

# Synchronized and reconfigurable motion of molecular (quantum) robots: a field theoretic approach

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**Abstract—** Using an elementary version of quantum field theory that uses creation and annihilation operators and takes care of damping, we present typical solutions representing motion of molecular robots.

**In our opinion, our model bears great potentialities for further extensions. We have treated robot molecules with one leg. Molecules with several legs, even showing different gaits can be dealt with in a similar way. A steering of the quantized signal field allows us to manipulate various configurations of the multi molecular robot system. Further, the excitation of the biological substrate by external signals opens a new bio-hybrid method to control the substrate from outside if it shows e.g. special kinds of mal-functioning.**

## I. INTRODUCTION

Robotics is presently reaching the nano-scale which is witnessed by recent experiments on molecular robots, [1] – [6]. This work is inspired by biological processes such as muscle contraction where myosin molecules using their flexible “heads” move along actin-filaments, or where kinesin or dynein molecules “run” along tubulin strands transporting e.g. organelles. At this small dimensions the use of quantum theory to cope with these phenomena, when to be treated theoretically, becomes obligatory. In our paper, a first step is done so to treat the correlated (or better “synchronized”) motion of molecular robots.

The topics that are described in this paper can be considered at a first glance as the presentation of construction of molecular machines out of DNA’s (like a tweezer) as it is presented in [5], or a DNA Walker presented in [6]. In these two papers as well in the before mentioned references [1] - [4] the general common goal can be characterized by a sophisticated experimental approach to work with DNA material as well as self-organized “structural material to construct nano-machines” but also to use it as a substrate that operates as “fuel” for machines like tweezers or nano-mechanical switches.

Here we are concentrated not on the experimental methods to generate such biological DNA-machines but we focus our efforts on the theoretical treatment of the translational motion of molecular robots. In previous work [7] we treated the movement of myosin on actin fibers. The whole process,

which is fueled by ATP-consumption, is fundamentally of quantum mechanical nature. Thus our approach served as test of how to apply quantum mechanical methods to such processes. Based on the experience we have gained there, in the present paper we present a model that can be applied to molecular robots (including those composed of DNA).

This approach is based on an elementary version of quantum field theory that allows us to take the impact of the surrounding on the quantum mechanical activity of a single molecule into account. The great efficiency of our approach [7] had been demonstrated before in the realm of laser theory (cf. [8]). In addition parts of the methods used in [7] can be seen in a clear connection to applications of Langevin resp. generalized Langevin equations to atomic systems that are extensively described in [9].

In our paper we assume that the molecules move on an energy rich substrate. As will be demonstrated, two quite different types of solutions to the quantum mechanical equations can be found:

1. A quantum mechanical version of the classical “grass fire” phenomenon.
2. A quantum wave.

It is worthwhile to mention that our “grass fire” solution has to be considered in a more abstract sense than the classical solution of the spread of real, natural grass fires that are modeled e.g. by the application of Huygens’s principles to fire fronts as it is defined e.g. in [10]. Here we look at the substrate molecules as “fuel-stations” that deliver energy to motor proteins or other molecules for their next “step” and must later on again refilled by “fuel”. We consider such set of molecules as a swarm of molecular robots that must be configured, synchronized and in time supported by energy. These restrictions can be very well fulfilled by the approach of quantum field theory (QFT).

Further it should be mentioned that only this method describes the molecules as waves (dualism between particle and field), therefore we present also a second solution (matter waves) that can only be derived by this technique.

A third type of solution is available if we consider passive transport mechanisms that originate from tunneling effects and by fluctuating forces. Both effects occur also in biological cells. This is a further argument to work with QFT methods. However, in this contribution we do not consider this solution; it can be found in [7].

To treat cooperative effects among several molecules (up to many) we assume that signals (e.g. deformations, chemical, etc.) can be transmitted via the substrate. In detail, we formulate our model as follows.

