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Abstract. A recently suggested simple model of an open microscopic system interacting with a bath and behaving like an isothermal Maxwell daemon is simplified and treated numerically. Results obtained confirm expectations that the system can, at the cost of thermal energy of the bath, spontaneously and in a cyclic process, pump particles from a particle reservoir to states with even higher energy. This contradicts the usual opinion based on the second law of macroscopic thermodynamics. For this effect, the interaction with the bath cannot be treated as weak. The role of dephasing owing to this interaction is illustrated.

1. Hamiltonian

Recently, we have found a model with an interesting property of pumping particles, purely on account of the thermal reservoir energy of a single bath, in an open system from one side (particle reservoir) to another one preserving or even slightly increasing the mean particle energy [1, 2]. Other types of this model working with pairs of particles also exist [3, 4]. The principle on which the system works reminds us, as far as the final effect is concerned, of the Maxwell daemon [5, 6]. The underlying physics is, on the other hand, remarkably different. The main difference consists in the fact that in our case, also called the isothermal Maxwell daemon, the central system (daemon) working as a pump is, in contrast to [5, 6], an inherent part of the system. The system interacts with the bath and together all are described by the standard Liouville equation for the system + bath complex. The above behaviour resulting from rigorous analytical treatments is, of course, hardly compatible with the macroscopic equilibrium thermodynamics for a quasi-independent system and bath. That is what makes the problem attractive and why studies of such one-way transport mechanisms are important.

In [2], a semiclassical version corresponding to the original quantum model [1] is also briefly mentioned. Its solution has, however, been only very briefly reported in [7]. There has been no detailed discussion of the resulting one-directional transfer even against external forces on account of the fact that only the thermal energy of a single bath exists. This is the aim of the present work. The semiclassical model, in its simplest form, is described by the Hamiltonian of the system

$$H_S(t) = \delta\epsilon c_1^\dagger c_1 + J(c_{-1}^\dagger c_0 + c_0^\dagger c_{-1})[1 - z(t)] + I(c_1^\dagger c_0 + c_0^\dagger c_1)[1 + z(t)] - \epsilon z(t)c_0^\dagger c_0. \quad (1)$$

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It involves only one particle on three sites with particle creation (annihilation) operators $c_m^\dagger$ (c_m), $m = -1$, 0 or $+1$. $\delta\epsilon$ describes increase of the particle (site) energy upon the transfer '-1' $\rightarrow$ '$+1$' found below with an initial condition corresponding to the particle localized at, e.g. site '-1'. J and I play the role of the usual particle hopping (transfer) integrals; both values $I = J$ and $I \neq J$ are admissible. The hopping integrals are, however, multiplied by factors $1 \pm z(t)$ where $z(t)$ is a c-number (i.e. classical) variable $\in \langle -1, +1 \rangle$ describing the state of a central system (the isothermal Maxwell daemon) able to open (close) the transfer channels '-1' $\leftrightarrow$ '0' and '0' $\leftrightarrow$ '$+1$'. The physical meaning of $z(t)$ is the mean value of $\hat{z} \equiv |u\rangle\langle u| - |d\rangle\langle d|$ where $|u\rangle$ and $|d\rangle$ are two states of a two-level system (representing our central system or daemon) separated, on the energy axis, by the energy difference ϵ. Quantum mechanically, one can easily describe instability of the central system upon the particle transfer to site '0' assumed to form a receptor inherently connected with the central system (daemon). This instability (change of the topological orientation or conformation) is well known in, e.g. the macromolecular world (e.g. valinomycine upon accepting the K^+ ion [8]). Owing to the semiclassical way of describing the daemon conformation [2], the above states of the daemon do not explicitly appear in (1).

From (1), one obtains the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \psi_{-1}(t) \\ \psi_0(t) \\ \psi_1(t) \end{pmatrix} = \begin{pmatrix} 0 & J(1 - z(t)) & 0 \\ J(1 - z(t)) & -\epsilon z(t) & I(1 + z(t)) \\ 0 & I(1 + z(t)) & \delta\epsilon \end{pmatrix} \cdot \begin{pmatrix} \psi_{-1}(t) \\ \psi_0(t) \\ \psi_1(t) \end{pmatrix} \tag{2}$$

where $\psi_n(t)$ represent site probability amplitudes to find the particle at site n. As for $z(t)$, one must introduce a relaxation equation representing the instability as well as the effect of the system bath and the bath Hamiltonians H_{S-B} and H_B. We assume a simple dynamical equation

$$\frac{\partial}{\partial t} z(t) = -\gamma[z(t) + 1 - 2|\psi_0(t)|^2] \tag{3}$$

describing exponential relaxation (with, in general, ϵ- and temperature-dependent relaxation rate γ) to values corresponding to an instantaneous population of the receptor site '0'. In particular, as far as the particle is fully localized to (or absent at) site '0', $z(t)$ relaxes to $+1$ (or -1). The exponential form of the relaxation according to (3) is not important. It is dictated anyway by the Markovian form of (3) which is now easy to derive by modern methods of the nonequilibrium statistical mechanics [9].

