

# Analytical evaluation of the time evolution of a non-adiabatic non-linear quantum dimer under the averaging approximation

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**Abstract.** While the evolution of the non-linear quantum dimer can be solved exactly in the adiabatic limit, only numerical methods and general analytical arguments have been used in the non-adiabatic case. We present approximate analytical expressions for the dependence of the complete density matrix of the system through an application of an averaging method. The method consists of selecting a constant of the motion for the adiabatic case, studying its time evolution, and using the results to obtain the evolution of the entire system.

## 1. Introduction

In two recent papers, Kenkre and Wu [1] proposed the following equations for studying the evolution of quasiparticles such as electrons or excitons in a two-site system (dimer) with strong interaction with vibrations:

$$i dc_1/dt = Vc_2 + Ex_1c_1 \quad (1.1)$$

$$i dx_2/dt = Vc_1 + Ex_2c_2 \quad (1.2)$$

$$dx_1/dt + \Gamma x_1 = -(\chi\Gamma/E)|c_1|^2 \quad (1.3)$$

$$dx_2/dt + \Gamma x_2 = -(\chi\Gamma/E)|c_2|^2. \quad (1.4)$$

In (1.1)–(1.4),  $c_1$  and  $c_2$  are the probability amplitudes for the quasiparticle to be on the two sites 1 and 2,  $V$  is the intersite transfer matrix element of the quasiparticle,  $x_1$  and  $x_2$  are the displacements of the two Einstein oscillators with whose vibrations the quasiparticle interacts,  $\Gamma$  is the vibrational relaxation rate, and the coupling strength between the quasiparticle and the vibrations is specified by  $E$  and  $\chi$ . As has been mentioned in [1], (1.1)–(1.4) are similar to the equations introduced by Scott [2] and collaborators in the context of energy transport in  $\alpha$ -helix proteins, but differ in that, in (1.1)–(1.4), the oscillators have no dispersion, possess damping and incorporate a single relaxation rate  $\Gamma$ . In the adiabatic limit, which corresponds to the vibrational relaxation rate being infinite ( $\Gamma \rightarrow \infty$ ), (1.1)–(1.4) yield the discrete non-linear Schrödinger equation for a dimer which has been studied extensively by Kenkre and collaborators

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[3–6]. Those studies dealt with exact solutions [3] and various applications to experiments [4–6]. Equations (1.1)–(1.4) have also been adopted by the present authors [7] as the starting point for the study of the effect of temperature on self-trapping. In that study, (1.1)–(1.4) have been supplemented by Gaussian white noise terms to represent temperature effects. The main result of [7] is that, although no abrupt transition exists as a function of temperature, a characteristic temperature does exist, above which the localised state is practically destroyed, the temperature dependence of the destruction process being Arrhenius in character.

As in our earlier work [1], we define the following quantities:

$$p = \rho_{11} - \rho_{22} \quad q = i(\rho_{12} - \rho_{21}) \quad r = \rho_{12} + \rho_{21} \quad (1.5)$$

where  $\rho_{11}$ ,  $\rho_{22}$ ,  $\rho_{12}$  and  $\rho_{21}$  are the density matrix elements (e.g.  $\rho_{12} = c_1^* c_2$ ) of the quasiparticle. We further define [1]

$$y = -(E/\chi)(x_1 - x_2). \quad (1.6)$$

to be the difference of the oscillator displacements. Henceforth in this paper we express  $\chi$ ,  $\Gamma$  and  $1/t$  in units of  $2V$ . Then (1.1)–(1.4) can be rewritten as

$$d\rho/dt = q \quad (1.7)$$

$$dq/dt = -p - \chi r y \quad (1.8)$$

$$dr/dt = \chi q y \quad (1.9)$$

$$dy/dt = -\Gamma(y - p). \quad (1.10)$$

In [1], it has been hoped that analytic solutions of (1.7)–(1.10) would be available. The following is an attempt in that direction. We intend to solve (1.7)–(1.10) for fast but finite vibrational relaxation rates for the following reason. Physically, it is the first-order correction of the adiabatic limit, and technically, it allows us to apply a perturbation scheme in orders of  $1/\Gamma$ . Notice that [1], for a time scale longer than  $1/\Gamma$ , (1.10) has the following approximate solution to order  $1/\Gamma$

$$y(t) \approx p(t - 1/\Gamma) \approx p(t) - (1/\Gamma)(dp(t)/dt). \quad (1.11)$$

