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Finite Hubbard Model with Phonon Coupling

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Abstract

The spectrum of the two point Hubbard model with phonon coupling is studied. In particular the connection with quantum chaos is discussed.

Barma and Bari [1] studied the Hubbard model coupled to lattice vibrations for an infinite linear chain. Starting from the Hubbard model they expanded the hopping integral to first order in the phonon operators. The thermodynamic and transport properties for this model can only be obtained approximately. In the present paper we discuss a finite Hubbard model with phonon coupling. To be precise, a two point model coupled with one phonon mode is discussed. Finite dimensional Hubbard models without phonon couplings have been widely studied in literature [2–4]. The model under consideration is given by

$$H = t\sum_{\sigma}(c_{1\sigma}^{+}c_{2\sigma} + c_{2\sigma}^{+}c_{1\sigma}) + U\sum_{i=1}^{2} n_{i\uparrow}n_{i\downarrow} + \omega b^{+}b + k\sum_{\sigma}(c_{1\sigma}^{+}c_{2\sigma} + c_{2\sigma}^{+}c_{1\sigma})(b^{+} + b), \quad (1)$$

where b, b^{+} are the Bose annihilation and creation operators for the vibrational mode, respectively. The $c_{i\sigma}^{+}$, $c_{i\sigma}$ are the Fermi annihilation and creation operators and $n_{i\sigma} = c_{i\sigma}^{+}c_{i\sigma}$. The quantity t is the hopping integral and U is the on-site Coulomb repulsion. The third is the oscillatory energy and the fourth term describes the interaction. The two-site Hubbard model with vibronic coupling has been investigated by several authors [5–7]. Kral [5] and Rice [7] studied this model in connection with TCNQ salts.

We study the spectrum of this Hamiltonian in dependence on k. In particular the connection with "quantum chaos" [4, 8–13] is discussed.

A large number of authors (compare [4, 8–13] and references therein) have studied the interrelation between classical Hamiltonian systems which show chaotic behaviour above a threshold value E_c and the corresponding quantum system. Various approaches have been applied to "define" what we understand by "quantum chaos". Among others, there are the method of avoiding energy-level crossings and the distributions of nearest-neighbour spacings. When we consider the method of distribution of the nearest-neighbour spacings we find that in the regular case (i.e., the classical system is integrable) the energy eigenvalues are distributed randomly, leading to a Poisson-type distribution function [11]. A regular spectrum ("quantum chaos") occurs when energy levels are correlated, resulting in a repulsion of adjacent levels [12]. The nearest neighbour-spacings distribution function peaks at a finite value and exhibits the typical feature of a Wigner distribution. In this case the classical system shows chaotic behaviour. A warning is in order: In literature the impression is given that a Wigner distribution is the "hallmark" of quantum chaos. While rigorous proofs exist for integrable systems [11], no such proofs exist for the non-integrable systems. Based on a "plausible assumption" about the spatial distribution of the wave function for chaotic Hamiltonians, Peschukas [12] was able to derive the level spacings distribution in the irregular spectrum, and he showed that it is close to a Wigner distribution. The possibility cannot be excluded that strongly non-separable but integrable systems rise to highly non-Poisson, and maybe Wigner-like distribution. These remarks indicate that the question of chaos in quantum mechanics is still far from being solved. In the given model (1) we have the additional problem that there is no classical analog (compare [4, 13] for the discussion of this point). Thus we study the spectrum of Hamiltonian (1) in dependence on k and ask whether or not there is level repulsion.

First of all let us briefly discuss the (well-known) case without the phonon coupling. The two point Hubbard model is given by

$$H_{\mathrm{H}} = t\sum_{\sigma}(c_{1\sigma}^{+}c_{2\sigma} + c_{2\sigma}^{+}c_{1\sigma}) + U\sum_{i=1}^{2} n_{i\uparrow}n_{i\downarrow}. \quad (2)$$

The Hamiltonian H_{H} commutes with the number operators $\hat{N}_e = \Sigma_{i=1}^{2}(n_{i\uparrow} + n_{i\downarrow})$ and with the spin operator in z-direction $\hat{S}_z = (1/2)\Sigma_{i=1}^{2}(n_{i\uparrow} - n_{i\downarrow})$. In the following we study the half-filled case, i.e., $N_e = 2$. Consider first the subspace with $S_z = 0$. The Hamiltonian is invariant under spin reversal ($\uparrow \rightleftarrows \downarrow$) and under lattice site reversal ($1 \rightleftarrows 2$). Consequently, we can decompose the four dimensional space in invariant subspaces, namely $S_1 = \{|\Psi_1\rangle, |\Psi_2\rangle\}$ $S_2 = \{|\Psi_3\rangle\}$ and $S_3 = \{|\Psi_4\rangle\}$ where

$$|\Psi_1\rangle = 2^{-1/2}(c_{1\uparrow}^{+}c_{1\downarrow}^{+}|0\rangle + c_{2\uparrow}^{+}c_{2\downarrow}^{+}|0\rangle) \quad (3a)$$

