The non-adiabatic nonlinear quantum dimer in the absence of dissipation: exact solutions

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Abstract

We examine the time evolution of the nonlinear propagation of a particle or excitation in strong interaction with vibrations. We carry out calculations for the density matrix elements of the quantum nonlinear dimer without imposing the adiabatic limit. In contrast to earlier analyses which have treated the problem in the limit of extremely large or moderately large dissipation, i.e., respectively, the cases of infinite damping and severe overdamping, we investigate the case of no dissipation. Exact solutions are obtained for a restricted range of parameters. We exhibit the existence of the transition between a localized and delocalized state of the dimer, known from the adiabatic case. Similar behavior is observed in (numerically obtained) solutions valid outside the parameter range where analytical solutions can be obtained. The study is of direct interest in the context of any two-state quantum mechanical system interacting with a boson field, such as photons (light) or phonons (vibrations of a solid) whenever the boson field can be treated classically.

1. Introduction

The quantum nonlinear dimer is a two-state system interacting with a boson field whose original linear quantum evolution is rendered nonlinear by the elimination of the field variables. The system has seen intense study in the last few years in condensed matter physics. One of the reasons for the interest is that the dimer can be regarded as a special case of an extended quantum nonlinear system which, unlike the general counterpart, can be analyzed more easily, even exact analytic solutions being made possible in several cases. The general extended nonlinear system, characterized, for instance, by the so-called discrete nonlinear Schrödinger equation,

\[ i\hbar \frac{dc_m}{dt} = \sum_n V_{mn} c_n - \chi |c_m|^2 c_m, \]

where \( c_m(t) \) is the amplitude for the quantum particle to be at site \( m \) (which can be generally a vector), \( V_{mn} \) is the intersite matrix element for particle transfer from site \( n \) to site \( m \), and \( \chi \) is the nonlinearity parameter, is of relevance to fundamental questions concerning the propagation of solitons and the dynamics of polarons. The dimer counterpart of (1) is

\[ i\hbar \frac{dc_1}{dt} = Vc_2 - \chi |c_1|^2 c_1, \]

\[ i\hbar \frac{dc_2}{dt} = Vc_1 - \chi |c_2|^2 c_2. \]
These equations can be solved exactly in terms of Jacobian elliptic functions and their solution can be used to elucidate various features of polaron localization and related phenomena. Among examples of such elucidation are those to do with symmetry breaking in stationary states [1], dynamic evolution [2], application to experiments on neutron scattering and fluorescence depolarization [2,3], fluctuation effects [4], bifurcations [5], and nonlinear muon spin relaxation and rotational polarons [6].

The above-mentioned studies were relevant to systems known by the term adiabatic and characterized by time scales of the quantum particle and of the eliminated boson field (lattice vibrations) being disparate. The nonadiabatic case, in which this disparate-time-scale assumption cannot be made, were analyzed by Kenkre and Wu [7] in the presence of dissipation. The nonadiabatic case in the absence of dissipation was mentioned only briefly and not treated at length because it was felt that it was less realistic than the dissipative counterpart. Our recent studies have shown, however, that exact solutions can be found for this case. A discussion of these solutions constitutes the present paper.

In Section 2, we present the model and the equations of motion for the nonlinear nonadiabatic non-dissipative quantum dimer. In Section 3 we show the method of solution and display the exact solutions. We also compare the exact solutions to their adiabatic counterparts and numerically obtained nonadiabatic counterparts in the regions where we were not able to find exact solutions. Section 4 contains comments.

2. Equations of motion and analytic solutions

Eqs. (2) and (3) are the adiabatic limit of coupled equations for the quantum dimer and the classical vibrational field whose general form is

$$i\hbar \frac{d c_m}{dt} = \sum_n V_{mn} c_n + G x_m c_m,$$

$$\frac{d^2 x_m}{dt^2} + \alpha \frac{dx_m}{dt} + \omega_0^2 x_m = -\chi \frac{\omega_0^2}{G} |c_m|^2.$$
The nonlinear system of Eqs. (14)–(17) has two integrals of motion:

\[ I_1 = p^2 + q^2 + r^2 = 1, \]  
and

\[ I_2 = \frac{1}{\chi} r - py + \frac{1}{2} y^2 + \frac{1}{2\omega} y^2, \]  
the first of which is the total probability of excitation and the second one reflects conservation of energy in the whole system.