We can then rewrite (1.7)–(1.9) as

$$dp/dt = q \quad (1.12)$$

$$dq/dt = -p - \chi r p + (1/\Gamma)\chi q r \quad (1.13)$$

$$dr/dt = \chi q p - (1/\Gamma)\chi q^2. \quad (1.14)$$

While the evolution of the non-linear quantum dimer can be solved exactly in the adiabatic limit ( $\Gamma \rightarrow \infty$ ), only numerical methods and general analytical arguments have been used in the non-adiabatic case. We present an application of the ‘averaging method’ [8, 9] by selecting a constant of motion for the adiabatic case, studying its time evolution, and using that slow variable to obtain approximate expressions for the dependence of the complete density matrix of the system. In section 2, we discuss the application in detail. We search for a ‘constant of motion’ in the adiabatic limit, and derive the evolution equation of that quantity for finite  $\Gamma$ . In section 3, we solve the equation and obtain the expression for the time dependence of the slow variable. We also derive an expression for the time dependence of the probability difference  $p$  in section 4. A summary is presented in section 5.

## 2. The averaging method

Equations (1.12)–(1.14) constitute the starting point of our analysis. Since  $1/\Gamma$  is a small quantity, our strategy is based on a perturbation theory in orders of  $1/\Gamma$ . The method we apply is the so-called averaging method.

The first step of the averaging method is to search for a slow variable which is a constant of the motion in the limit that the small quantity vanishes. The small quantity in the present context is  $1/\Gamma$  in units of  $\chi$  or  $V$ . It is trivial to verify that

$$p^2 + q^2 + r^2 = 1 \tag{2.1}$$

is a constant of motion. However, this quantity is useless for our purpose because it is a constant of the motion for all values of the vibrational relaxation rate  $\Gamma$ . This corresponds to the conservation of the magnitude of a ‘spin’ rotating in three-dimensional space [10, 11]. Another quantity which is a constant of motion only in the adiabatic limit can be found in the following way. In the adiabatic limit, the last term of (1.14) vanishes and (1.14) can be written as

$$q = (1/\chi p)(dr/dt). \tag{2.2}$$

On substituting (2.2) into (1.12), we get

$$(\chi/2)(dp^2/dt) = dr/dt \tag{2.3}$$

and one sees immediately that the sum of  $r - (\chi/2)p^2$  and an arbitrary time-independent term is a constant of the motion in the adiabatic limit. We choose the additive term to be  $\chi/2 + 1/2\chi$  and call [7] the constant of the motion  $E$ :

$$E = r - (\chi/2)p^2 + \chi/2 + 1/2\chi. \tag{2.4}$$

The particular choice of the additive term makes  $E$  vanish in the non-trivial stationary state (i.e. when  $p \neq 0$ ) in which  $r$  equals  $-1/\chi$  and  $p = \pm(1 - 1/\chi^2)^{1/2}$ .

The quantity  $E$  evolves in time when the adiabatic limit does not apply, i.e. when  $1/\Gamma \neq 0$ . Combining (1.12)–(1.14) and (2.4), we find that the evolution is given by

$$dE/dt = -(1/\Gamma)\chi q^2. \tag{2.5}$$

It is clear from (2.5) that, if  $\chi/\Gamma$  is small, the rate of change of  $E$  is small, and that  $E$  is a slow variable relative to  $p$ ,  $q$ , and  $r$ . The fact that  $p$ ,  $q$ , and  $r$  are oscillating functions suggests that we carry out an average of (2.5) over one period of oscillation [3]. If we replace  $\langle E \rangle$ , the average of  $E$ , by  $E$  itself, assuming that  $E$  is a constant during a period, (2.5) gives

$$dE/dt = -(1/\Gamma)\chi \langle q^2 \rangle. \tag{2.6}$$

Among the variables  $p$ ,  $q$ , and  $r$ , we may use (2.1) and (2.2) to express  $q^2$  in terms of  $E$  and one other variable. We choose that variable to be  $p$ . With this choice,

$$q^2 = -(\chi/2)^2 p^4 - [\chi(E - 1/2\chi - \chi/2) + 1]p^2 + [1 - (E - 1/2\chi - \chi/2)^2] \tag{2.7}$$