Let us now remind ourselves of the dephasing existing in nature but formally omitted in the noiseless equation (3). In many situations (as verified numerically), it is not necessary. In order to model more realistic situations, it will be reintroduced into our numerical studies below. (The reader is referred below for detailed arguments and technical details.) As is well known, the noise can be easily added to the Schrödinger equation provided we model it by an external stochastic potential; the theory as well as practice is now well established [10–12]. As we shall, however, argue below one also gets the dephasing with the fully quantum and responsive bath. Averaging over the noise obtained can of course be well performed only on the level of the density matrix. The latter task shall not be solved here. We do not need it, however, for our purposes because we get (as reported below and for specified values of parameters of the model) the one-directional transfer for any realization of the noise with properly chosen intensity of the dephasing. Thus, the averaging cannot change the existence of the one-directional transfer as the main result of this work.

Concerning the dephasing as modelled below, one should stress that we *neither* need *nor* assume the real stochastic picture in our model here. One should realize the following.

• If the dephasing exists in the classical (stochastic potential) description of the bath, it inevitably also exists in its quantum description. The point is that the classical description is nothing but a limiting case of the quantum one. The notion of dephasing is now well established and built into the quantum theory of open systems [13].

• Our basic equations like (3) above are in fact written as for a genuinely quantum bath; with the stochastic description of the bath, $z(t)$ would relax to $z = 0$ only.

2. Analytical semiclassical solution

This section is necessary before resorting to numerical calculations in order to understand some peculiarities reported below. The point is that our set (2), (3) is, owing to the above semiclassical approximation $\hat{z} \to z(t) \equiv \langle z \rangle(t)$, nonlinear. This may provide a variety of possibilities and connections between general and stationary solutions, including even chaos [14].

Except for $\sum_{n=-1}^{+1} |\psi_n(t)|^2$, no conserving quantity is seen in the above dynamical problem. Owing to the nonlinearity, no nonstationary analytical solutions to (2), (3) have been found analytically. Let us add that the task is technically complicated, being represented by a motion of a representing point in a seven-dimensional space. The first task in investigating time dependence of physical observables in nonlinear systems is, however, an analysis of stationary states. For that, let us for a while put $\delta\epsilon = 0$.

For arbitrary values of input parameters, there are at least three stationary states of our semiclassical problem. The three solutions (up to a phase factor) read

$$E_1 = 0 \qquad z(t) = -1$$
$$\begin{pmatrix} \psi_{-1}(t) \\ \psi_0(t) \\ \psi_{+1}(t) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{4}$$

and

$$E_{2,3} = \pm\sqrt{J^2 + I^2} \qquad z(t) = 0$$
$$\begin{pmatrix} \psi_{-1}(t) \\ \psi_0(t) \\ \psi_{+1}(t) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm J/(\sqrt{J^2 + I^2}) \\ 1 \\ \pm I/(\sqrt{J^2 + I^2}) \end{pmatrix} \cdot e^{\mp i\sqrt{J^2+I^2}t/\hbar}. \tag{5}$$

In state (4), the particle is already on the right-hand side and the system (provided we admit more-particle states) is able to accept another particle from the left. This solution corresponds to the expected asymptotic state (see [2]), as we are going to argue below (limit cycle or circle of physically equivalent attractors in the seven-dimensional space of Re ψ_m, Im ψ_n ($n = -1, 0, +1$) and $z(t)$). One should mention that this is owing to the lucky fact that the semiclassical replacement $\hat{z} \to z(t)$ underlying (1) becomes exact as long as we are in a state where the operator on the left-hand side assumes a sharp value (i.e. -1 in our case). Such an advantageous situation does not appear in other (including nonstationary) states, in particular (5). In the corresponding states, the central system is in an 'equilibrium' with the particle which is partly on both sides. Such an 'equilibrium' immediately becomes disturbed once quantum fluctuations are taken into account, as is also illustrated below. Such fluctuations in particular violate sharp phase relations (underlying in fact this 'equilibrium' situation) among individual components $\psi_m(t)$ of (5). In contrast, one should notice that no such relations can be established among components of (4). That is why (4) may survive as the asymptotic solution (attractor) even under the presence of the noise to be introduced below. One should also add that (5) is a stationary solution

in the physical sense only (stationarity for the squared amplitudes $|\psi_n(t)|^2$). In the above seven-dimensional space, (5) provide a periodic solution (limit cycle) in the usual sense as the phase factor never dies out.