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## II. THE MODEL

We assume that each molecule possesses a movable side group ("leg") that can acquire two different positions (quantum states) "a" and "b". (Our approach can be easily extended to several legs). The substrate for each individual molecule is a periodic one-dimensional array of two-level molecules with an excited state "e" and a ground state "g". The different sites of the substrate molecules are distinguished by an index "l",  $l = 1, \dots, L$ . In the spirit of quantum field theory, the generation of the quantum state "a" of the robot molecule situated at site "l" is described by the creation operator  $r_{al}^\dagger$ , and the destruction of that state by the annihilation operator  $r_{al}$ . Similarly, we describe generation and destruction of state "b" of the robot molecule at site "l" by creation operator  $r_{bl}^\dagger$  and the annihilation operator  $r_{bl}$ , respectively. Quite analogously we introduce the creation and annihilation operators for the substrate molecules by means of  $s_{el}^\dagger, s_{el}$ , and  $s_{gl}^\dagger, s_{gl}$  in an obvious notation

In the following we use the Heisenberg picture in which the operators are time-dependent, whereas the so called state vector is time independent. As we shall see below, the corresponding Heisenberg equations allow us to interpret their physical meaning in a simple manner. In addition, they allow us to take care of the impact of the environment on the robot molecule by means of damping and fluctuations. Lack of space does not allow presenting the whole procedure in detail so that we sketch the individual steps.

First we establish the Hamiltonian operator that comprises the Hamiltonian of the quantum states of the molecular robots, of the substrate molecules, and of the signal field. Furthermore it contains the interaction between a robot molecule and its substrate molecules. We model this interaction as follows: when the leg in state "a" hits an excited substrate molecule, energy is transferred and the leg is brought to its state "b". Under the impact of a substrate signal, state "b" is converted into state "a", that, however locks at a new substrate molecule thus promoting the robot molecule one step further (fig. 2.1).

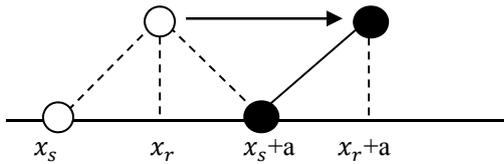


Figure 2.1. Power stroke of robot molecule  $r$  from position  $x_r$  (in state „b“) to the new position  $x_r+a$  (in state „a“).

The signals are transmitted via a Bose field of phonons or chemical waves. The Heisenberg equation can be derived from the Hamiltonian by means of the well-known rule

$$\frac{d\Omega}{dt} = \frac{i}{\hbar}(H\Omega - \Omega H), \quad (2; 1)$$

where  $\Omega$  belongs to a set of suitably chosen operators (in our present model we choose them as Bose operators that obey the commutation relations

$$\Omega_j \Omega_k^\dagger - \Omega_k^\dagger \Omega_j = \delta_{jk}, \text{ etc.} \quad (2; 2)$$

Equation (2; 1) must be supplemented by damping terms (see below) and fluctuating forces.

## III. EQUATIONS OF MOTION

We distinguish the robots (and their corresponding substrate molecules by an index  $m = 1, \dots, M$ ). The coupling constants are denoted by  $g_1, g_2$  (real), the damping constants by  $\gamma$  (supplemented by indices).  $F^\dagger$  (supplemented by indices) are random forces with vanishing mean value and  $\delta$ -correlated in time.  $J_{ll'}$ ;  $l, l' = 1, \dots, L$  are coupling constants between the signal field modes. Note that the dot denotes the time derivation  $\frac{d}{dt}$ . The complete set of equations is given by

$$\dot{r}_{al,m}^\dagger = ig_1 s_{el,m} r_{bl,m}^\dagger s_{gl,m}^\dagger + ig_2 r_{bl-1,m}^\dagger B_l - \gamma_a r_{al,m}^\dagger + F_{al,m}^\dagger, \quad (3; 1)$$

$$\dot{r}_{bl,m}^\dagger = ig_1 s_{el,m}^\dagger s_{gl,m} r_{al,m}^\dagger + ig_2 r_{al+1,m}^\dagger B_{l+1} - \gamma_b r_{bl,m}^\dagger + F_{bl,m}^\dagger, \quad (3; 2)$$

$$\dot{s}_{gl,m}^\dagger = ig_1 r_{al,m}^\dagger s_{el,m}^\dagger r_{bl,m} - \gamma_g s_{gl,m}^\dagger + F_{gl,m}^\dagger, \quad (3; 3)$$

