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A note on the existence of phase transitions in finite-site Peierls-Hubbard systems

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We discuss spectral properties of a generalized N-site n-electron Peierls-Hubbard system and examine the possibility of phase transitions of the ground state. For $N=2$, it is proved that no phase transition exists. For $N>2$, the only possibility of a phase transition is a crossing of two discrete energy levels corresponding to different symmetries.

1. Introduction

In this note, we are concerned with analytical properties of generalized finite-site Peierls-Hubbard systems; we examine their spectral properties and propose a method to test for the existence of a phase transition of the ground state.

The Peierls-Hubbard system, which is under consideration, describes n electrons on N lattice sites, which are coupled to N lattice ions. The lattice is taken one-dimensional and with periodic boundary conditions. The associated Hamiltonian reads as follows

$$H=H_T+H_U+H_L+H_S \tag{1}$$

where

$$H_T=-\sum_{\sigma=1}^{2}\sum_{i,j=1}^{N}[T_{\sigma ij}(Q_1,\ldots,Q_N)\,c_{i\sigma}^{+}\,c_{j\sigma}+\text{h.c.}], \tag{2}$$

$$H_U=\sum_{i=1}^{N}U_i\,n_{i1}\,n_{i2}, \tag{3}$$

$$H_L=\sum_{i=1}^{N}[\tfrac{1}{2}\omega_i\,P_i^2+V(Q_i)]+\sum_{i\neq j}W(Q_i,Q_j), \tag{4}$$

$$H_S=S^{\frac{1}{2}}\cdot f(Q_1,\ldots,Q_N;n_1,\ldots,n_N). \tag{5}$$

In (3) and (5), we defined

$$n_{i\sigma}=c_{i\sigma}^{+}\,c_{i\sigma} \tag{6}$$

and

$$n_i=n_{i1}+n_{i2}. \tag{7}$$

Let us briefly explain the notation and the physics contained in the Hamiltonian H. $c_{i\sigma}^{+}$, $c_{i\sigma}$ are (fermionic) creation and annihilation operators for the electrons; i is the site numeration and σ the spin index for the electrons. P_i, Q_i are the momentum and position operators of the lattice ions. H_T describes electronic hopping processes with transfer energy $-T_{\sigma ij}(Q_1,\ldots,Q_N)$. This transfer energy is taken in a generalized form, for it may depend on the lattice site, the spin and on the displacements of the oscillators. The Hubbard term H_U takes into account the Coulomb repulsion U_i of electrons at the same lattice site i with different spins. H_L describes the lattice ions, moving in a generalized potential $V(Q_i)$. Additionally an ion-ion-interaction is taken into account by $W(Q_i,Q_j)$. In general, V and W may include harmonic and non-harmonic contributions to the lattice vibrations. Finally, H_S describes the electron-ion coupling in a generalized form, S being the coupling parameter. Note that this coupling may be nonlinear in the electron density and may be on-site as well as off-site, since $f(Q_1,\ldots,Q_N;n_1,\ldots,n_N)$ is, in principle, an arbitrary function. Of course the number of electrons is conserved. Therefore one may seek solutions corresponding to fixed electron number n.

In the literature, frequently the socalled T-U-S-ω-model of an Peierls-Hubbard system is studied. It is a special case of the Hamiltonian H, which is obtained

by setting

$$T_{\sigma ij}(Q_1, \ldots, Q_N) \equiv \begin{cases} T & \text{if } (ij) \text{ nearest neighbours} \\ 0 & \text{otherwise,} \end{cases}$$

$$U_i \equiv U, \ \omega_i \equiv \omega, \tag{8}$$

$$V(Q_i) \equiv \tfrac{1}{2} Q_i^2, \quad W(Q_i, Q_j) \equiv 0 \tag{9}$$

and

$$f(Q_1, \ldots, Q_N; n_1, \ldots, n_N) \equiv \sum_{i=1}^{N} n_i Q_i. \tag{10}$$

In the adiabatic limit ($\omega \equiv 0$) one may regard the Q_i's as parameters and it is known that in this approximation phase transitions (i.e. nonanalyticities of the ground state energy as a function of T, U, S) may occur. The lattice configuration of the ground state can change from an undistorted state to a distorted state, as S increases. We refer to Toyozawa [1], who treats the case $N=2$, as well as to Schreiber [2] for $N=3$, and to Takimoto and Toyozawa [3] for $N=4$. Does this situation change for the physical case when the kinetic energy of the lattice is not ignored?