For special values of the parameters, one can also identify other stationary solutions with similar characteristics as above. In particular, for $8|IJ| < \epsilon^2$, two other stationary solutions exist with

$$z_\pm = (-4I^2 + 4J^2 \pm \sqrt{\epsilon^4 - 64I^2 J^2})/(\epsilon^2 + 4I^2 + 4J^2) \neq 0 \qquad z\pm \in (-1, +1). \qquad (6)$$

The corresponding energies read

$$E_\pm = -0.5\epsilon(z_\pm + 1) \qquad (7)$$

and the solutions are

$$\begin{pmatrix} \psi_{-1}(t) \\ \psi_0(t) \\ \psi_{+1}(t) \end{pmatrix} = \sqrt{\frac{1 + z_\pm}{2}} \begin{pmatrix} -\frac{2J(1-z_\pm)}{\epsilon(z_\pm+1)} \\ 1 \\ -\frac{2I}{\epsilon} \end{pmatrix} \cdot e^{i\epsilon(z_\pm+1)t/2\hbar}. \qquad (8)$$

If, e.g. $8|IJ| = \epsilon^2$ then $z_+ = z_-$. We then only get one additional solution for $|I| \neq |J|$ or no additional solution for $|I| = |J|$. If $8|IJ| > \epsilon^2$, the additional solutions disappear. Properties of these additional solutions as far as the existence of fixed phase relations among $\psi_n(t)$ are concerned are the same as above.

Unfortunately, similar simple analysis cannot be performed analytically for $\delta\epsilon \neq 0$. Quasiperiodic or periodic solutions to (2), (3) may then, however, persist until the first dephasing event takes place. For a sufficient density of the dephasing events, one always finds that the solution finally yields the full ' − 1' → ' + 1' transfer.

3. Numerical studies

Let us now continue with general $\delta\epsilon$, $|\delta\epsilon| < \epsilon$. Disturbing the last inequality makes the model unphysical [2] (no one-way transfer exists in the original quantum model [2]). The first point to be discussed is that the formulation of our problem to be solved here as given by (2) and (3) differs from the original quantum problem with inclusion of H_B and H_{S-B} not only by formal omission of any additional dephasing in our noiseless equation (3). The semiclassical approximation consisting in replacing $\hat{z} \equiv |u\rangle\langle u| - |d\rangle\langle d|$ by its mean value $z(t)$ appreciably *underestimates* the tendency to the one-way particle transfer ' − 1' → ' + 1'. The point is that in the original quantum problem [2], the $|u\rangle \leftrightarrow |d\rangle$ transitions, i.e. closing and opening of the trap (gate) to the left and right, appear after the particle comes to and from site '0' in the *same* system in the ensemble. On the other hand, replacing $\hat{z}$ by its mean value $z(t)$ means to relate the process of closing and opening of the trap to the mean situation in all the systems in the whole ensemble. Moreover, as the values of $z(t)$ lie in the whole interval $z(t) \in \langle -1, +1 \rangle$, the opening or closing the gate in each system of the ensemble is, as in our semiclassical model (2), (3) and in contrast to the original quantum one [2], only partial. Consequently, once we get the one-way transfer from the semiclassical formulation of the problem here, we have good grounds to assert that a similar and even more pronounced effect is described by the original quantum model [2] as well. The opposite is, however, clearly not true. All our numerical results below are reported for the initial condition $\psi_{-1}(0) = 1 - \psi_0(0) = 1 - \psi_{+1}(0) = 1$ (the particle is initially at site '−1') and $z(0) = -1$. Qualitatively similar results are also obtained for other initial conditions. Next, we assume everywhere the symmetric hopping situation with $J = I > 0$. Possibly different values $J \neq I$ cannot yield qualitatively different overall picture of the process.

The next point is connected with reintroduction of the above dephasing omitted at the moment of postulating (2), (3). First, let us notice that including the longitudinal relaxation (longitudinal relaxation time T_1) means, according to the famous relation

$$T_1 \gtrsim 0.5 T_2 \tag{9}$$

(see [15, 16]) automatic inclusion of the corresponding dephasing characterized by the transversal relaxation (dephasing) time T_2. Thus, the dephasing connected with the $|d\rangle \leftrightarrow |u\rangle$ transitions (longitudinal relaxation) of our central system is already included. It underlies the very introduction of the transfer rates between the $|u\rangle$ and $|d\rangle$ states of our central system, i.e. γ in (3). These transitions are due to the coupling of the central system to the thermodynamic bath.

On the other hand, let us realize that as usual;
• the transversal relaxation is usually much faster than the corresponding longitudinal one,
• it can even exist for such types of the coupling to the bath when the longitudinal relaxation does not exist (T_2 is finite while T_1 turns to infinity in (9)), and
• not only the central system (for which the bath-assisted transitions are already included) but also the particle transferred is in general coupled to the bath.