$$\dot{s}_{el,m}^\dagger = ig_1 r_{al,m}^\dagger s_{gl,m}^\dagger r_{bl,m} - \gamma_e s_{el,m}^\dagger + F_{el,m}^\dagger, \quad (3; 4)$$

$$\dot{B}_l^\dagger = ig_2 \sum_m r_{bl-1,m}^\dagger r_{al,m} - \gamma_l B_l^\dagger + F_l^\dagger + i \sum_{l'} J_{ll'} B_{l'}^\dagger. \quad (3; 5)$$

## IV. SOLUTIONS

To get an overview over the behavior of our molecular robots, we take the expectation values with respect to coherent states. This allows us to ignore the fluctuating forces, and still more important, to replace all operators by ordinary time-dependent variables. First we treat the motion of a single robot molecule so that (at least in most cases) we drop the robot index "m". We have found two types of solutions:

- 1) "Grass fire",
- 2) Running waves.

### A. "Grass fire" solution

We solve the equations (3; 1)-(3; 5) in a self-consistent way by iteration starting from position  $l = 1$  and assume  $B_l^\dagger$  as given. Because of the relatively long life-time of the ground state and excited state of the substrate molecules we may assume  $\gamma_e = \gamma_g = 0$ . Furthermore we assume  $\gamma_a = \gamma_b = \gamma$ . According to steps "a"  $\rightarrow$  "b" and "b"  $\rightarrow$  "a" we subdivide to solutions to equations (3; 1) - (3; 4) into two steps.

**Step I:** "a"  $\rightarrow$  "b";  $r_{al}^\dagger \rightarrow r_{bl}^\dagger, t_l \rightarrow t_{l+1}$ .

In equation (3; 1) we put  $r_{bl-1}^\dagger = 0$  because it has damped out. In equation (3; 2) we set  $r_{al+1}^\dagger = 0$  because the excitation has not yet reached the site  $l+1$ . Under these assumptions and the initial conditions ( $t = t_l$ ):

$$r_{al}^\dagger = 1, r_{bl}^\dagger = 0, s_{el}^\dagger = 1, s_{gl}^\dagger = 0, \quad (4; 1)$$

equations (3; 1)-(3; 4) can be solved exactly:

$$s_{el}^\dagger = \cos G(t), s_{gl}^\dagger = i \sin G(t), \quad (4; 2)$$

$$r_{al}^\dagger = \cos f e^{-\gamma t}, r_{bl}^\dagger = \sin f e^{-\gamma t}. \quad (4; 3)$$

(For sake of simplicity we have put  $t_l = 0$ ).

Terms  $G$  and  $f$  obey the coupled equations

$$\dot{f} = \frac{1}{2} g_1 \sin(2G), \dot{G} = \frac{1}{2} g_1 \sin(2f) e^{-2\gamma t}. \quad (4; 4)$$

For  $\gamma$  small, in lowest approximation we may put  $f = \pm G$  and solve the now resulting single equation explicitly

$$\text{tg}(G(t)) = \text{tg}G(t_k) \exp\{-(g_1(t - t_k))\}. \quad (4; 5)$$

**Step2:** "b"  $\rightarrow$  "a";  $r_{bl}^\dagger \rightarrow r_{al+1}^\dagger, t_{l+1} \rightarrow t_{l+2}$ .

In equation (3; 1) - (3; 4) we replace  $l$  by  $l+1$  and assume, in a self-consistent way, that  $r_{bl}^\dagger$  has not yet decayed (still present), whereas  $r_{al+2}^\dagger$  has not yet been generated. The initial conditions are ( $t = t_{l+1}$ )

$$r_{al+1}^\dagger = 0, r_{bl+1}^\dagger = 0, s_{el+1}^\dagger = 1, s_{gl+1}^\dagger = 0. \quad (4; 6)$$