3. Exact solutions of the equations of motion

It is not possible to find the exact solution of the system (14)–(17) for arbitrary initial conditions. In fact it was shown that the equivalent system can exhibit chaos for some values of parameters and initial conditions [8,9], which precludes finding exact analytic solutions. Nevertheless, some useful, exact solutions valid for restricted values of the parameters can be obtained through the application of techniques used in a related context in quantum optics [10,11].

Our interest here is in finding some exact solutions of the system (14)–(17). The adiabatic limit [2] assumes that \( y(t) = \gamma^2 (t - 1/\Gamma) \). Here we shall assume that \( p \) and \( y \), while not identical to each other, are interrelated through a simple functional relationship: \( p = f(y) \). If we take this function to be a simple power form, and realize that (17) requires that \( f(y) = -f(-y) \) we can write

\[ p = \sum_k \alpha_k y^{2k+1}, \]  
where \( \alpha_k \) are coefficients to be determined from (14)–(17). Nontrivial solutions can be obtained when we allow only the first two terms of (24):

\[ p = \alpha_0 y + \alpha_1 y^3. \]  

Now, from Eq. (15), we have

\[ q = \dot{p} = (\alpha_0 + 3\alpha_1 y^2) \dot{y}, \]  
and consequently

\[ \dot{q} = \dot{y}(\alpha_0 + 3\alpha_1 y^2) + 6\alpha_1 y^2y, \]  
or after using Eq. (17) to express \( \dot{y} \) in terms of \( y \) and \( p \)

\[ \dot{q} = y[6\alpha_1 y^2 + \omega^2(\alpha_0 - 1)\alpha_0 + \omega^2(4\alpha_0\alpha_1 - 3\alpha_1)y^2 + 3\omega^2\alpha_1^2 y^4]. \]  

Substitution of (26) to (16) enables us, after a straightforward integration, to express \( r \) in the form

\[ r = \gamma + \frac{1}{2} \chi \alpha_1 y^2 + \frac{3}{4} \chi \alpha_2 y^4, \]  
where \( \gamma \) is an integration constant.

Now we can compare right hand sides of (15) and (28) to obtain a single equation for the function \( y(t) \)

\[ y^2 = F_0 + F_2 y^2 + F_4 y^4, \]  
where

\[ F_0 = \frac{1}{6\alpha_1} [\omega^2(1 - \alpha_0)\alpha_0 - \chi \gamma], \]  
\[ F_2 = \omega^2 \left( \frac{1}{3} - \frac{3}{2} \alpha_0 \right) - \frac{1}{6} - \frac{\alpha_0}{12\alpha_1} \chi^2, \]  
\[ F_4 = -\frac{1}{2} \omega^2 \alpha_1 - \frac{1}{8} \chi^2. \]  

General solution of (30) can be written in terms of elliptic functions. When the requirements that \( p, q, r, \) and \( y \) and must be real and that (22) must be satisfied are imposed, one finds that (30) is obeyed by

\[ y = y_0 cn(\Omega t | k), \quad y_0 = \frac{4\Omega k^{1/2}}{\chi}, \]  
\[ \Omega^2 = \frac{\omega^2 - \frac{1}{3}}{2(2k - 1)}, \]  
where the modulus \( k \) of the elliptic function \( cn(\Omega t | k) \) depends on the parameters \( \omega \) and \( \chi \) of the system. The conditions that the modulus \( k \) and the frequency \( \Omega \) of the elliptic function \( cn \) are real and positive in Eq. (34) impose restrictions on the parameters for which the solution (34) exists. The ranges of parameters \( \chi \) and \( \omega \) in which the solution (34) is valid, together with the corresponding values of the modulus \( k \) are given by the following expressions:
\[ \omega^2 \leq \frac{1}{9}, \quad \chi^2 \geq \frac{9}{16\omega^4} \left( \omega^2 - \frac{1}{9} \right)^2 \left( \omega^2 + \frac{1}{2} \right)^2, \]

\[ k = \frac{1}{2} - \frac{1}{2\sqrt{1 + B_+}}, \quad (35) \]

\[ \frac{1}{9} < \omega^2 < \frac{1}{3}, \quad 4 \left( \frac{\omega^2 - \frac{1}{9}}{\omega^4} \right)^3 \leq \chi^2 < 4\omega^2 - \frac{1}{3}, \]

\[ k = \frac{1}{2} - \frac{1}{2\sqrt{1 + B_-}}, \quad (36) \]

\[ \frac{1}{3} \leq \omega^2 \leq \frac{17}{9}, \quad 4 \left( \frac{\omega^2 - \frac{1}{9}}{\omega^4} \right)^3 \leq \chi^2 < 4\omega^2 - \frac{1}{3}, \]