The latter coupling, in its simplest form leading to the transversal relaxation (T_2 for the particle) may only be written in the site-diagonal form proportional to, e.g. $c_0^\dagger c_0$. (Here, without any impact on the qualitative result of our analysis, we have for simplicity assumed that only the particle coupling to the bath at site '0' is essential.) Let us now first describe perhaps not the most physically sound (owing to its classical character) but certainly the simplest, as well as the most instructive way, to get the dephasing from this form of the coupling assuming that it is caused by a classical stochastic field. We have chosen this possibility at the very beginning to become as convincing as possible. A way of generalizing these arguments beyond the classical stochastic level of description is sketched below.

Conditions are well established when and to what extent a real coupling to the bath can be replaced by, e.g. a stochastic field $U(t)$ acting (in our case) as a site local random field [10]. Thus, the term $\approx c_0^\dagger U(t) c_0$ should in such a case be added to (1). This is the basis for the so-called stochastic Liouville equation model [11, 17]. As far as this field (bath) is fast as compared with our particle dynamics, this stochastic field can have the character of statistically distributed shot noise (known to act on, e.g. Brownian particles as described by the Langevin equation [22]). Adding such a noise to the 2, 2-element (or 0, 0 in our notation) in the Hamiltonian matrix on the right-hand side of (2), it is trivial to verify that each such a stochastic potential shot leads to nothing but a stochastic change of the phase of the complex variable $\psi_0(t)$ provided that its duration be appreciably shorter than $\hbar/|J|$ and $\hbar/|I|$. (In order to see that, one can, during the potential shot, fully neglect J and I in (2). Direct integration of the second equation in (2) then yields the required result.)

A highly important objection can now be raised against the *classical* character of random field $U(t)$ added to the problem. In order to reject such objections, one can simply replace $U(t)$ by a potential resulting from impacts of inherently *quantum* particles in the reservoir. The (almost) shot-like character of the interaction may be then due to their distribution in space (well localized wavepackets impinging on our system), and their relatively high velocity with respect to that of the particle transferred. In general, for an arbitrary nontrivial bath, we always get dephasing in all of the advanced methods of the reduced density matrix theory (see [18, 19] for methods of the quantum Redfield–Bloch equations).

The above shows why we have eventually complemented our model (2), (3) by a full randomization of the phase of $\psi_0(t)$ at well defined time points. Three comments should

now be mentioned concerning this procedure.

• This way of introducing the randomization of the phase fully corresponds to purely quantum theories [20, 21, 9] as well as to the classical Langevin-type description of the Brownian motion with a stochastic and formally delta-correlated force (acting on the Brown particle and modelling influence of the bath) [22]. An important physical condition for such a kind of description is that the bath is very fast (the real duration of the scattering events is extremely short) as compared with the particle transferred. This is what we also assume here. This allows then to take the randomization events as fully localized in time (i.e. happening at only discrete time points).

• Real impact (scattering) of any (classical or quantum) particle lasts, on the other hand, only a finite time (the scattering duration is finite). Thus, in contrast to physical expectations, our randomizing procedure seems to introduce zero-correlation time and, consequently, infinite frequencies or energies into the problem. If true, this would certainly be nonadmissable at finite temperatures required by (and used in), e.g. (3). The same (and, in fact, also *only formal*) problem appears, on the other hand, in the standard classical Langevin theory of the Brownian motion [22]. This theory also works with finite temperatures (in, e.g. the resulting Einstein diffusivity versus mobility relation) and, simultaneously, with formally zero duration of the scattering events, i.e. zero-correlation time of the random force (formula (1.3.41) of [22]). In the Langevin theory, the stochastic force (irrespective of the zero-correlation time) produces no heating of the particle as a consequence of, e.g. the presumed lack of correlation between the stochastic force and particle position. In our model, one can see that there is no unphysical energy transfer to the system owing to the above dephasing from, e.g. the energy variational estimate. For finite J and I, there is a possibility of a finite increase of the particle energy owing to the dephasing, by the amount of energy which is $\leqslant 4(|J| + |I|)$ only. For, e.g. appreciably up-in-energy transfers with $4(|J| + |I|) \ll \delta\epsilon$, this is certainly a negligible amount. Moreover, this finite particle energy increase owing to disturbing intersite particle phase relations is fully physical, existing both in the rigorous quantum theory and in nature (bond breaking). Hence, no danger of any unphysical energy pumping to the system appears in our case, too. In general situations, however, the problem of the unlimited energy transfer to the system upon including stochastic perturbations with, e.g. white frequency spectrum, may be sometimes quite crucial [10].

• Any distribution of the above randomization times is possible, leading to the same qualitative result. We have, purely for technical reasons, chosen their regular distribution at (positive) multiples of the randomization time step Δt, keeping only the heights of the potential shots random (i.e. the random change of the phase of ψ_0). In this connection, one should notice that in many situations, only a few randomization events are necessary to observe a clear tendency to the full ' -1' $\rightarrow$ ' $+1$' transfer (see, e.g. figure 1). This illustrates how details of the distribution of the randomization times are of little importance. In general, the randomization accelerates the transfer process or causes the transfer if there is no transfer without it. For this to occur, however, it must be sufficiently intense. On the other hand, too intense randomization preserves the overall tendency to the transfer reported but makes the pictures obtained too noisy.

