A UNIFIED VIEW ON VARIOUS ITERATIVE APPROACHES
TO THE GROUND-STATE AND FINITE TEMPERATURE PROPERTIES OF QUANTUM SPIN SYSTEMS

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We show that several iterative techniques, which were proposed for calculating ground-state properties of quantum models, can all be derived as the zero-temperature limit of a real-space quantum renormalization method. As a consequence, all these techniques are systematically improvable by a perturbative approach, and may be extended in a natural way to nonzero temperatures.

In recent years several renormalization methods have been proposed for studying the ground state properties of quantummechanical models, such as the Ising model in a transverse field [1,2], the Heisenberg and XY-model [2,3], or the Kondo problem [4].

With the exception of Ref.[1], there seems at first sight to be no clear connection between these methods and the renormalization techniques introduced for studying the properties of the same systems at nonzero temperatures [5].

Nevertheless, it would be highly desirable to have a unified approach to ground-state and finite temperature properties, possibly within a unique approximation scheme. It is the purpose of this contribution to show that there exists indeed such a unique approximation scheme, which includes all the above mentioned methods as possible zero temperature realizations.

We will illustrate our argument by the example of the XY-model without transverse field. We will show that the zero temperature limit of a properly chosen transformation of the type defined in Ref.[5] yields the ground state transformation scheme of Ref.[3].

We divide, as usual, the lattice in Kadanoff cells, and we split the Hamiltonian as $H = H_0 + V$, $H_0 = \sum_{\alpha} H_{0\alpha}$, where α numbers the cells and V contains the inter-cell interactions. Due to the up-down symmetry in the z-component of the spins, if each cell contains an odd number of lattice sites, the eigenvalues ϵ_i of $H_{0\alpha}$ will be degenerate, and we will denote the corresponding eigenstates by $|+,i\rangle$ and $|-,i\rangle$. The $(\pm)$ sign may correspond to the sign of the majority of the z-components of the spins in the cell, and we will identify this sign with σ_{α}^z , the z-component of the new effective cell spin vector.

A finite temperature renormalization transformation on the reduced Hamiltonian (βH) can then be defined according to the basic formula [5]:

$$\langle \sigma_{\alpha}^z | \exp(-(\beta'H')) | \sigma_{\alpha}^z \rangle = \sum_{\{i_{\alpha}\}} \langle \sigma_{\alpha}^z, \{i_{\alpha}\} | \exp(-\beta H) | \sigma_{\alpha}^z, \{i_{\alpha}\} \rangle. \quad (1)$$

$\beta'H'$ may now be calculated in a cumulant expansion in V , e.g. by making use in the r.h.s. of (1) of the identity

$$e^{-\beta H_0 - \beta V} = e^{-\beta H_0} T \exp \left(- \int_0^{\beta} d\lambda e^{\lambda H_0} V e^{-\lambda H_0} \right), \quad (2)$$

where T is the ordering operator with respect to decreasing values of λ .

From these formulae, one can now compute $\beta'H'$ up to any desired order in V . In doing so, we obtain an expression which is linear in β , since all higher-order terms in β are canceled by the cumulant expansion. If one then takes the limit $\beta \rightarrow \infty$, one obtains recursion formulae between H' and H , which coincide exactly with the formulae derived for zero temperatures from the Rayleigh-Schrödinger perturbation theory [3].

Besides giving a new interpretation to this zero-temperature iteration procedure, the present approach allows us to extend in a natural way the ground-state calculations into a method for obtaining numerical estimates for the free energy at all temperatures. In this way we have verified, e.g., that already in a first order calculation the free energy of the 1-dimensional XY-chain deviates less than 13% from the exact result over the whole temperature range (at $T=0$ this deviation is 11% [3]).

For systems with transverse fields, either Ising or XY, the ground state of $H_{0\alpha}$ is no longer degenerate. For such systems different iterative methods have been proposed [1,2] and it has even been claimed that these methods are not perturbative [2].

We have been able to show, however, that these methods may also be obtained as a first-order approximation to a transformation as defined

in formula (1), if one makes an appropriate choice for the labelling of the cell states $|\pm, i\rangle$. The ground state and the first excited state of $H_{0\alpha}$ have to be classified as belonging to $\sigma_{\alpha}^z = +1$ and -1 respectively (consistently with the direction of the magnetic field), and to the same i -value. In this way, of course, σ_{α}^z is not necessarily defined according to the previously described majority rule.

It is then possible to look for corrections to the method of [2], by expanding (2) up to second order in V . In second order, higher energy eigenstates in the cell play an important role in the calculation; the results depend on the specific way in which these states have been classified as $|\pm, i\rangle$ states. The second order correction seems to give a remarkable improvement on the ground state energy. As an example, we tabulate a few ground state energy values for the 1-dimensional transverse Ising model, obtained with a two-spin cell:

h/J	$(-E_0/J)$ Ref. [2]	$(-E_0/J)$ 2d.order	$(-E_0/J)$ exact
0.2	1.0014	1.0347	1.0405
0.4	1.0156	1.1056	1.1680
0.6	1.0544	1.1863	1.4199

In this table, h and J are respectively the transverse field and the ferromagnetic interaction strength; E_0 is the ground state energy per spin.

We may thus conclude that the various methods, which have been proposed for studying the ground state properties of quantum systems by renormalization group methods may all be viewed as different realizations of the same idea. This idea amounts to set up a free energy preserving mapping of the spin Hamiltonian into a cell Hamiltonian on the basis of (1). If this mapping is computed in a suitable

cumulant approximation, the $\beta \rightarrow \infty$ limit can then be performed, leading to zero temperature transformations. The difference between the various methods lies mainly in whether one chooses for the basic cell states $|\sigma_{\alpha}^z, i\rangle$ the eigenstates of $\sum_j s_j^z$ ($j \in \alpha$) (as in [1]), or the eigenstates of $H_{0\alpha}$ (as in [2]). All methods are equally suited for a systematic improvement or for a generalization to nonzero temperatures.

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