In the atomic limit ($T \equiv 0$), on the other hand, one may regard the n_i's as parameters. The T-U-S-ω-model is completely solvable for $T \equiv 0$ yielding a first order phase transition of the ground state which is connected with a structural charge of the ground state from a charge density wave to a spin density wave (as U increases). Does this phase transition persist for finite T?

Up to now, these two questions were merely attacked by numerical calculations. For very small N, e.g. $N=2$, the T-U-S-ω-model can be solved (see e.g. Schmidt and Schreiber [4] for numerical results). It turns out, that numerically the sharp structure of phase transitions vanishes for strictly positive ω and T. In this paper, we propose a general criterion which definitively decides the existence or non-existence of phase transitions. In particular, we do prove that for $N=2$ no phase transition of the ground state exists, supporting nicely the numerical results of Schmidt and Schreiber [4].

Our result holds not only for the T-U-S-ω-model, but also for the generalized Hamiltonian (1). Thus the effects of a Q-dependent transfer energy, ion-ion-interactions and nonlinear off-site couplings, which would require a much greater numerical effort, are automatically included into our proof. They do not change the negative result, concerning the existence of phase transitions.

Furthermore, our method should be useful for larger N, where the numerical procedures become more and more complicated (see e.g. Schmidt and Schreiber [5]).

This paper is organized as follows: Studying spectral properties of the Hamiltonian H, the phase transition problem is reduced to a degeneracy problem in Sect. II. In Sect. III, the special case $N=2$ is considered. It is proved that the ground state is nondegenerate which excludes a phase transition. Finally, in Sect. IV, we give an outlook to larger systems ($N>2$) and conclude our results.

II. Spectral properties and existence of phase transitions

In this chapter, we provide a condition for the Hamiltonian (1) to have a purely discrete spectrum. Especially, the ground state is discrete in this case. This enables us to apply analytical perturbation theory in order to prove smoothness properties of the ground state.

Since we are dealing with a finite number of sites, the electronic operators, which are representable as finite-dimensional matrices, cannot generate a continuous spectrum. For arbitrary functions $T_{\sigma ij}$, V, W and f in (2), (4) and (5), however, there may be a continuous spectrum due to the infinite-dimensional Hilbert space of the ions. If, however, the potentials tend to infinity for $|Q_i| \to \infty$, such a continuous spectrum is not expected. In the following, we shall give a rigorous formulation of these facts.

Firstly, we specify the underlying Hilbert space $\mathscr{H}$, on which H is defined, to the usual product space of ions and electrons

$$\mathscr{H} = L^2(\mathbb{R}^N) \otimes \mathbb{C}^M \tag{11}$$

where M is the dimension of the electronic space. Whether or not we restrict ourselves to fixed particle number n ($1 \leqq n \leqq 2N$), bears no consequence for this section. Let

$$\mathbf{P} \equiv (P_1, \ldots, P_N), \quad \mathbf{Q} \equiv (Q_1, \ldots, Q_N), \quad \mathbf{n} \equiv (n_1, \ldots, n_N). \tag{12}$$

We assume henceforth $\omega_i > 0$ for all $i = 1, \ldots, N$. After a suitable scaling transformation, we may even take $\omega_i \equiv 1$.

Consider the Hamiltonian

$$H_P \equiv H_L + H_S \equiv \tfrac{1}{2} \mathbf{P}^2 + G(\mathbf{Q}, \mathbf{n}) \tag{13}$$

where the last equation defines an "effective potential" $G(\mathbf{Q}, \mathbf{n})$.

Now, we are able to prove our first statement: If $G(\mathbf{Q}, \mathbf{n})$ is locally bounded and bounded from below by $d > -\infty$ and if the assumption

$$\lim_{|\mathbf{Q}| \to \infty} G(\mathbf{Q}, \mathbf{n}) = \infty \quad \text{(for any fixed } \mathbf{n}) \tag{14}$$

holds, then the Hamiltonian H_P has a purely discrete spectrum [6].