Figure 1 illustrates the transfer among sites with the same site energy (horizontal in energy). The role of the individual randomization events is worth noticing. In such situations and with general initial conditions, the entropy of the particle distribution clearly turns to its minimum as a result of activity of our central system. Figure 2 shows a more complicated case of a transfer going down-in-energy. An important observation is that in our starting model, we have no bath-assisted mechanism acting directly on the particle transferred which
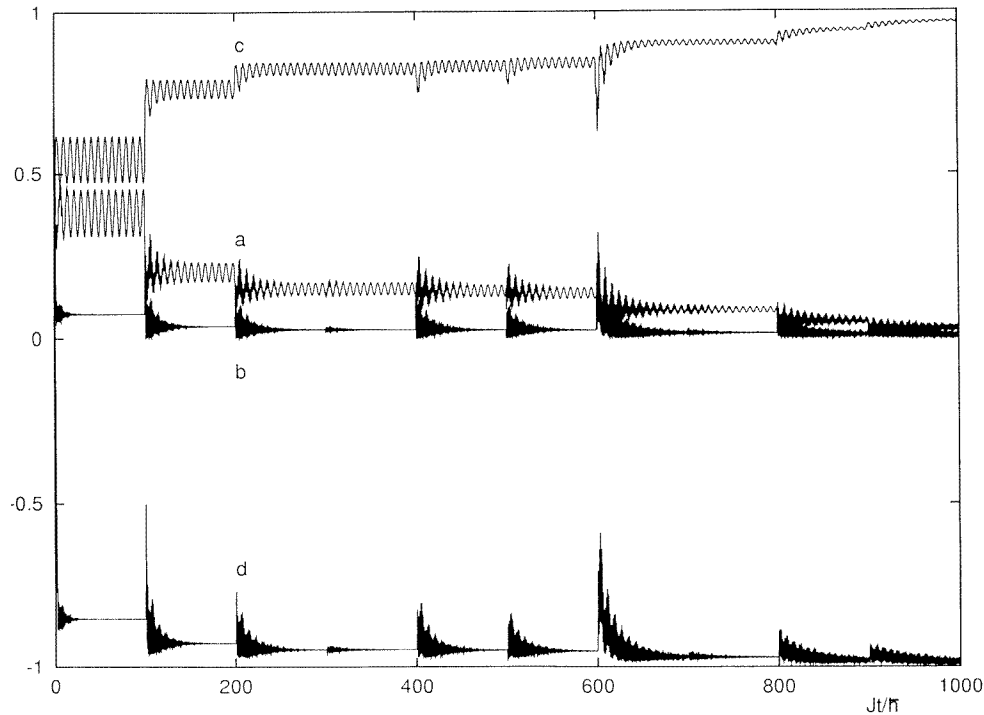
Figure 1. Time dependence of probabilities $P_m(t) \equiv |\psi_m(t)|^2$ ($m = -1$, 0, and $+1$ for curves 'a', 'b' and 'c', respectively) of finding the particle at individual sites, and the daemon parameter $z(t)$ (curve 'd'); $z(t) = 1$ or $z(t) = -1$ designate the daemon fully open to the right (to release the transferred particle to the right) or left (to accept another particle from the left if any), respectively. See the main text for the initial condition. Parameters $\gamma = 5J/\hbar$, $\delta\epsilon = 0$, $\epsilon = 4J$, $\Delta t = 100\hbar/J$, $I = J > 0$.

would prefer its down-in-energy transitions (the asymmetry of the up- and down-in-energy transitions being due to the spontaneous processes with respect to the bath). The coupling to the bath in our model only influences the central system. Thus, this picture illustrates the decisive role of the timing of the gate provided by the central system. It also shows how it forces the particle to go in one direction only, this time in correspondence with expectations. The timing also works, however, for the up-in-energy transitions. This time, the one-directional transfer is, however, contradicting standard statistical physics. Figure 3 shows such a case. Worth noticing is, that on the one hand, standard chaos (in the mathematical sense) appears [14]. Three different curves (obtained for three different initial integration steps) for $P_{+1}(t)$ (i.e. the probability of the particle transfer) are shown that start to deviate for $t \gtrsim 50\hbar/J$. All of them, on the other hand, turn to the same value $P_{+1}(t) \rightarrow +1$. That is to say, owing to the exponentially-like increase (with increasing time) of the influence of uncertainties in initial conditions, rounding errors etc, the genuine time-dependence of the solution to our problem becomes numerically unpredictable. What, however, is predictable is the overall tendency of all the possible curves to the corresponding asymptotic value, i.e. unity.