\[ k = \frac{1}{2} + \frac{1}{2\sqrt{1 + B_-}}, \quad (37) \]

\[ \frac{17}{9} < \omega^2, \quad 4 \left( \frac{\omega^2 - \frac{1}{9}}{\omega^4} \right)^3 \leq \chi^2, \]

\[ k = \frac{1}{2} + \frac{1}{2\sqrt{1 + B_+}}, \quad (38) \]

where

\[ B_\pm = \left( \omega^2 - \frac{1}{3} \right)^2 \left[ \pm \frac{4}{3} \sqrt{\chi^2 \omega^4 - 4 \left( \omega^2 - \frac{1}{9} \right)^3} \right. \]

\[ - \left. \left( \omega^2 - \frac{1}{9} \right) \left( \omega^2 - \frac{17}{9} \right) \right]. \quad (39) \]

Regions of the parameter space in which the exact solutions can be found are presented in Figs. 1 and 2.

We used standard notation for the elliptic function also in the case when \( k > 1 \). Surely, in this case, one could perform the reciprocal modulus transformation and write the solution in terms of the function \( \text{dn} \) via the relation [12]

\[ \text{cn}(\Omega \tau|k) = \text{dn}(\Omega k^{1/2}\tau | k^{-1}). \quad (40) \]

According to Eqs. (25), (26) and (29) we can express the remaining variables \( p, q \) and \( r \) as

\[ p = a \text{cn}(\Omega \tau|k) + b \text{cn}^3(\Omega \tau|k), \quad (41) \]

\[ q = -\Omega \text{sn}(\Omega \tau|k) \text{dn}(\Omega \tau|k) \left[ a + 3b \text{cn}^3(\Omega \tau|k) \right], \quad (42) \]

\[ r = c_0 + c_1 \text{cn}^2(\Omega \tau|k) + c_2 \text{cn}^4(\Omega \tau|k), \quad (43) \]

The dependence of the coefficients \( a, b, c_0, c_1, \) and \( c_2 \) can be determined by substituting (41)–(43) to the original Eqs. (14)–(17) which results in

\[ a = \frac{6}{\chi \omega^2} \Omega k^{1/2}, \quad (44) \]

\[ b = -8 \frac{\Omega^3 k^{3/2}}{\chi \omega^2}, \quad (45) \]

\[ c_0 = \frac{1}{\chi \omega^2} \left[ \pm \sqrt{\chi^2 \omega^4 - 4 \left( \omega^2 - \frac{1}{9} \right)^3} - \frac{3}{2} \left( \omega^2 - \frac{1}{9} \right)^2 \right], \quad (46) \]

\[ c_1 = \frac{12}{\chi \omega^2} \left( \omega^2 - \frac{1}{9} \right) \Omega^2 k, \quad (47) \]

\[ c_2 = -\frac{24}{\chi \omega^2} \Omega^4 k^2, \quad (48) \]

where the sign in Eq. (46) corresponds to that in Eq. (39).

Figs. 3–5 show typical time evolution of the occupation probability difference between the two states.
Fig. 3. Time evolution of the occupation probability difference \( p(t) \) for two different exact solutions. The values of the parameters are given in the figures.

\( p(t) \) in various regions of the parameter space.

Eqs. (41)–(43) and (44)–(48) do not, obviously, give the general solution of the system (14)–(17). Indeed, from (34) and (41)–(43) we deduce that the above solutions fulfill the initial conditions

\[
\begin{align*}
p(0) &= a + b, \\
q(0) &= 0, \\
r(0) &= c_0 + c_1 + c_2, \\
y(0) &= y_0, \\
y(0) &= 0,
\end{align*}
\]

which certainly are not the most general ones. Nevertheless, by changing parameters we can observe several different typical patterns of the evolution of the system. An interesting property of the system is its possibility of exhibiting the so-called self-trapping transition when the relevant parameters are varied. The probability difference between two states of the dimer \( p(t) \) evolves periodically in time with the period:

Fig. 4. Same as in Fig. 3.