The exact solutions read:

$$r_{al+1}^\dagger(t) = \int_{t_{l+1}}^t I_a(t, \tau) r_{bl}^\dagger(\tau) B_l(\tau) d\tau, \quad (4; 7)$$

$$r_{bl+1}^\dagger(t) = \int_{t_{l+1}}^t I_b(t, \tau) r_{bl}^\dagger(\tau) B_l(\tau) d\tau, \text{ where } \quad (4; 8)$$

$$I_a = i g_2 e^{-\gamma(t-\tau)} \cos(F(t) - F(\tau)), \quad (4; 9)$$

$$I_b = i g_2 e^{-\gamma(t-\tau)} \sin(F(t) - F(\tau)). \quad (4; 10)$$

Because of the sin-fluctuation in (4; 10) and thus in (4; 8) and the exponential damping, we may assume that  $r_{bl+1}^\dagger$  remains very small. This implies that the r.h.s. of equations (3; 3) and (3; 4) are practically zero so that (because of the initial conditions)

$$s_{gl+1}^\dagger \approx \text{const.} = 0, s_{el+1}^\dagger \approx \text{const.} = 1.$$

Note that without damping quantum oscillation ("ringing") will occur.

So far, we have neglected the fluctuating forces. As a detailed discussion shows they fix time and again new initial conditions that counteract between the final decay of the amplitudes between the individual steps.

Fig. 3.1 sketches the effects of step1 and step 2 mentioned above.

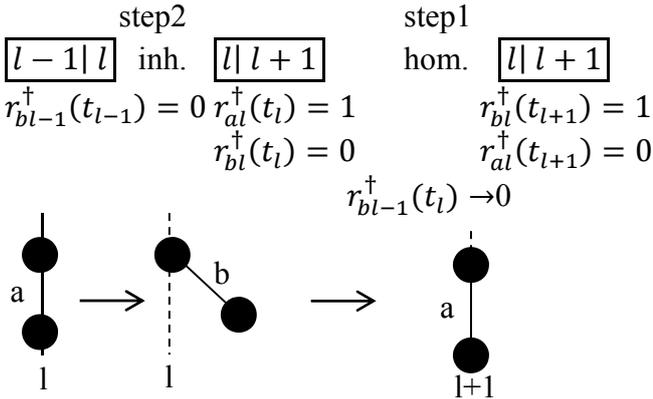


Fig. 3.1. Simplified representation of the effects of the two operator based steps in dependence of the two leg status "a" and "b". The active terms in the differential equations (3; 1) - (3; 4) define whether a homogenous or inhomogeneous solution during the performance of the two steps is used.

### B. "Grass fire" solution continued (synchronized modes)

We treat the motion of  $M$  robot molecules, labeled by an index  $m$ , running on parallel lanes and coupled by the B-field (cf. equation (3; 5)). We assume that the local B-fields are both coupled within a lane and, most importantly, across different lanes. In order not to overload our presentation and to bring out the essentials we assume that because of the coupling terms  $J_{ll'}$  in (3; 5) a single signal wave of practically infinite wavelength can be produced. This allow us to drop the indices  $k$  of  $B_l^\dagger, B_l$  everywhere in the equations (3; 1) - (3; 4). As a detailed analysis shows, equation (3; 5) must be replaced by

$$\dot{B}^\dagger = i g_2 \sum_{l,m} r_{bl-1,m}^\dagger r_{al,m} - \gamma_l B^\dagger + F^\dagger(t). \quad (4; 11)$$

As before, we take expectation values and drop  $F^\dagger$ . Under the assumption that  $B^\dagger(t)$  is a slowly varying amplitude, and that in (4; 7) we may replace  $r_{bl}^\dagger(\tau)$  by  $r_{bl}^\dagger(t)$  we may rewrite (4; 7) in the form (with appropriate indices)

$$r_{al,m}^\dagger(t) = -i g_2 B^\dagger(t) r_{bl-1,m}^\dagger(t) \int_{t-\sigma}^{t+\sigma'} I_a(t, \tau) d\tau. \quad (4; 12)$$

