's ideas (with the same purpose) is introduced in Ref. 5, in connection with the generator coordinate method.

The purpose of the present Comment is to point out a much simpler way of attaining the same goal (i.e., "detecting" phase transitions), than that of Refs. 5 and 7, by recourse to the elegant method devised years ago by Mann and Gross[8] (which will herefrom be referred to as the MG approach) as an approximation to the HF problem. They employ the Thouless representation of the HF Slater determinant in order to connect it with the unperturbed ground state (u.g.s) and perform a second order approximation that yields a *linear* set of equations.[8] An enormous simplification of the corresponding problem is thus achieved. This beautiful scheme is slightly marred, however, by the fact that one finds poles in the amplitudes determining the relevant unitary transformation, which limit the range of applicability of the corresponding theoretical approach.[8]

Our claim, in this respect, is that these poles (whose location is easily determined) *signal the presence of a phase transition.* We thus propose, as an alternative to the methods introduced in Refs. 5 and 7, the use of the poles that appear in the MG approach.

We shall illustrate our claim by reference to the same model employed in Ref. 8, the so-called AFP model.[9] In order to save space we shall employ the notation of Refs. 8 and 9, and refer the reader to these papers for the relevant details. In terms of the number of particles N and the coupling constant V, the HF energy E takes the form

$$E=-\tfrac{1}{2}N\cos(\beta)+V\tfrac{1}{2}N(N\cos^2\beta+1+\sin^2\beta+2\sin\beta)\ , \qquad (1)$$

where β is the angle that defines the corresponding HF transformation in quasispin space.[8–10] Consider first the thermodynamic limit[11] of this SU(2) model ($N\to\infty$). One finds a discontinuity in $\delta^2E/\delta V^2$, and thus a second order phase transition, given by

$$\beta=0,\quad V<V_c=\frac{1}{2N}\ ,\qquad \cos(\beta)=\frac{1}{2VN}\ ,\quad V>V_c\ . \qquad (2)$$

It is easy to see that in the thermodynamic limit the above referred to pole, that appears in the MG approach, is located *exactly* at $V=1/2N$. Moreover, the corresponding g.s. energy $E_{\rm MG}$ coincides with E and $V\leq V_c$.

For a *finite* number of particles, it has been shown in Ref. 5 that the *exact* (Schrödinger) g.s. energy exhibits a phase transition (in the sense discussed in Refs. 1–4) which can be associated with an absolute minimum of $\delta^2 E_{\text{exact}}/\delta V^2$. The corresponding HF energy displays a similar behavior. The associated critical coupling constant agrees with that found with the exact treatment (the degree of agreement is better than 95% for $N > 20$). If we take $N = 20$, then the HF critical coupling constant $V_c(\text{HF}) = 0.0264$ and the MG pole lies at $V_{\text{MG}} = 0.0263$. For $N = 40$ we have $V_c(\text{HF}) = 0.0129$ and $V_{\text{MG}} = 0.0128$. The degree of agreement between $V_c(\text{HF})$ and V_{MG} steadily improves as N grows and is always excellent.

In conclusion, we believe, that, as a contribution to the discussion originated by Kümmel's paper,[7] it may be of interest to comment on the relevance of the MG approach.

This work was supported in part by the Comisión de Investigaciones Científicas and the Consejo Nacional de Investigaciones, Argentina.

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