Fig. 5. Same as in Fig. 3.
\[ 4K(k) = 4 \int_{0}^{\pi/2} \frac{d\theta}{\sqrt{1 - k \sin^2 \theta}}. \quad (54) \]

If \( k < 1 \) the time average of the probability difference is equal to zero and we say that the dimer is in delocalized ("free") state. For \( k > 1 \) the solution takes the form of a dn function and oscillates around its nonzero mean value

\[ p_{av} = \frac{\pi}{2K} \left[ a + b \left( 1 - \frac{k^2}{2} \right) \right] \quad (55) \]

- the dimer is in the localized ("trapped") state. Such a transition occurs whenever \( 1/3 < \omega^2 < 17/9 \) and

\[ \chi^2 = \frac{9}{16\omega^2} \left( \omega^2 - \frac{4}{3} \right)^2 \left( \omega^2 + \frac{5}{3} \right)^2, \quad (56) \]

i.e.

\[ \omega^2 = \frac{1}{3} \left( 2\chi - \frac{4}{3} \right) + \frac{2}{3} \sqrt{\left( 2\chi - \frac{4}{3} \right)^2 + \frac{5}{3}}. \quad (57) \]

The border between the regions of the parameter states where the considered exact solutions exhibit localized and delocalized state is marked by the dashed line in Figs. 1 and 2.

The time evolution for \( \omega = 1.0 \) and three different values of the parameter \( \chi \) in the close vicinity of the critical value calculated from the Eq. (56) are shown in Fig. 6, exhibiting clearly the transition from the delocalized to the localized state when the nonlinearity of the system measured by the parameter \( \chi \) increases.

Although it may seem that the above described transition is specific to particular values of parameters and initial conditions allowing the exact analytic solutions, it is worth stressing that a strictly similar transition was observed in the adiabatic nonlinear quantum dimer model [2]. As it was pointed out in the literature [3,6], such a transition has consequences which can be experimentally exhibited in the measurements of the neutron scattering spectra or fluorescence depolarization. From this point of view it is interesting to find whether the transition can be observed in the non-adiabatic dimer also for the more general initial conditions. To this end we investigated numerically the system (14)-(17). As it was already mentioned, the system can exhibit chaotic behavior. As a consequence, typical trajectories cannot be classified as describing clearly localized or delocalized state. Nevertheless, it is relatively easy to find initial conditions for which the system exhibits the tendency to stay in a well localized state characterized by a nonvanishing mean value of \( p \) for a relatively long time. Typical case is shown in Fig. 7. The trajectories in Fig. 7 do not fulfill above described conditions giving exact solutions in terms of elliptic functions. In both cases however, the oscillations, although not so regular as previously, lead to different mean values of \( p \). For \( \chi^2 = 1 \) and \( \omega^2 = 5 \) the dimer is in a delocalized state and the occupation probability \( p(t) \) oscillates around the zero mean. It is contrasted with the case \( \chi^2 = 10 \) and \( \omega^2 = 5 \). For these values of the parameters the evolution clearly prefers positive values of \( p(t) \) - the dimer is in a localized state. The above results indicated clearly that the self-trapping transition is not unique to the adiabatic model, but rather an universal phenomenon common to the considered dimer-like systems.

4. Conclusions

A fundamental problem of condensed matter physics concerns the description of the influence of strong interactions of the lattice on quasiparticles such as electrons or excitons moving in solids. Recent approaches to this problem have been based on discrete...
nonlinear quantum evolution equations. In this paper we present new results regarding the coupled evolution of such quasiparticles and of the lattice oscillators with which they interact, obtained without making the usual “adiabatic” approximation. The essential feature of the systems of interest to the present investigation is a strong interaction between a quasiparticle which moves on a lattice in keeping with a quantum evolution equation, and oscillators whose displacements modulate the quasiparticle parameters such as the site energy. Several different sets of coupled equations for the moving quasiparticle and the lattice vibrations have been arrived at from microscopic analysis or postulated. We focus here on the prototypical set used by Scott [1,13] and his collaborators. Of their two coupled equations, one for the moving quasiparticle and the other for the (optical) vibration which interacts with the quasiparticle. Our consideration concerned the case when the adiabatic elimination of the lattice vibration could not be justified.

We presented the exact analytic solutions of the equations of motion of the non-linear, non-adiabatic dimer in the absence of dissipation. The obtained solutions are valid only in some regions of the parameter space of the system, parameters being the (normalized) frequency of the lattice vibrations and the nonlinear coupling coefficients between the vibrations and quasiparticle motion. Despite the limited regions of validity, the obtained solutions are of considerable interest. First, from purely formal point of view, it is interesting to have specific analytic solutions corresponding to the special initial conditions of the system which for other initial conditions behaves chaotically. More important is our observation that the transition between localized and delocalized state, known from the adiabatic case is present also in the non-adiabatic system.

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References

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