The proof is quite analogous to the one of theorem XIII.16 of Reed and Simon [7]. We only sketch the main steps: Because of (14), there exists, for any positive real number c, a ball B such that $G(\mathbf{Q}, \mathbf{n}) \geqq c$ if $\mathbf{Q} \notin B$. Let $F_c(\mathbf{Q})$ be the potential that is $-c+d$ if $\mathbf{Q} \in B$ and zero otherwise. Then we have [8]:

$$H_P \geqq \tfrac{1}{2}\mathbf{P}^2 + c + F_c(\mathbf{Q}). \tag{15}$$

Since the number of sites is finite, the Hamiltonian $\frac{1}{2}\mathbf{P}^2 + F_c(\mathbf{Q})$ has only a finite number of eigenvalues which are smaller than -1. Hence by (15), the number of eigenvalues of H_P which are smaller than $c-1$ is finite. As c can be chosen arbitrarily large, we finally get that H_P has purely discrete spectrum.

Next, we have to examine the influence of $H_T + H_U$ on the discreteness of the spectrum. Since H_U depends merely on electronic operators, it is a bounded operator, i.e. there exists a number $C < \infty$ such that

$$H_U \leqq C. \tag{16}$$

Concerning H_T, we assume that H_T is form bounded with respect to H_P i.e. there exist numbers $A < 1$ and $B < \infty$ such that

$$|H_T| \leqq A \cdot H_P + B. \tag{17}$$

A straight forward calculation shows that (17) is fulfilled if

$$2L|T(\mathbf{Q})| \leqq A \cdot G(\mathbf{Q}) + B \tag{18}$$

for some $A < 1$, $B < \infty$ where L is the number of different index combinations of σ, i, j such that $T_{\sigma ij} \not\equiv 0$. Furthermore

$$T(\mathbf{Q}) \equiv \max_{\sigma, i, j} T_{\sigma ij}(\mathbf{Q}) \tag{19}$$

and

$$G(\mathbf{Q}) \equiv \min_{\mathbf{n}} G(\mathbf{Q}, \mathbf{n}). \tag{20}$$

Now we show that under the condition (17) the Hamiltonian H has purely discrete spectrum, too.

Because of (16) and (17), the following von-Neumann resolvent expansion converges in norm

$$(\zeta - H)^{-1} = (\zeta - H_P)^{-1} \left\{ \sum_{n=0}^{\infty} [(H_T + H_U)(\zeta - H_P)^{-1}]^n \right\} \tag{21}$$

and the second factor of the right hand-side of (21) defines a bounded operator for $\mathrm{Re}\,\zeta$ sufficiently small. An equivalent statement (see Reed, Simon [6]) for the fact that a Hamiltonian H has purely discrete spectrum, is that its resolvent $(\zeta - H)^{-1}$ is compact for some ζ. By our statement above, $(\zeta - H_P)^{-1}$ is compact for $\mathrm{Re}\,\zeta$ sufficiently small. Because of (21), $(\zeta - H)^{-1}$ is representable as a product of a compact and a bounded operator for $\mathrm{Re}\,\zeta$ sufficiently small. Therefore $(\zeta - H)^{-1}$ is compact for $\mathrm{Re}\,\zeta$ sufficiently small. Consequently, H has purely discrete spectrum, too.

Let us summarize our result. If ω_i is strictly positive and if the assumptions (14) and (17) hold, the spectrum of H is purely discrete. We remark that (14) is not fulfilled, if the system is translational invariant. Then one has to separate the conserved total momentum and to discuss the spectrum of the associated momentum-decomposed Hamiltonian with our methods.