and the average of  $q^2$  reads

$$\begin{aligned} \langle q^2 \rangle = \int q^2 dp / \int dp = & -\frac{1}{3}(\chi/2)^2(p_+^4 + p_+^3 p_- + p_+^2 p_-^2 + p_+ p_-^3 + p_-^4) \\ & -\frac{1}{3}[\chi(E - 1/2\chi - \chi/2) + 1](p_+^2 + p_+ p_- + p_-^2) \\ & + [1 - (E - 1/2\chi - \chi/2)^2] \end{aligned} \tag{2.8}$$

where  $p_{\pm}$  are the turning points of one oscillation. It can be shown [7] that, in the trapped regime

$$p_{\pm} = [1 - 1/\chi^2 - 2E/\chi \pm (2/\chi)(2E/\chi)^{1/2}]^{1/2} \quad (2.9)$$

or

$$p_{\pm} = -[1 - 1/\chi^2 - 2E/\chi \pm (2/\chi)(2E/\chi)^{1/2}]^{1/2} \quad (2.10)$$

depending on at which of the two sites the quasiparticle is trapped. We carry out a similar procedure for the 'free' regime and obtain

$$p_{\pm} = \pm[1 - 1/\chi^2 - 2E/\chi + (2/\chi)(2E/\chi)^{1/2}]^{1/2}. \quad (2.11)$$

The turning points in the 'free' regime are symmetric about  $p = 0$ .

### 3. Approximate solutions for the slow variable $E$

The evolution of the slow variable  $E$  is given by (2.6) with  $\langle q^2 \rangle$  given by (2.8)–(2.11). However, exact analytical solutions of (2.6) are difficult to obtain since  $\langle q^2 \rangle$  in (2.8) is a complicated function of  $E$ . A natural procedure that enables us to proceed approximately, but analytically, is a polynomial expansion of  $\langle q^2 \rangle$  about  $E$ . Inspection of figure 1, in which we plot  $\langle q^2 \rangle$  numerically as a function of  $E$  (full curves), shows that  $\langle q^2 \rangle$  may be approximated by a linear function of  $E$  for the trapped regime and a quadratic one in the 'free' regime, provided that  $\chi$  is not negligibly small. It can be shown [7] that, in the trapped regime,  $\langle q^2 \rangle$  can be approximated by

$$\langle q^2 \rangle \simeq (4/3\chi)E \quad (3.1)$$

where  $4/3\chi$  is the linear coefficient in an expansion of  $\langle q^2 \rangle$  in powers of  $E$  near the non-trivial stationary states, i.e. near  $E = 0$ . In the 'free' regime, we expand  $\langle q^2 \rangle$  as a quadratic expression for  $E$  around  $E_0$ , the highest possible value of  $E$ , i.e. the one obtained by setting  $p = 1$  and  $r = 0$  in (2.4)

$$E_0 = 1/2\chi. \quad (3.2)$$

That expansion, namely,

$$\langle q^2 \rangle = A + B(E - E_0) + C(E - E_0)^2 \quad (3.3)$$

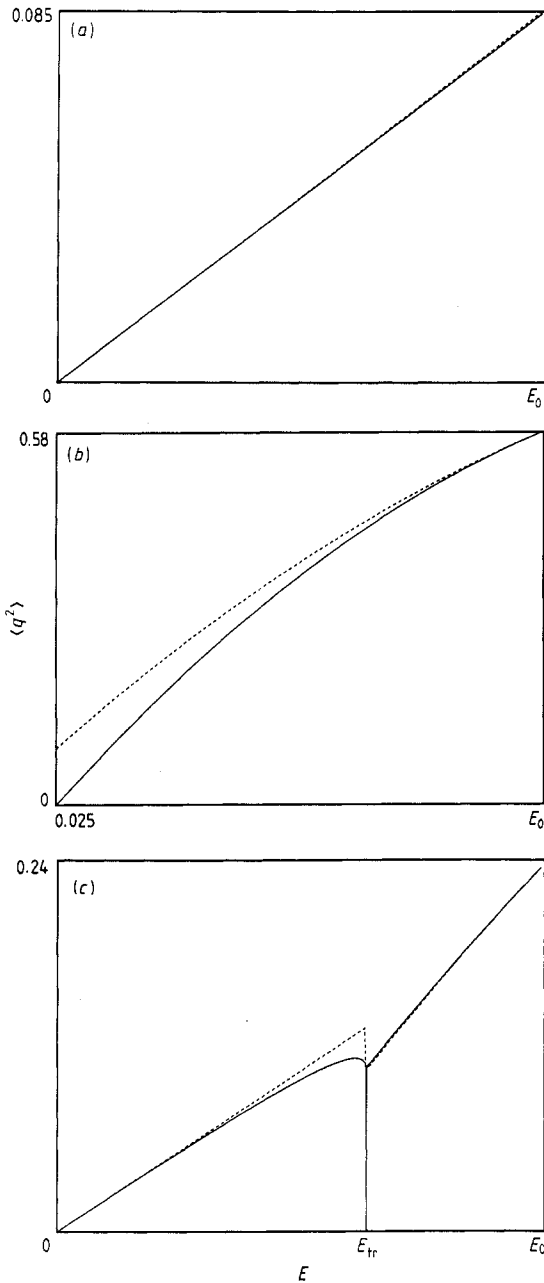
has the coefficients  $A$ ,  $B$  and  $C$  given by