We insert (4; 12) into (4; 11) and add the term  $-CB^\dagger B^\dagger$  on the r.h.s. of (4; 11) in order to counteract too large amplitudes (which can be physically justified). We obtain

$$\dot{B}^\dagger(t) = AB^\dagger(t) - CB^\dagger B^\dagger, C > 0, \text{ where } \quad (4; 13)$$

$$A(t) = \sum_{l,m} a_{l,m}(t) - \gamma, \text{ and}$$

$$a_{l,m}(t) = g_2^2 |r_{bl-1,m}(t)|^2 \int_{t-\sigma}^{t+\sigma'} I_a(t, \tau) d\tau. \quad (4; 14)$$

Because we may assume the integral to be positive, we may state

$$a_{l,m} > 0 \text{ iff } |r_{bl-1,m}(t)| > 0. \quad (4; 15)$$

The r.h.s. of (4; 13) can be written as derivation of the potential

$$V = -AB^\dagger B + \frac{C}{2} (B^\dagger B)^2. \quad (4; 16)$$

To find its minimum, we put  $B^\dagger = r e^{i\varphi}$ , so that

$$V = -Ar^2 + \frac{C}{2} r^4. \quad (4; 17)$$

Its minimum lies at  $r = 0$  for  $A < 0$  and at  $r^2 = \frac{A}{C}$  for  $A > 0$ .

The B-field is maximized when

$$\sum_{l,m} a_{l,m}(t) = \text{max}. \quad (4; 18)$$

which because of (4; 14) means that all  $|r_{bl-1,m}(t)|$  must be maximal, i.e. must be synchronized, possibly up to different sites  $l$ . Note that  $r_{bl-1,m}(t)$  has a time independent phase. So it can be chosen real. This may change in case of fluctuations. Our present approach applies to *parallel* "m" lanes. If all robot molecules run only on a single lane, the substrate must be replenished quickly enough.

### C. Solution I: running waves

Our starting point is the set of equations (3; 1) - (3; 4), where we take the expectation values as  $F^\dagger = 0$  and ignore the time-dependence of the B-field, i.e. we put  $B^\dagger = B = 1$ . Again we assume  $\gamma_e = \gamma_g = 0, \gamma_a = \gamma_b = \gamma$ . We make wave like ansatz

$$r_{al}^\dagger = \varrho_a^\dagger(t) e^{iKl}, r_{bl}^\dagger = \varrho_b^\dagger(t) e^{-\gamma t} e^{iKl}. \quad (4; 19)$$

$$s_{gl}^\dagger = S_g(t) e^{iKl}, s_{el}^\dagger = S_e(t) e^{iKl}. \quad (4; 20)$$

Inserting (4; 19) and (4; 20) in (3; 1) and (3; 2) yields

$$\dot{\rho}_a^\dagger = iQe^{i\varphi}q_b^\dagger, \dot{\rho}_b^\dagger = iQe^{-i\varphi}q_a^\dagger, \text{ where} \quad (4; 21)$$

$$Qe^{i\varphi} = (g_1S_eS_g^\dagger + g_2e^{-iK}), Q \text{ and } \varphi \text{ are real.} \quad (4; 22)$$

We assume, in a self-consistent way  $\dot{\varphi} = 0$ . This allows us to satisfy equation (4; 21) by means of the ansatz

$$q_a^\dagger(t) = e^{\pm iF(t)}\rho_0, q_b^\dagger(t) = \pm e^{\pm iF(t)}e^{-i\varphi}\rho_0, \quad (4; 23)$$

where

$$F(t) = \int_0^t Q(\tau)d\tau; \rho_0 \text{ real, } \dot{\rho}_0 = 0. \quad (4; 24)$$

Inserting (4; 19) and (4; 20), with (4; 23) in (3; 3) and (3; 4) yields

$$\dot{S}_g^\dagger = ig_1\rho_0^2e^{i\varphi}e^{-2\gamma t}S_e^\dagger \quad (4; 25)$$

$$\dot{S}_e^\dagger = ig_1\rho_0^2e^{-i\varphi}e^{-2\gamma t}S_g^\dagger. \quad (4; 26)$$

The solutions to (4; 25) and (4; 26) read

$$S_g^\dagger = e^{iU}e^{i\varphi}S_0^\dagger, S_e^\dagger = e^{iU}S_0^\dagger, \text{ where} \quad (4; 27)$$

$$U = \int_0^t g_1e^{-2\gamma\tau}\rho_0^2d\tau, \quad (4; 28)$$

where again  $\dot{\varphi} = 0$  holds.

