On the thermodynamic limit at a quantum critical point

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Open questions regarding the uniqueness and existence of the thermodynamic limit at a quantum critical point are discussed in the context of the Lipkin model, a popular model in many-body theory. This model illustrates a quantum phase transition, including spontaneous symmetry breaking. The thermodynamic limit seemingly yields different answers depending on the approach used. The discussion is based on recent developments, including a joint publication by the authors.

The following presents a résumé of one particular research activity in theoretical physics at the University of Stellenbosch. The emphasis is placed on open problems rather than on established results, and the discussion is based on a paper published jointly by the authors recently.[1]

One of the most intriguing problems in many-body physics concerns phase transitions (see e.g. ref. 2). While from a classical view point a phase transition is usually associated with a system of infinitely many particles, in quantum systems finite systems are more often investigated. The typical quantum phase transition is encountered at a particular value of a suitable parameter being usually an interaction strength and not the temperature; in fact zero temperature transitions fall exclusively into the realms of quantum physics.

Typical examples are found in nuclear physics,[3] where one speaks about transitions from a normal to a superfluid nucleus, from a spherical to a deformed nucleus, shape transitions of deformed nuclei, and onset of tilted rotations, to mention just a few. For an infinite system the quantum analogue of the classical liquid–gas transition is still awaiting experimental confirmation in nuclear or quark matter. Phase transitions have also received considerable attention within the interacting boson model (IBM)[4] (see also ref. 5 for recent developments and further references). Spin systems are naturally favoured subjects for the study of quantum phase transitions,[2] and here the thermodynamic limit, that is the limit $N \to \infty$, $V \to \infty$ at constant density (with N being the particle number), is, for certain models, well understood. Once the spectrum is known, consideration of finite temperatures is then straightforward, employing the standard procedures of statistical physics.

In many cases, however, the thermodynamic limit is problematic, even in models that have been thoroughly investigated owing to their attractive features for finite N. One case in point is the popular Lipkin model[6] that has served as a prime example for a quantum phase transition including spontaneous symmetry breaking.[7] Using methods developed recently[8,9] that allow calculation of the spectrum for virtually unlimited (yet finite) values of N, the properties of the model have been scrutinized for a larger range of the interaction strength and energy than was done traditionally, where the emphasis was focused upon the phase transition affecting only the low-lying states. Investigation of singularities effecting the phase transition,[10] singularities affecting also the partition function,[11,12] provides a special view point of the limit.

The Lipkin model in its original form[6] considers interacting Fermions occupying two Ω-fold degenerate levels. Its major appeal lies in the easy solubility[7] and the demonstration of a quantum phase transition including spontaneous symmetry breaking. The essential form is given in terms of $2j + 1 = N + 1$-dimensional representations of the SU(2) operators J_z and $J_\pm = J_x \pm iJ_y$, N being the number of particles. It reads in dimensionless form

$$H_N(\lambda) = J_z + \frac{\lambda}{2N}(J_+^2 + J^2\ ). \qquad (1)$$

Here the interaction is scaled by N to ensure that H is extensive, the operators J_+^2 and J_-^2 effectively scale as N^2. In this form the model has a phase transition just beyond $\lambda = 1$, the larger N the closer the transition point at $\lambda = 1$. This has been discussed under various points of view in the literature, see e.g. refs 7, 13. Many more details can be found in ref. 1. Here we turn our attention to the thermodynamic, that is, the large N limit.