$$A = \frac{2}{3}(1 - \chi^2/5) \quad (3.4)$$

$$B = \frac{2}{3}\chi \quad (3.5)$$

$$C = \frac{1}{3}(1 + 7\chi^2/10). \quad (3.6)$$

In figure 1 we present  $\langle q^2 \rangle$  in this combined linear and quadratic approximation (broken curves) compared with the exact numerical results from (2.8) (full curves). We see that this approximation is remarkably good for high non-linearities ( $\chi > 2$ ), i.e. the trapping regime (figure 1(a)). The deviation of the approximate result from the exact one is apparent for small non-linearities ( $\chi < 1$ ), i.e. the free regime (figure 1(b)). For  $2 > \chi > 1$  (figure 1(c)), the agreement is fairly good except near the transition. That  $\langle q^2 \rangle$



**Figure 1.** The quantity  $\langle q^2 \rangle$  plotted as a function of the slow variable  $E$ . The full curves are the exact numerical results from (2.8), which lead to the approximation by a linear fit in the trapped regime and a quadratic fit in the free regime. These fits are plotted as broken curves. Values of the non-linearities are: (a)  $\chi = 2.8$ , (b)  $\chi = 0.8$  and (c)  $\chi = 1.8$ . In (c),  $\langle q^2 \rangle = 0$  at the transition between the trapped and free regimes.

drops to 0 sharply at the transition is because of the fact that the transition point represents an unstable stationary state. The value of  $E$  at this transition point, namely  $E_{tr}$  is found from (2.5) with  $p = 0$  and  $r = -1$ ,

$$E_{tr} = 1/2\chi + \chi/2 - 1. \tag{3.7}$$

The approximate solution of (2.6) with the linear fit (3.1) or the quadratic fit (3.2) is

straightforward. There are three cases depending on the initial values of  $E$  and the non-linearities. The first is for  $\chi < 1$ . In this case, only ‘free’ motion is allowed for all initial values of  $E$ . Using (3.2), we have

$$E(t) = B/(2C) + (D/2C) \tanh\{D\chi t/2\Gamma - 2 \ln[(D - B + 2CE_i)/(D + B - 2CE_i)]\} \tag{3.8}$$

where

$$D = (B^2 + 4AC)^{1/2}. \tag{3.9}$$

$A$ ,  $B$  and  $C$  are defined in (3.3)–(3.5), and  $E_i$  is the initial value of  $E$ . The second case is for  $\chi > 2$  or  $\chi > 1$  but  $E_i < E_{tr}$  where the quasiparticle is trapped at the beginning and, therefore, will always be trapped. In this case, (3.1) is the appropriate fit and the solution is

$$E(t) = E_i e^{-(4/3\Gamma)t}. \tag{3.10}$$

The third case is for  $1 < \chi < 2$  and  $E_i > E_{tr}$ . In this case, the quasiparticle undergoes a free-to-trapped transition when the value of  $E$  crosses  $E_{tr}$ . The solution then is (3.8) before the transition and (3.10) after the transition:

$$E(t) = 2C + (D/2C) \tanh\{D\chi t/2\Gamma - 2 \ln[(D - B + 2CE_i)/(D + B - 2CE_i)]\} \tag{3.11a}$$

for  $t < t_{tr}$

$$E(t) = E_{tr} \exp[(4/3\Gamma)(t - t_{tr})] \tag{3.11b}$$

for  $t > t_{tr}$ .