$$|\Psi_2\rangle = 2^{-1/2}(c_{1\uparrow}^{+}c_{2\downarrow}^{+}|0\rangle + c_{2\uparrow}^{+}c_{1\downarrow}^{+}|0\rangle) \quad (3b)$$

$$|\Psi_3\rangle = 2^{-1/2}(c_{1\uparrow}^{+}c_{2\downarrow}^{+}|0\rangle - c_{2\uparrow}^{+}c_{1\downarrow}^{+}|0\rangle) \quad (3c)$$

$$|\Psi_4\rangle = 2^{-1/2}(c_{1\uparrow}^{+}c_{1\downarrow}^{+}|0\rangle - c_{2\uparrow}^{+}c_{2\downarrow}^{+}|0\rangle). \quad (3d)$$

From the subspace S_1 we obtain the eigenvalues

$$\frac{E_{\pm}}{t} = \frac{U}{2t} \pm \left(\frac{U^2}{4t^2} + 4\right)^{1/2} \quad (4a)$$

or

$$\frac{E_\pm}{U} = \frac{1}{2} \pm \left(\frac{4t^2}{U^2} + \frac{1}{4}\right)^{1/2}. \tag{4b}$$

The function $|\Psi_3\rangle$ is eigenfunction with eigenvalue $E = 0$ and $|\Psi_4\rangle$ is eigenfunction with eigenvalue $E = U$. Consider now the subspace with $S_z = 1$. The only state is $|\Psi_5\rangle = c_{1\uparrow}^+ c_{2\uparrow}^+ |0\rangle$ and $H|\Psi_5\rangle = 0$. Analogously, for the subspace $S_z = -1$ with $|\Psi_6\rangle = c_{1\downarrow}^+ c_{2\downarrow}^+ |0\rangle$ we find $H|\Psi_6\rangle = 0$.

Let us now study the Hamiltonian (1). Consequently, we have a product space. We set $|n\rangle = (n!)^{-1/2}(b^+)^n|0\rangle$ with $b|0\rangle = 0$ and $\langle 0|0\rangle = 1$. For $S_z = 0$ the basis in the product space is now given as

$$S_1' = \{|\Psi_1\rangle|n\rangle, |\Psi_2\rangle|n\rangle, \quad n = 0, 1, 2, \ldots\} \tag{5a}$$

$$S_2' = \{|\Psi_3\rangle|n\rangle, \quad n = 0, 1, 2, \ldots\} \tag{5b}$$

$$S_3' = \{|\Psi_4\rangle|n\rangle, \quad n = 0, 1, 2, \ldots\}. \tag{5c}$$

The we obtain

$$\begin{aligned} H|\Psi_1\rangle|n\rangle &= 2t|\Psi_2\rangle|n\rangle + (U + n\omega)|\Psi_1\rangle|n\rangle \\ &\quad + 2k(n+1)^{1/2}|\Psi_2\rangle|n+1\rangle \\ &\quad + 2kn^{1/2}|\Psi_2\rangle|n-1\rangle \end{aligned} \tag{6b}$$

$$\begin{aligned} H|\Psi_2\rangle|n\rangle &= 2t|\Psi_1\rangle|n\rangle + n\omega|\Psi_2\rangle|n\rangle \\ &\quad + 2k(n+1)^{1/2}|\Psi_1\rangle|n+1\rangle \\ &\quad + 2kn^{1/2}|\Psi_1\rangle|n-1\rangle. \end{aligned} \tag{6b}$$

The order of the basis in the subspace S_1' is given by $|\Psi_1\rangle|0\rangle$, $|\Psi_2\rangle|0\rangle$, $|\Psi_1\rangle|1\rangle$, $|\Psi_2\rangle|1\rangle$, ... Consequently, for the subspace S_1' we find the infinite matrix representation

$$\begin{pmatrix} U & 2t & 0 & 2k & 0 & 0 & \ldots \\ 2t & 0 & 2k & 0 & 0 & 0 & \ldots \\ 0 & 2k & (U+\omega) & 2t & 0 & 2\sqrt{2k} & \ldots \\ 2k & 0 & 2t & \omega & 2\sqrt{2k} & 0 & \ldots \\ 0 & 0 & 0 & 2\sqrt{2k} & U+2\omega & 2t & \ldots \\ 0 & 0 & 2\sqrt{2k} & 0 & 2t & 2\omega & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix} \tag{7}$$

In the subspace S_2' we have the energy levels $n\omega$ ($n = 0, 1, 2, \ldots$) and in the subspace S_3' we find $U + n\omega$ ($n = 0, 1, 2, \ldots$). In both cases the eigenvalues do not depend on k. For the subspace with $S_z = 1$ we have the eigenstate $c_{1\uparrow}^+ c_{2\uparrow}^+ |0\rangle|n\rangle$ with eigenvalues $n\omega$. Analogously, for $S_z = -1$ we find the eigenvalue $n\omega$. Here, too, the eigenvalues do not depend on k.