All the pictures illustrate that there is no ban on the particle transfer in the direction up- or down-in-energy in our dynamical model. It also shows how the transfer goes on, typical timescales for the transfer in the semiclassical model as well as behaviour of the central
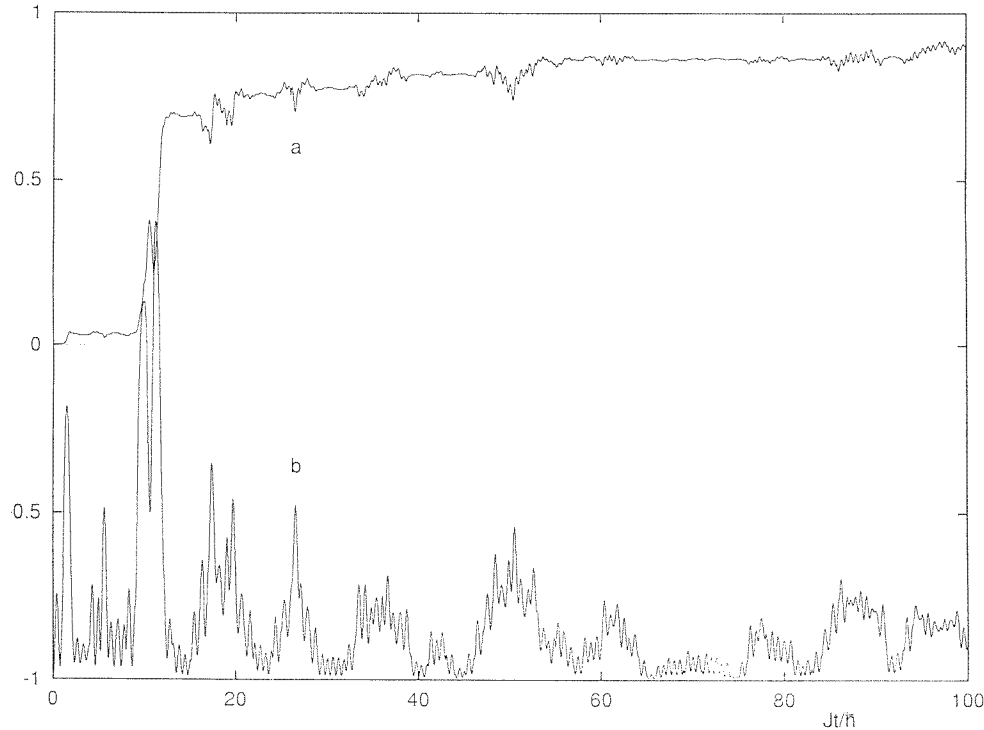
Figure 2. The probability $P_{+1}(t)$ of finding the particle already transferred (curve 'a'), and the corresponding value of the daemon parameter $z(t)$ (curve 'b') for $\gamma = 10J/\hbar$, $\delta\epsilon = -3J$, $\epsilon = 10J$, $\Delta t = 1\hbar/J$.

system. The latter, upon transferring the particle to site '+1', always turns to open to the left ($z(t)$ turning to -1) waiting for another particle (if any) to be transferred. The chain character of the process (lying, owing to our technical limitation to only one particle here, beyond the possibilities of our simple theory) makes the system highly important.