The quantity  $t_{tr}$  appearing in (3.11) is the time for the free-to-trapping transition to take place. One of the results of this paper is the following explicit expression for this trapping time:

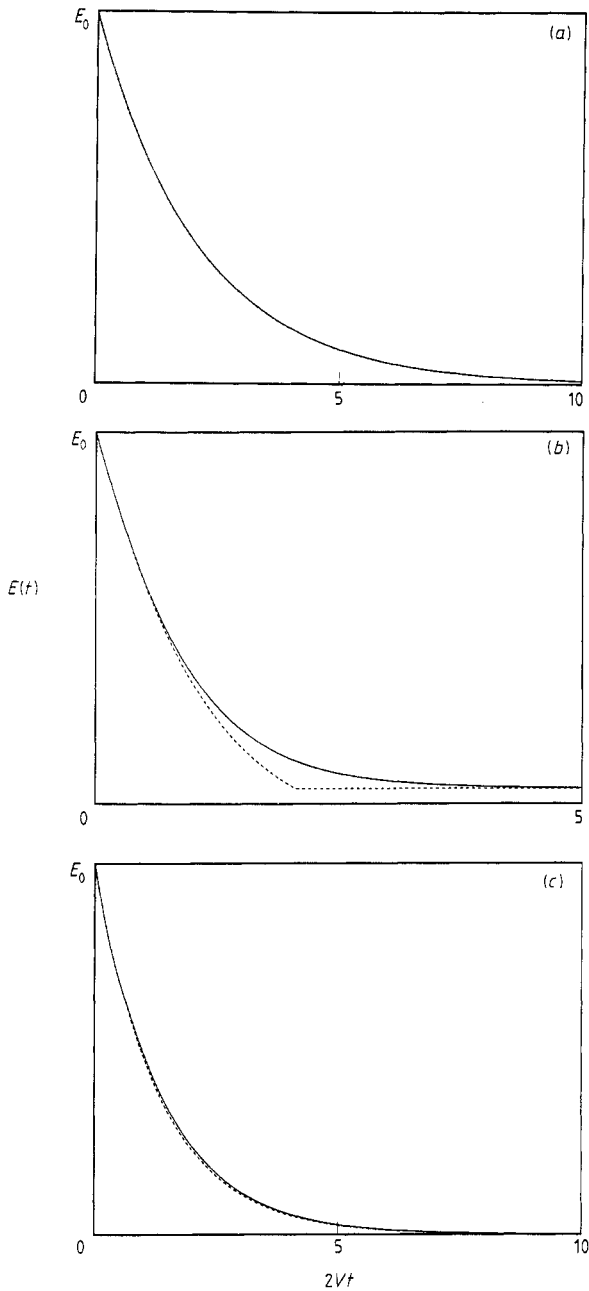
$$t_{tr} = (2\Gamma/\chi D) \{ \ln[(D - B + 2CE_i)/(D + B - 2CE_i)] + \ln[(D - B + 2CE_{tr})/(D + B - 2CE_{tr})] \} \tag{3.12}$$

The initial value of  $E$ , namely  $E_i$ , is obtained from (2.5) in terms of initial values of  $p$  and  $r$  respectively. In many physical experiments, the derivative of  $p$  at  $t = 0$  is 0; thus  $q_0 = 0$ . According to (2.1), we then have  $r_0 = \pm (1 - p_0^2)^{1/2}$ , and

$$E_i = \pm (1 - p_0)^{1/2} - (\chi/2)p_0^2 + 1/2\chi + \chi/2. \tag{3.13}$$

where the + and – signs on the right hand side correspond to the in-phase and out-of-phase motion, respectively [4].

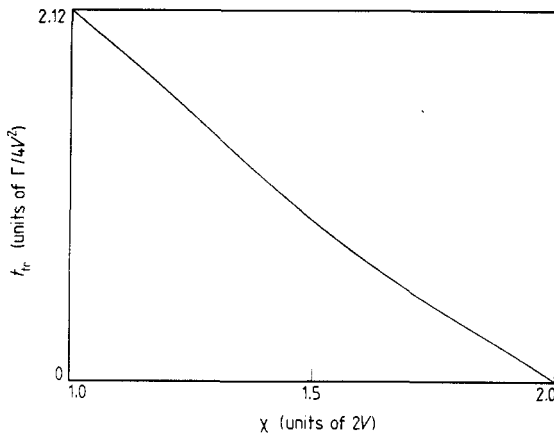
In figure 2, we present the time dependence of the approximate analytical solutions of the quantity  $E(t)$  for the same non-linearities as in figure 1 where the nonlinear parameters are, respectively: (a)  $\chi = 2.8$ , (b)  $\chi = 0.8$  and (c)  $\chi = 1.8$ , all in units of  $2V$ . The initial condition of the quasiparticle is taken to be localised, that is  $p_0 = 1$  and  $r_0 = 0$ . The extent to which the numerical results (full curves) and the analytical solutions agree in figure 2 is consistent with that in figure 1. In figure 3, we plot the quantity  $t_{tr}/\Gamma$  as a function of the non-linearity  $\chi$  for  $1 < \chi < 2$  for initial localised conditions. Note that the dependence of  $t_{tr}$  on  $\chi$  appears to be essentially linear. The meaning of the fact that the transition time  $t_{tr}$  vanishes at  $\chi = 2$  corresponds to the fact that for  $\chi \geq 2$ , the quasiparticle finds itself restricted to one side of the double-well potential for all times.