This limit is well understood for the normal phase, i.e. for $0 \le \lambda < 1$ where the Holstein–Primakoff transformation[14] to boson operators reduces the Hamiltonian (1) to a quadratic boson Hamiltonian which reads in the large N limit

$$H_\infty(\lambda) = b^\dagger b + \frac{\lambda}{2}(b^2 + (b^\dagger)^2\ ). \qquad (2)$$

This is diagonalized using the standard Bogoliubov transformation, readily yielding a harmonic spectrum $E_k = k\sqrt{(1-\lambda)}$, $k = 1, 2, \ldots$. Note that this result implies that the whole spectrum collapses to zero at $\lambda = 1$. However, as the Bogoliubov transformation becomes singular at this point, this would be a naive conclusion. In fact, the boson Hamiltonian reduces at $\lambda = 1$ to

$$H_\infty(1) = \frac{1}{2}(b + b^\dagger)^2 + \frac{1}{2} \qquad (3)$$

being equivalent to a free Hamiltonian containing only the kinetic energy $p^2/2$ and having the well-known continuous spectrum (in this case $½ \le E < \infty$). What is worse, for $\lambda > 1$, the Hamiltonian (2) is ill-defined: it can be rewritten as a single-particle Hamiltonian for a harmonic oscillator potential which has, however, the wrong sign of the potential, i.e. it reads

$$H_\infty(\lambda > 1) = \frac{p^2}{2} - \frac{\lambda^2 - 1}{2}. \qquad (4)$$

The reason for these odd results lies in the bosonization: rewriting the matrix representations of $J_{x,y,z}$ as boson operators is correct only up to orders l/N. Omitting correction terms yields incorrect results for $\lambda \ge 1$. A more careful analysis in the region $\lambda > 1$ can be done that does indeed yield the correct results to leading order in $1/N$. However, the critical point remains elusive as the higher order corrections in $1/N$ are always important at this point. This is symptomatic of the fact that the double limit $N \to \infty$ and $\lambda \to 1$ is non-uniform and depends on the order taken.

In ref. 1 the authors investigate the exceptional points (EP), that is, the singularities of the spectrum in the complex λ-plane. While it appears clear how the complex plane is being filled up with increasing N, we could not arrive at a conclusive result for the actual limit. It is clear that no singularities occur inside the unit circle; this is in line with the limit attained unproblematically for λ 1. Yet it could not be ascertained whether the EPs accumulate on the whole unit circle and the whole real axis $|R\lambda| \ge 1$ or only at $\lambda = \pm 1$ and $\lambda = \pm i$. If the unit circle is in fact densely filled

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with singularities in the limit $N \to \infty$, the consequences would be that the normal phase ($|\lambda| < 1$) is no longer analytically connected to the deformed phase ($|\lambda| > 1$). Furthermore, it is known that a Hamilton operator cannot be diagonalized at an EP.[15] Therefore, if the real λ-axis is densely populated by accumulation points of EPs, it could mean that in the limit $N \to \infty$ the Hamiltonian (1) ceases to be hermitian for $\lambda > 1$. For $\lambda = \pm 1$ this is likely to be the case.

So far, we have seen from the discussion above that the limit, if it exists, is much more subtle for $\lambda \geq 1$ than it may appear at first glance. Well-established methods like bosonization and quite different attempts like exceptional points do not provide obvious answers. We mention a semi-classical approach in which the operators $J_{x,y,z}$ are rewritten in polar coordinates.[16] It turns out that $\cos\theta$ and ϕ, the cosine of the polar and the azimuth angle, respectively, can be interpreted as canonical conjugate coordinates and the problem is thus reduced again to a single-particle problem. This approach yields at $\lambda = 1$ a $k^{4/3}$ behaviour for the levels E_k being numerically well confirmed (H. Krield, pers. comm.) and contrasting results based on Equations (2) and (3). It also confirms the $N^{-1/3}$ behaviour for the level distances at $\lambda = 1$ obtained independently in ref. 17.

It is not yet clear whether the problematic large N limit of the Lipkin model has obvious physical ramifications or whether it is simply a mathematical freak of an otherwise extremely useful model. Note, however, the comments made above in connection with analyticity. Yet, there are strong indications from the study of the EPs related to phase transitions[18] that the limit attained is less problematic if the model is perturbed in a stochastic way. In fact, the EPs would then be tossed around, they may not even accumulate on the real axis, and the phase transition would be generically smeared out. Related to this question is that of the extended states associated with EPs: will they become localized? These and related problems, seemingly of a universal nature and interest, must be the subject of future research.

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