Similar results can also be expected when choosing times of randomizing the phase also at random. That brings us to the problem which is the explanation of the final transfer of the particle to site '+1' from the point of view of the mathematical structure of (2) and (3) only (i.e. apart from physics of the starting quantum model [2]). The solution to (2) and (3) may be represented as a path in the seven-dimensional space of real variables $\mathrm{Re}\,\psi_n$, $\mathrm{Im}\,\psi_n$ ($n = -1, 0, +1$), and z. The above stationary solutions are in fact periodic solutions (limiting cycles) in this space. In all the stationary solutions (5) and (8), all the $\psi_n(t)$ are nonzero and are determined up to a common phase factor. Thus, the relative phase of, e.g. $\psi_0(t)$ and $\psi_1(t)$ is well determined. Hence, the randomization of just the phase of $\psi_0(t)$ at any randomization event means a relatively long jump in the seven-dimensional space. In other words, it brings the path out of the neighbourhood of the solution and the wandering in the seven-dimensional space starts again. At the stationary solution (4), however, the situation is totally different. Here $\psi_{-1}(t) = \psi_0(t) = 0$. Hence the randomization of the phase of ψ_0 only has no effect, i.e. the path gets resistive with respect to the randomization. In other words, the solution (4) remains stationary (i.e. as a resistive limit cycle in the seven-dimensional space) even with respect to any randomization procedure of the type used above. This helps us to understand what is happening with the solution, even for such
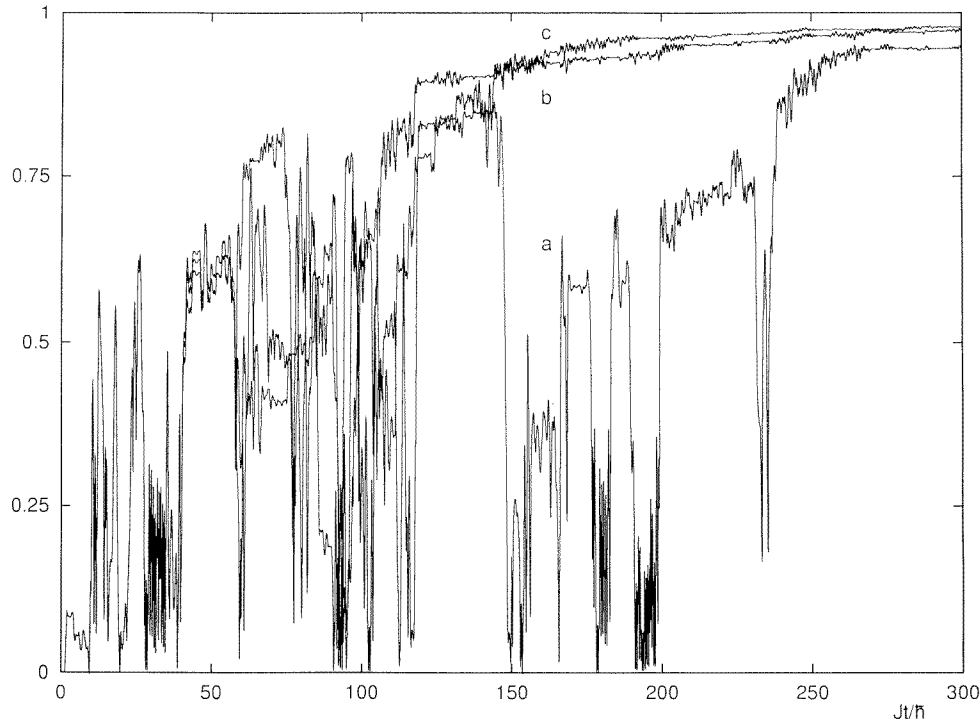
Figure 3. Three curves of $|\psi_{+1}(t)|^2$ for $\gamma = 10J/\hbar$, $\delta\epsilon = +3J$, $\epsilon = 10J$, $\Delta t = 1\hbar/J$ but three different values of the initial integration step (0.01, 0.02 and 0.05 in $\hbar/J$ units for 'a', 'b' and 'c' curves, respectively). Notice that for $t \gtrsim 50\hbar/J$, the curves are different (indicating chaotic behaviour of the solution) but all of them finally turn, with increasing time, to unity.

long times when numerical data become unreliable. Let us add only that all our pictures were calculated with a high accuracy (double precision calculations) which appreciably exceeds the accuracy of drawing the pictures. Within the time intervals indicated, the absolute error in figures 1 and 2 is always appreciably less than 10^{-8}. Figures 1 and 2 were drawn using at least 10 000 points, and at least 6000 points were used in figure 3.

4. Results versus energy conservation law and second law of thermodynamics

The first questions which should be answered here are;

• how it is possible that the energy of the particles is raised at the cost of that of the bath when the reorientations of the central system (closing and opening the way for the particle to the right or to the left) are always owing to down-in-energy (i.e. mostly spontaneous) transitions of the central system?

• How it is possible that the opening and closing acts of the central system come 'on average' at a proper time to cause, as a final effect, the '−1' → '+1' drain reported here. Let us add that the proper timing of the above acts is a precondition of the process.

For the second question, there is no ready answer except that we have observed this timing to be automatically ensured by equations (2), (3) themselves. This perhaps suggests something deeper in the physics of the model, in particular the tendency to the one-way '−1' → '+1' transfer already contained in the original quantum model [2]. As for

the energy conservation, arguments which could be raised in principle against the process observed, one should add that the dephasing (for the central system at least as a necessary prerequisite of the process as discussed above) means a continuous energy exchange between the system and bath. That makes the final energy conservation possible.