**Figure 2.** Comparison of the approximate (broken curves) but analytical time evolution of the slow variable  $E$  with 'exact' (full curves) numerical solutions. The parameters are the same as in figure 1. Time is in the units of  $1/2V$ .

#### 4. Time evolution of the probability difference

There are two time scales in the averaging method applied above: the slow time scale of  $E$  and the fast time scale of  $p$ ,  $q$  and  $r$ . When, as in section 3 above, one averages over the fast quantities in order to obtain a closed equation for  $E$ , one loses information about fast quantities. However, in most cases, the latter are directly related to experimental



**Figure 3.** Transition time (in units of  $\Gamma/(2V)^2$ ) for the free-to-trapping transition to take place given by (3.12) plotted as a function of the non-linearity  $\chi$  (in units of  $2V$ ) showing a quasi-linear dependence.

observables. For instance, in the present example, the Fourier transform of the time evolution of the probability difference  $p$  is essentially the scattering spectrum of interest in neutron scattering experiments [4(a)], while the quantity  $r$  determines fluorescence depolarisation [4(b)]. In this section, we obtain an approximate solution for such fast quantities, specifically for the probability difference  $p$ . For the sake of simplicity, we restrict our analysis to localised initial conditions.

We square (1.12) and combine with (2.7) to obtain

$$(dp/dt)^2 = -(\chi/2)^2 p^4 - \chi(E(t) + 1/2\chi - \chi/2)p^2 + [1 - (E(t) - 1/2\chi - \chi/2)^2]. \quad (4.1)$$

Equation (4.1) can also be written as

$$(dp/dt)^2 = (\chi/2)(p_{1+}^2 - p^2)(p^2 + p_{1-}^2) \quad (4.2)$$

for  $E > E_{tr}$ , where  $p_{1\pm}$  are the roots of the right-hand side of (4.1) and are given by

$$p_{1\pm}^2(t) = \pm (1 - 1/\chi^2 - 2E(t)/\chi) + (2/\chi)(2E(t)/\chi)^{1/2}. \quad (4.3)$$

For  $E < E_{tr}$ , we rewrite (4.1) as

$$(dp/dt)^2 = (\chi/2)(p_{2+}^2 - p^2)(p^2 - p_{2-}^2) \quad (4.4)$$

$$p_{2\pm}^2(t) = (1 - 1/\chi^2 - 2E(t)/\chi) \pm (2/\chi)(2E(t)/\chi)^{1/2}. \quad (4.5)$$

In the adiabatic limit,  $E$  is independent of time, (4.1) is integrable, and  $p$  can be expressed exactly in terms of Jacobi elliptical functions [3]. Although in the present case  $E$  does depend on time, it is a slow quantity compared with  $p$ ,  $q$  and  $r$ . We may therefore integrate (4.2) or (4.4), taking  $E$  as a constant during the integration, and obtain the following solutions of elliptical functions expressed as an expansion of Fourier series. For  $E > E_{tr}$ , the solution is a cn elliptical function [12]

$$p(t) = p_{1+} (2\pi/k_1 K(k_1)) \sum_n \frac{q_1^{n+1/2}}{(1+q_1^{2n+1})} \cos[(2n+1)(\chi\Omega_1 t/2 + \Phi_1(t))] \quad (4.6)$$

and for  $E < E_{tr}$ , it is a dn elliptical function,

$$p(t) = p_{2+} \left( \pi/(2K(k_2)) + [2\pi/K(k_2)] \sum_n \frac{q_2^n}{1+q_2^{2n}} \cos[2n(\chi\Omega_2 t/2 + \Phi_2(t))] \right) \quad (4.7)$$