Now we turn to analytical perturbation theory (see Kato [9]). This theory ensures us that a nondegenerate discrete state depends analytically on $t_{\sigma ij}$, U_i and S for $S > 0$, where $t_{\sigma ij}$ is an extracted transfer parameter: $T_{\sigma ij}(\mathbf{Q}) \equiv t_{\sigma ij} \cdot h_{\sigma ij}(\mathbf{Q})$. To guarantee analyticity around $S = 0$, one has additionally to require that there exist numbers $C < 1$ and $D < \infty$ such that

$$|f(\mathbf{Q}; \mathbf{n})| \leqq C(H_L + H_T) + D. \tag{22}$$

Consequently, the whole spectrum of H depends analytically on $t_{\sigma ij}$, U_i and S except possible degenerate points. Therefore the phase transition problem of the ground state is clearly reduced to the degeneration problem of the ground state. If the ground state is nondegenerate for any $t_{\sigma ij}$, U_i and S, no phase transition does occur.

In the next section, we shall prove that, for $N = 2$, the ground state is unique for any $t_{\sigma ij}$, U_i and S, if the transfer energies $-T_{\sigma ij}(\mathbf{Q})$ are negative.

III. The two-site case ($N = 2$)

The two-site case represents the simplest nontrivial Peierls-Hubbard system. In this section, we are concerned with the degeneracy problem of the ground state for this case. We write the transfer part H_T of the Hamiltonian H as follows

$$H_T = -\sum_{\sigma=1}^{2} T_\sigma(\mathbf{Q})(c_{1\sigma}^+ c_{2\sigma} + c_{2\sigma}^+ c_{1\sigma}). \tag{23}$$

Henceforth, we assume a strictly negative transfer energy, i.e.

$$T_\sigma(\mathbf{Q}) > 0 \quad \text{for any } \mathbf{Q}, \sigma \tag{24}$$

and we restrict ourselves to electron number $n = 2$. The cases $n = 1, 3$ can be treated in the same manner

and are not considered further. Then, the electronic space is six-dimensional and spanned by the vectors $|1\rangle, \ldots, |6\rangle$ where

$$|1\rangle = c_{12}^+ c_{11}^+ |0\rangle, \quad |2\rangle = c_{21}^+ c_{22}^+ |0\rangle, \tag{25}$$

$$\begin{aligned} |3\rangle &= 2^{-\frac{1}{2}}(c_{12}^+ c_{21}^+ - c_{11}^+ c_{22}^+)|0\rangle, \\ |4\rangle &= 2^{-\frac{1}{2}}(c_{12}^+ c_{21}^+ + c_{11}^+ c_{22}^+)|0\rangle, \end{aligned} \tag{26}$$

$$|5\rangle = c_{12}^+ c_{22}^+ |0\rangle, \quad |6\rangle = c_{11}^+ c_{21}^+ |0\rangle. \tag{27}$$

Here, $|0\rangle$ is the electronic vacuum. The last two states $|5\rangle$ and $|6\rangle$ are triplett states with nonvanishing total spin, which do not interact with the other states. Therefore it suffices to study the spectrum of H in the reduced electronic space spanned by $|1\rangle, \ldots, |4\rangle$. H reads as follows:

$$H \equiv H_L + A \equiv H_0 + F(\mathbf{Q}) + A \tag{28}$$

where the last equation defines $F(\mathbf{Q})$. H_0 is given by

$$H_0 \equiv \sum_{i=1}^{N} \tfrac{1}{2}\omega_i P_i^2 \tag{29}$$

and the operator A is represented in the chosen electronic representation ($A_{ij} = \langle i|A|j\rangle$) as

$$(A_{ij}) = \begin{pmatrix} U_1 + S^{\frac{1}{2}} f(\mathbf{Q}; 2, 0) & 0 & -a(\mathbf{Q}) & -b(\mathbf{Q}) \\ 0 & U_2 + S^{\frac{1}{2}} f(\mathbf{Q}; 0, 2) & -a(\mathbf{Q}) & -b(\mathbf{Q}) \\ -a(\mathbf{Q}) & -a(\mathbf{Q}) & S^{\frac{1}{2}} f(\mathbf{Q}; 1, 1) & 0 \\ -b(\mathbf{Q}) & -b(\mathbf{Q}) & 0 & S^{\frac{1}{2}} f(\mathbf{Q}; 1, 1) \end{pmatrix} \tag{30}$$

with

$$\begin{aligned} a(\mathbf{Q}) &= 2^{-\frac{1}{2}}(T_1(\mathbf{Q}) + T_2(\mathbf{Q})), \\ b(\mathbf{Q}) &= 2^{-\frac{1}{2}}(T_2(\mathbf{Q}) - T_1(\mathbf{Q})). \end{aligned} \tag{31}$$

Henceforth, we additionally assume

$$T_2(\mathbf{Q}) > T_1(\mathbf{Q}) \quad \text{for any } \mathbf{Q} \tag{32}$$

such that (together with (24)) $a(\mathbf{Q})$ and $b(\mathbf{Q})$ are strictly positive.

