Renormalization Group Approach to a One-Dimensional Cooperative T—e Jahn-Teller System

S. Brühl and E. Sigmund

Institute of Theoretical Physics, University of Stuttgart, Pfaffenwaldring 57, 7000 Stuttgart 80, Germany

(Z. Naturforsch. **32 a**, 111—112 [1977]; received December 22, 1976)

A linear chain of $T-e$ molecules exhibiting the cooperative Jahn-Teller effect is considered. Following Nauenberg's[1] treatment of the one-dimensional Ising model a renormalization group approach is used. The series-expansion of the free energy is put into a closed form.

We consider a one-dimensional chain of identical unit cells of cubic symmetry, each of which represents a $T-e$ Jahn-Teller center. This means that in each unit cell a triply degenerate electronic state interacts with a doubly degenerate vibrational mode. By an exponential transformation the local electron-phonon coupling is transcribed into a nonlocal electron-electron interaction[2, 3]. If we restrict ourselves to a coupling between nearest neighbours the resulting Hamiltonian reads

$$H = -J \sum_n (\tau_n \tau_{n+1} + \tfrac{1}{3} \Gamma_n \Gamma_{n+1}) \tag{1}$$

where τ and Γ are diagonal electronic operators with the eigenvalues -1, 0, 1 and 1, 1, -2 respectively. J is the coupling constant. The 3×3 transfer matrix of this system takes the form

$$P = \begin{Bmatrix} e^{2K} & e^{-K} & e^{-K} \\ e^{-K} & e^{2K} & e^{-K} \\ e^{-K} & e^{-K} & e^{2K} \end{Bmatrix} \tag{2}$$

with

$$K = \tfrac{2}{3} J \; (k_B T = 1) \, .$$

Following the method of Nauenberg[1] and others[4, 5] we have to look for a renormalization transformation $K \to K'$ such that

$$P^2(K) = e^{2g(K)} P(K') \, . \tag{3}$$

In this way a partial summation over the even lattice points $n = 2, 4, \ldots$ is performed and the system is reduced to the $N/2$ odd lattice points with an effective coupling constant K'. From exprs. (2) and (3) we get the relations

$$K' = \frac{1}{3} \ln \frac{e^{3K} + 2\, e^{-3K}}{2 + e^{-3K}} \tag{4}$$

and

$$g(K) = \tfrac{1}{2} K' + \tfrac{1}{2} K + \tfrac{1}{2} \ln (2 + e^{-3K}) \, . \tag{5}$$

Just as for the one dimensional Ising model the fixed points of Eq. (4) are $K^* = 0$ and $K^* = \infty$ with the eigenvalues $\lambda = 0$ and $\lambda = 1$ respectively. This means that there exists no phase transition for our system.

Applying the renormalization transformation n times, the mapping from the initial coupling constant $K^{(0)} = K$ to the final value $K^{(n)}$ is given by

$$K^{(n)} = \frac{1}{3} \ln \frac{\exp\{3\, K^{(n-1)}\} + 2 \exp\{-3\, K^{(n-1)}\}}{2 + \exp\{-3\, K^{(n-1)}\}} \, . \tag{6}$$

In order to solve this recurrence relation we perform a transformation to a new variable. In accordance to Ref. [1] we require

$$\zeta' = \zeta^2 \, . \tag{7}$$

Inserting the formal ansatz

$$\zeta = (a_0 + a_1\, e^{3K}) / (b_0 + b_1\, e^{3K}) \tag{8}$$

into Eq. (7) and comparing with Eq. (4) the transformation is found to be

$$\zeta = (e^{3K} - 1)/(e^{3K} + 2) \, . \tag{9}$$

Then the solution of the recurrence formula (6) takes the form

$$K^{(n)} = \frac{1}{3} \ln \frac{1 + 2\, \zeta^{2^n}}{1 - \zeta^{2^n}} \, . \tag{10}$$

As shown in Ref. [1] the free energy per lattice point in the thermodynamic limit can be given in a series expansion

$$f(K) = \sum_{n=0}^{\infty} g(K^{(n)})/2^n$$

which in our case leads to

$$f(K) = \frac{1}{2} K + \frac{3}{2} \sum_{n=1}^{\infty} \frac{K^{(n)}}{2^n} + \frac{1}{2} \sum_{n=0}^{\infty} \frac{1}{2^n} \cdot \ln (2 + e^{-3K^{(n)}}) \, . \tag{11}$$

With help of solution (10) one gets

$$f(K) = -K + \ln 3 + \ln \prod_{n=0}^{\infty} \left(\frac{1 + \zeta^{2^n}}{1 - \zeta^{2^n}} \right)^{(\frac{1}{2})^{n+1}} . \tag{12}$$

The product over n can be transcribed into the closed form $1/(1-\zeta)$ and the final result is

$$f(K) = \ln (e^{2K} + 2\, e^{-K}) \, . \tag{13}$$

This expression can also be obtained using the conventional transfer matrix method

$$f(K) = \lim_{N \to \infty} \frac{1}{N} \ln \mathrm{Trace}(P^N) = \ln \lambda_{\mathrm{Max}} \tag{14}$$

Reprint requests to Dr. E. Sigmund, Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, *D-7000 Stuttgart 80*, Germany.

where $\lambda_{\mathrm{Max}} = e^{2K} + 2\,e^{-K}$ is the largest eigenvalue of P.

So far the linear $T-e$ electron-phonon chain is the only nontrivial cooperative Jahn-Teller system, which is solved exactly by a renormalization group approach. Up to now the more complicated system consisting of $E-e$ and $T-t$ molecules cannot be solved in an analytic form by this method. There numerical techniques are required.

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Verantwortlich für den Inhalt: A. Klemm
Satz und Druck: Konrad Triltsch, Würzburg