where  $K$  is the complete elliptical integral of the first kind. In (4.6) and (4.7), certain quantities are related. For instance,



$$q_i = \exp(-\pi K(k'_i)/K(k_i)) \quad i = 1, 2 \quad (4.8)$$

$$\Omega_i = \pi\omega_i/2L(k_i) \quad i = 1, 2 \quad (4.9)$$

$$k_i'^2 + k_i^2 = 1 \quad i = 1, 2 \quad (4.10)$$

and  $k_i$  and  $\omega_i$  are functions of  $p_{\pm i}$  ( $i = 1, 2$ ) through the following relations:

$$\omega_1 = (p_{1+}^2(t) + p_{1-}^2(t))^{1/2} \quad (4.11)$$

$$k_1 = p_{1+}(t)/(p_{1+}^2(t) + p_{1-}^2(t))^{1/2} \quad (4.12)$$

$$\omega_2 = p_{2+}(t) \quad (4.13)$$

$$k_2 = (p_{2+}^2(t) + p_{2-}^2(t))^{1/2}/p_{2+}(t). \quad (4.14)$$

When (4.6)–(4.14) are used as solutions in the adiabatic limit,  $E$  is a constant. The  $p_{i\pm}$  ( $i = 1, 2$ ) are also constant. In the non-adiabatic case with small  $1/\Gamma$ , we present (4.6) and (4.7) as our approximate *but analytical* solutions for  $p$  of (1.12)–(1.14). The difference between the present solution and the ones of the adiabatic limit is that now  $E$  becomes a slowly varying quantity evolving in time according to (3.8) or (3.10) depending on whether  $E < E_{\text{tr}}$  or  $E > E_{\text{tr}}$  with  $E_i = E_0 = 1/2\chi$  for localised initial conditions. The quantities  $p_{i\pm}$ ,  $\omega_i$ , and  $k_i$  ( $i = 1, 2$ ) also become time varying because of the dependence on  $E$ .

To complete our solutions, we now evaluate the phase terms  $\Phi_1(t)$  and  $\Phi_2(t)$ . We obtain them by substituting (4.6) and (4.7) into (4.1) and equating the terms of the same order in  $1/\Gamma$ . The procedure is tedious but straightforward. For  $E < E_{\text{tr}}$

$$\begin{aligned} \Phi_1(t) = & (\pi t^2/K(k_1))\{(\chi/\Gamma)[A + B(E(t) - E_0) + C(E(t) - E_0)^2]\} \\ & \times [1/(2\chi E(t))^{3/4} - (\omega_1/K(k_1))\{(\mathcal{E}(k_1) - k'^2 K(k_1))/k_1 k_1'^2\}] \\ & \times \{[1/(2\chi E(t))^{1/2} - 1]/\omega_1 p_{1+} \chi - p_{1+}/[\omega_1^2 (2\chi E(t))^{3/4}]\} \end{aligned} \quad (4.15)$$

where  $A$ ,  $B$  and  $C$  are given in (3.4)–(3.6),  $E_0 = 1/2\chi$ ,  $E(t)$  follows (3.8) with  $E_i = E_0$ , and  $\mathcal{E}$  is the complete elliptical integral of the second kind. For  $E > E_{\text{tr}}$ ,