We remark that the trivial case $T_2(\mathbf{Q}) \equiv T_1(\mathbf{Q})$ can be treated analogously by reducing the matrix A to a 3×3 matrix, since then the state $|4\rangle$ doesn't interact with the other states. Also the cases $T_2(\mathbf{Q}) \geqq T_1(\mathbf{Q})$ and $T_2(\mathbf{Q}) \leqq T_1(\mathbf{Q})$ are included into the subsequent proof. (In the first case the second factor of the right hand side of (37) is no longer strictly positive for any $\mathbf{q}$, k and l, but nevertheless (33) remains strictly positive. The latter case is obtained from the first case by an index permutation.)

Now we turn to the basic question of the uniqueness of the ground state which was raised in Sect. II. There exists a manageable criterion which guarantees that for a given Hamiltonian H the ground state is nondegenerate (see e.g. Reed, Simon [7]): If in a chosen representation of the Hilbert space $\mathscr{H}$ the integral kernel of the operator $\exp(-H)$ is strictly positive, then its ground state is nondegenerate. Furthermore, let $H = H_1 + V$ where V is a multiplication operator in the chosen representation (i.e. V has vanishing nondiagonal matrix elements in the chosen representation). Then, $\exp(-H)$ has a strictly positive integral kernel, if $\exp(-H_1)$ has a strictly positive integral kernel. For a proof, we again refer to Reed, Simon [7] and to Gerlach, Löwen [10] who applied these criteria recently to the polaron problem.

Utilizing this method for our problem, we firstly have to choose the representation. For the oscillators we choose the position representation ($\mathbf{Q}$-representation). As electronic representation we just choose the one given by the states $|1\rangle, \ldots, |4\rangle$ in (25) and (26). Neglecting all multiplication operators according to the criterion above, all we have to do, in order to prove the nondegeneracy of the ground state, is to show that the integral kernel

$$\langle \mathbf{y}| \langle j| \exp(-H_0 + B(\mathbf{Q}))|i\rangle |\mathbf{x}\rangle \tag{33}$$

is strictly positive for any $\mathbf{y}$, $\mathbf{x}$, i and j. In (33), $B(\mathbf{Q})$ is defined by

$$(B_{ij}(\mathbf{Q})) = \begin{pmatrix} 0 & 0 & a(\mathbf{Q}) & b(\mathbf{Q}) \\ 0 & 0 & a(\mathbf{Q}) & b(\mathbf{Q}) \\ a(\mathbf{Q}) & a(\mathbf{Q}) & 0 & 0 \\ b(\mathbf{Q}) & b(\mathbf{Q}) & 0 & 0 \end{pmatrix} \tag{34}$$

$|\mathbf{y}\rangle$, $|\mathbf{x}\rangle$ are (formal) eigenstates of $\mathbf{Q}$. To prove the positivity of (33), we use the Trotter product formula

$$\begin{aligned} &\langle \mathbf{y}| \langle j| \exp(-H_0 + B(\mathbf{Q}))|i\rangle |\mathbf{x}\rangle \\ &= \lim_{m \to \infty} \langle \mathbf{y}| \langle j| (\exp(-H_0/m) \exp(B(\mathbf{Q})/m))^m |i\rangle |\mathbf{x}\rangle. \end{aligned} \tag{35}$$