Evidently, however, the results reported also contradict the standard formulation of the second law of thermodynamics in the sense that the particle (or particles, if more of them were present) acquires additional energy at the cost of that of the bath. There are, however, several formulations of the second law. In order to be as precise as possible, we should therefore add now that we mean the following one. *There is no (Planck–Thomson) perpetuum mobile of the second kind allowing to get another form of energy from the thermal one without compensation* (i.e. without additional heat transfer between two reservoirs, from a warmer to a colder one). In our case, we have assumed, in the original quantum model [2] as well as in its approximate form treated here, just one bath with (in its thermodynamic limit) infinite number of modes characterized by a single initial bath temperature entering, e.g. our parameter γ in (3) above. Hence, no compensation is possible by the very definition of the model. As for the energy gained, it is, in the limit of small I and J at least, determined by the site-energy difference $\delta\epsilon$ (we suppose $\delta\epsilon > 0$ here). In fact, $\delta\epsilon$ then means the particle potential energy acquired at the cost of thermal energy of our single bath†. The present model does not include the very act of further transformation or utilization of this potential energy. Anyway, the model can always be trivially complemented by any mechanism (e.g. light emission) connected with the direct back $+1 \rightarrow -1$ transfer (leakage) with, e.g. characteristic times appreciably greater than those encountered here. In this situation, there would be no change of the particle dynamics till the particle is fully transferred to site $+1$. Then the above leakage mechanism would, at the longer time scale, release the desired energy as required by the definition of the perpetuum mobile of the second kind. Hence, there is a real contradiction with the above formulation of the second law. As for connection with its other formulations, see any detailed textbook of thermodynamics, e.g. [23]. Let us only add that invoking the Caratheodory principle stemming from the above formulation of the second law, one easily arrives at the standard formula

$$\delta Q = T \cdot dS \tag{10}$$

(usually taken as another standard formulation of the second law) of the equilibrium thermodynamics for the infinitesimal heat increment δQ and introduces thus the entropy S. Thus:

• our results above question the usual basis of the axiomatic thermodynamics in connection with the Planck–Thomson form of the second law, ascribing it (as all the above effects disappear in the classical limit) with at most a classical meaning. Let us again stress that compared with the quantum model [2], the model treated here rather underestimates the tendency to the uphill-in-energy particle transfer obtained. Anyway, it still yields the effect discussed.

• Questioning the axiomatic thermodynamic basis for (10) based on the Planck–Thomson formulation of the second law means, however, questioning of neither the notion of entropy nor of the formula (10) itself. Let us remind the reader that the notion of entropy is now well established in statistical physics [24].

As far as the second law in form of (10) is concerned, one can still understand it in two different ways.

† Worth noticing is that as the particle at sites ± 1 is *not* under the influence of, e.g. the site-local coupling to the bath, there is no site-energy renormalization (small-polaron energy shift) in our model. Thus, $\delta\epsilon$ is not the 'bare' (unrenormalized) but real particle energy.

- First, as a generalization of our everyday experience in the macroscopic world; the second law then becomes an inherent part of macroscopic thermodynamics. Our system is, on the other hand, fully microscopic. That deprives us of any possibility to raise objections against the above numerical results using macroscopic phenomenological arguments of this type.

- Second, as a consequence of the nonequilibrium statistical mechanics and microscopic equations of motion. Here, one must admit, however, that this programme has so far only been accomplished at the level of the classical statistical mechanics [25, 26]. Then (10) results from the first-order expansion in powers of a small parameter of the problem defined as a ratio of the diameter of the particles and typical dimension of the system. Thus, the parameter is really small in truly macroscopic systems but is not, on the other hand, small in systems like the one investigated here.

- Concerning the latter point, one important comment concerning methods of quantum dynamical semigroups [27] should be added. These methods are based on time-local differential equations determining the time-dependence of the density matrix of the system only. Conclusions then support standard understanding of transport phenomena, thus contradicting our above results. One should add, however, that the starting time-local equations can be derived only approximately (using, e.g. the Born–Markov approximations to time-convolution generalized master equations, or unphysical unbounded-from-below model Hamiltonians etc.) or by taking the singular coupling limit [27]. Real applicability of such approximate methods is, however, highly limited (compare, e.g. rigorous arguments in [28–30] concerning the applicability of such methods to at most finite time intervals). As for the singular coupling limit methods, they require, e.g. simultaneous coupling strength as well as time rescaling. In physical terms, the bath, as well as the system relaxation under its influence, should become infinitely fast. For our model here, we could check such a limiting case by taking the $\gamma \to +\infty$ limit, keeping other (system) parameters constant. Our numerical results then indicate that the effect reported above disappears. Hence, there is no contradiction between the quantum dynamical semigroups method and the present model.

In connection with the above discussion, one should again stress that our starting model [2] is fully quantum and ceases to work in the classical limit. To our knowledge, no unambiguous derivation of the Planck–Thomson form of the second law applicable to the purely quantum regime and truly microscopic systems exists so far. On the other hand and also to the best of our knowledge, no quantum and truly microscopic systems have been reported so far which show a behaviour contradicting this law as our model here. The only exceptions are variations of the present model for pairs of particles (leading to conversion of the thermal bath energy into the chemical one) for which analytical solutions supporting the above picture exist [3, 4]. As for the ratchets models ([31] and papers cited therein), they require an external noise (absent here) in addition to the influence of the bath, in order to compete with the second law. This is what perhaps makes these models less realistic. The above, therefore, makes the model treated here and its behaviour still more important.

Acknowledgments

References

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