

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

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A linear chain of T–e molecules exhibiting the cooperative Jahn-Teller effect is considered. Following Nauenberg's<sup>1</sup> 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<sup>2,3</sup>. If we restrict ourselves to a coupling between nearest neighbours the resulting Hamiltonian reads

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

where  $\tau$  and  $\Gamma$  are diagonal electronic operators with the eigenvalues  $-1, 0, 1$  and  $1, 1, -2$  respectively.  $J$  is the coupling constant. The  $3 \times 3$  transfer matrix of this system takes the form

$$P = \begin{pmatrix} e^{2K} & e^{-K} & e^{-K} \\ e^{-K} & e^{2K} & e^{-K} \\ e^{-K} & e^{-K} & e^{2K} \end{pmatrix} \quad (2)$$

with

$$K = \frac{2}{3} J (k_B T = 1).$$

Following the method of Nauenberg<sup>1</sup> and others<sup>4,5</sup> we have to look for a renormalization transformation  $K \rightarrow K'$  such that

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

In this way a partial summation over the even lattice points  $n = 2, 4, \dots$  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

$$K' = \frac{1}{3} \ln \frac{e^{3K} + 2e^{-3K}}{2 + e^{-3K}} \quad (4)$$

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and

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

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

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

In order to solve this recurrence relation we perform a transformation to a new variable. In accordance to Ref.<sup>1</sup> we require

$$\zeta' = \zeta^2. \quad (7)$$

Inserting the formal ansatz

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

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

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

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

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

As shown in Ref.<sup>1</sup> 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

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

With help of solution (10) one gets

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

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

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

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

$$f(K) = \lim_{N \rightarrow \infty} \frac{1}{N} \ln \text{Trace}(P^N) = \ln \lambda_{\text{Max}} \quad (14)$$



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where  $\lambda_{\text{Max}} = e^{2K} + 2e^{-K}$  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.

<sup>1</sup> M. Nauenberg, J. Math. Physics **16**, 703 [1975].

<sup>2</sup> M. Wagner, to be published.

<sup>3</sup> G. A. Gehring and K. A. Gehring, Rep. Progr. Phys. **38**, 1 [1975].

<sup>4</sup> M. Nauenberg and B. Nienhuis, Phys. Rev. Lett. **33**, 1598 [1974].

<sup>5</sup> Th. Niemeijer and Th. W. Ruijgrok, Physica **81 A**, 427 [1975].