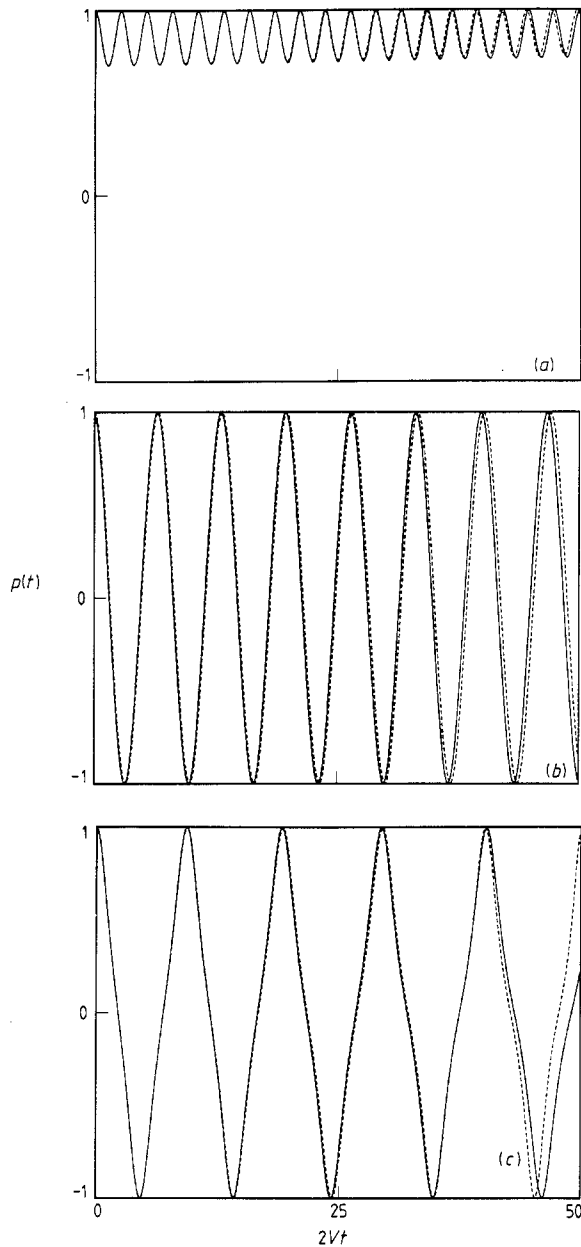
$$\begin{aligned} \Phi_2(t) = & (\pi t^2/K(k_2))(4E(t)/3\Gamma)[[1/(p_{2+} \chi)][1/(2\chi E(t))^{1/2} - 1] \\ & - (\omega_2/K(k_2))\{(\varepsilon(k_2) - k'^2(k_2))/k_2 k_2'^2\}\{1/[p_{2+} (2\chi E(t))^{3/4}]\} \\ & - (\omega_2/\chi p_{2+}^3)[1/(2\chi E(t))^{1/2} - 1]] \end{aligned} \quad (4.16)$$

where  $E(t)$  follows (3.10) with  $E_i = E_0 = 1/2\chi$ .

Comparisons of the approximate solutions (4.6) and (4.7) and the numerical results obtained by summing 100 terms in (4.6) and (4.7) are presented in figure 4 for three values of  $\chi$ : (a)  $\chi = 2.8$ , (b)  $\chi = 0.8$  and (c)  $\chi = 1.8$ .

## 5. Summary

We have investigated the non-adiabatic dimer in the case of fast but finite vibrational relaxation through the application of an averaging method. We studied a slowly varying quantity  $E$ , which is a constant of motion in the adiabatic limit. The definition of  $E$  is in (2.4) and the approximate time evolution we found is in (3.8)–(3.11), obtained using



**Figure 4.** The probability difference  $p$  plotted as a function of time, showing both 'exact' numerical solutions (full curves) and the approximate but analytical results (broken curves) of this paper. Analytical solutions are good for  $2Vt < (\Gamma/\chi)^{1/2}$ . The rate  $\Gamma$  (in units of  $2V$ ) is taken to be 200 and other parameters are as in figures 1 and 2.

simple polynomial fits of  $\langle q^2 \rangle$  (figure 1). The time dependence we obtained is shown in figure 2. For intermediate non-linearities, the evolution of the quasiparticle undergoes a 'free'-to-trapping transition. We have derived an expression, (3.12), for the time taken for this transition to take place. The time dependence for the probability difference is given in (4.6) and (4.7) and is shown in figure 4.

One of the important characteristics of our method is the presence of the phase terms  $\Phi_1(t)$  and  $\Phi_2(t)$  in (4.6) and (4.7). Phase terms are unnecessary in applications of the averaging method to other non-linear problems such as the von del Pol oscillator [9],

since in the latter case, the zero-order solution (which corresponds to the adiabatic solution in the present problem) is a harmonic oscillation: the period of oscillation does not change as one varies the amplitude. Since the zero-order solution in our case is an elliptical function, the treatment of phases is essential to our problem. We mention in passing that  $\Phi_i(t)$  in (4.14) is the first-order phase correction and must be small compared with unity. Since  $dE/dt$  is of the order of  $\chi/\Gamma$  and  $\Phi_i(t)$  is proportional to  $t^2$ , it is clear that the approximate solution of  $p$  in (4.3) and (4.4) is valid for  $2Vt < (\Gamma/\chi)^{1/2}$ . The approximation could be improved by considering higher order corrections.

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