Let us now discuss the spectrum. We have only to discuss the subspace S_1'. The spectrum is discrete and bounded from below. For $k = 0$ the eigenvalues are given by

$$\frac{E_{\pm n}}{t} = \frac{n\omega}{t} + \frac{U}{2t} \pm \left(4 + \frac{U^2}{4t^2}\right)^{1/2}. \tag{8}$$

For the infinite matrix (7) we have calculated numerically the eigenvalues. We have truncated the infinite matrix, where we have neglected the matrix elements for $n, m > 1200$. Then we have solved the eigenvalues of the 1200×1200 matrix. Due to the truncation it is obvious that the higher eigenvalues are not sufficiently accurate. In our consideration we take into account the first 100 eigenvalues. If k is not large compared to U, t, and ω we can expect that these eigenvalues are sufficiently accurate. For fixed values of U, t, and ω we have calculated the eigenvalues in dependence on k. In Fig. 1 we have plotted the eigenvalues as a function of k for $U = 5$, $t = 1$, and $\omega = 0.5$. Figure 2 shows the eigenvalues as a function of k for $U = 1$, $t = 1$, and $\omega = 0.5$. In both figures we have included the eigenvalues from the other subspaces. Let us first discuss the case $U = 5$, $t = 1$, $\omega = 0.5$ and $0 \leqq k \leqq 0.5$. As expected the eigenvalues decrease with increasing k. In the subspace S_1' the eigenvalues are not degenerate. The second excited state of the subspace S_1' crosses the eigenvalue 0 (eigenvalue 0 is threefold). "Quantum chaos" is indicated if in the subspace under consideration

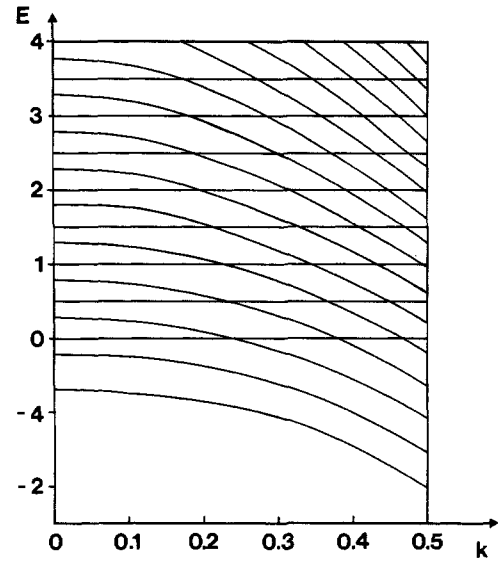

Fig. 1. Energy eigenvalues as a function of k for $U = 5$, $t = 1$, $\omega = 0.5$.

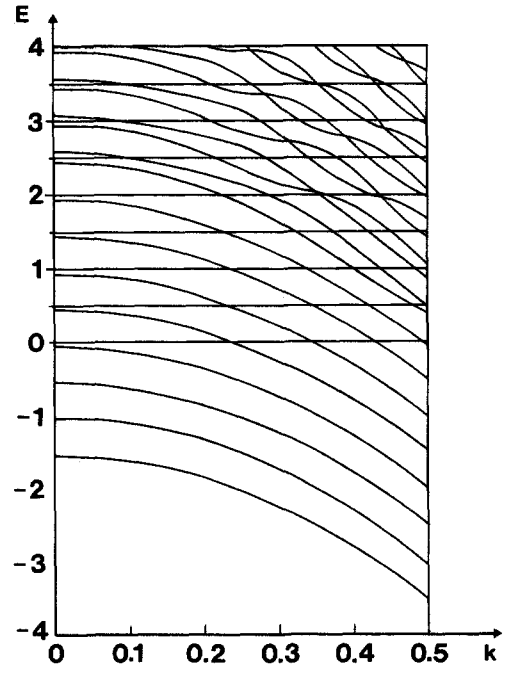

Fig. 2. Energy eigenvalues as a function of k for $U = 1$, $t = 1$, $\omega = 0.5$.

there is a repulsion of adjacent levels. In the present case it makes only sense to study this question in the subspace S_1'. Our numerical results show that there is no repulsion with increasing k. However, for the first 20 energy levels in the subspace S_1' we have no crossing for the range $0 \leqq k \leqq 0.5$. For the case $U = 1$, $t = 1$ and $\omega = 0.5$, and $0 \leqq k \leqq 0.5$ the eigenvalues in the subspace S_1' again decrease with increasing k. The eigenvalues in the subspace S_1' are not degenerate. However, we find crossings for the higher energy levels. In this sense the system (subspace S_1') does not show "quantum chaos". The lowest eigenvalue is in the subspace S_1'. The lowest eigenvalue which does not belong to S_1' is again 0 (three times degenerate). For $k = 0$ three eigenvalues of the subspace S_1' are below $E = 0$. When we decrease U and ω more and more eigenvalues of the subspace S_1' are below $E = 0$.

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