We firstly observe that

$$\begin{aligned} \langle \mathbf{z}| \langle k| \exp(-H_0/m)|l\rangle |\mathbf{q}\rangle &= \delta_{kl} \cdot \left[\prod_{i=1}^{N} (m/(2\pi\omega_i))^{\frac{1}{2}}\right] \\ \cdot \exp\left(-\sum_{i=1}^{N} m(z_i - q_i)^2/(2\omega_i)\right) \end{aligned} \tag{36}$$

and that

$$\langle \mathbf{z}| \langle k| \exp(B(\mathbf{Q})/m) |l\rangle |\mathbf{q}\rangle$$
$$= \delta(\mathbf{q}-\mathbf{z}) \cdot \langle k| \sum_{p=0}^{\infty} (p!)^{-1} m^p (B(\mathbf{q}))^p |l\rangle. \quad (37)$$

The second factor of the right hand side of (36) is strictly positive for any $\mathbf{z}$, $\mathbf{q}$ and for $\omega_i > 0$. Since $a(\mathbf{Q})$ and $b(\mathbf{Q})$ are strictly positive, we get by an explicit computation, that the second factor of the right hand side of (37) is strictly positive for any $\mathbf{q}$, k, l, too. Therefore, according to the standard Feynman-Kac construction of integral kernels, the combination of (35), (36) and (37) shows that (33) is strictly positive.

Consequently, the ground state of H is nondegenerate in the case $N=2$.

We add a final remark. The positivity of (33) implies that the ground state is strictly positive in the chosen representation (see again Reed and Simon [7]). Physically this means that the ground state is not a pure spin density wave or a pure charge density wave but a mixture of all states $|1\rangle, \ldots, |4\rangle$. As indicated above, this holds only for strictly positive frequencies $\omega_i > 0$ and transfer energies $T_\sigma(\mathbf{Q}) > 0$.

IV. The case $N>2$, conclusions

For $N>2$, the method from Sect. III cannot be used directly, even for the simple T-U-S-ω-model: In the usual electronic representations, where H_U and H_S acts as multiplication operators, the corresponding matrix A has also negative nondiagonal matrix elements and therefore $\exp(-H)$ can no longer have a positive kernel in this representation. To prove the nondegeneracy of the ground state, one has to find another better representation where $\exp(-H)$ has a strictly positive kernel. We leave this as an unsolved problem.

It may, however, happen that the ground state energies of the Hamiltonian fixed to the subspace of a given symmetry intersect each other. To decide whether or not this is connected with a phase transition, one has to proceed as follows: In each subspace of a given symmetry, one has to find a representation such that the kernel of $\exp(-PHP)$ is strictly positive in the restricted Hilbert space. Here P is the projection operator on the subspace of a given symmetry. Then the ground state is unique and analytical in the subspace of a given symmetry. The identity theorem for holomorphic functions tells us that a intersection of two energy levels of different symmetry is a true nonanalyticity, i.e. a phase transition. The crossing of two noninteracting, discrete energy levels is the only mathematical possibility for a nonanalytical ground state energy.

For $N=n=3$, in the adiabatic approximation, there exist phase transitions for the T-U-S-ω-model (see Schreiber [2]). However, the calculation of Schmidt, Schreiber [11] indicates that the symmetry of the ground state doesn't change. Therefore, for $T>0$ and $\omega>0$ no phase transition is expected.

For $N=n=4$, however, Schmidt and Schreiber [11] show that the symmetry of the ground state changes, even in a nonadiabatic calculation. This indicates that, in this case, a phase transition really takes place.

A final remark is in order concerning finite temperatures. A phase transition, generated by a possible crossing of two discrete energy levels of different symmetries, will vanish. The free energy is analytical in all parameters. It is the zero temperature limit which may generate a nonanalyticity. This is in accordance with results, proven for discrete electron-phonon models (see [12]), and it can be shown in the same way as in [12].

In conclusion, we have studied spectral properties of Peierls-Hubbard systems. We have given sufficient conditions such that the spectrum of the associated Hamiltonian is purely discrete. The phase transition problem is directly connected with a degeneracy problem of the ground state. For $N=2$, we have shown that the ground state is unique which excludes a phase transition. Our result is not limited to the simple T-U-S-ω-model. It also includes more general transfer energies, being for example essential in the Su-Schrieffer-Heeger-model [13], and nonlinear electron-ion coupling.

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