Insertion of (4; 27) in (4; 22) yields, after a small rearrangement of terms

$$g_1|S_0|^2 - Q + g_2e^{-i(K+\varphi)} = 0, \quad (4; 29)$$

from which we conclude

$$\varphi = -K, Q = g_1|S_0|^2 + g_2. \quad (4; 30)$$

The initial values  $S_0^\dagger$  and  $\rho_0^\dagger$  can be arbitrarily chosen. An equivalent solution is given by replacing  $F(t)$  by  $-F(t)$ .

Taking the space and time dependence of the solutions together we clearly deal with (damped) running waves – a typical quantum phenomenon.

#### D. Solution II: running waves. Impact of a dynamical signal field

In the preceding section we have put  $B = 1$ , i.e. we treated the signal field as externally given. Now we study what happens if the B-field is generated by the molecular robot. To get some insight, we assume that the coupling constant  $g_2$  is small, but  $g_1$  large. This allows us to treat terms proportional to  $g_2$  as small perturbations. We will show that in this approximation the wave-character of the robot-field is retained even if the interaction robot-field is switched on. (Actually, the precise condition is  $|\gamma_2/\gamma_1|^2 \ll 1$ ).

Again, our starting point is the set of equations (3; 1) – (3; 4), where we take expectation values and put  $F^\dagger = 0$ . We assume  $\gamma_e = \gamma_g = 0, \gamma_a = \gamma_b = \gamma$ .

To take into account the interaction term  $J_{ll}$  in (3; 5), we transform (3; 5) to running waves, but keep only the infinite wave-length amplitude. This implies that (3; 5) is replaced by

$$\dot{B}^\dagger = i\sum_l g'_2 r_{bl-1}^\dagger r_{al} - \gamma_B B^\dagger \quad (4; 31)$$

with a new  $g'_2$  and  $F_l^\dagger$  dropped. We keep the wave-like ansatz (4; 19), (4; 20), which we insert in (3; 1) and (3; 2). But now, we write the resulting equation in a form different from (4; 21):

$$\dot{\rho}_a^\dagger = ig_1\tilde{Q}\rho_b^\dagger + ig_2\rho_b^\dagger e^{-iK}B, \quad (4; 32)$$

$$\dot{\rho}_b^\dagger = ig_1\tilde{Q}^*\rho_a^\dagger + ig_2\rho_a^\dagger e^{iK}B, \quad (4; 33)$$

$$\text{where } \tilde{Q} = S_eS_g^\dagger. \quad (4; 34)$$

Inserting (4; 19), (4; 20) in (3; 3), (3; 4) yields

$$\dot{S}_g^\dagger = ig_1GS_e^\dagger, \dot{S}_e^\dagger = ig_1G^*S_g^\dagger, \quad (4; 35)$$

where

$$G = \rho_a^\dagger\rho_b e^{-2\gamma t}. \quad (4; 36)$$

In the equations (4; 32), (4; 33), (4; 35) we treat the terms  $\alpha g_2$  as small perturbations. In the spirit of perturbation theory we put

$$\rho_a^\dagger = \bar{\rho}_a^\dagger + \varepsilon_a^\dagger, \rho_b^\dagger = \bar{\rho}_b^\dagger + \varepsilon_b^\dagger, \quad (4; 37)$$

$$\tilde{Q} = \bar{Q} + q, \quad (4; 38)$$

$$S_g^\dagger = \bar{S}_g^\dagger + \eta_g^\dagger, S_e^\dagger = \bar{S}_e^\dagger + \eta_e^\dagger, \quad (4; 39)$$

$$G = \bar{G} + g. \quad (4; 40)$$

We assume that all quantities indicated by a bar  $\bar{\phantom{x}}$ , obey the unperturbed equations with  $g_2 = 0$ . This allows us to use the solutions of the preceding section (with  $g_2 = 0$ ). As a closer inspection shows, the essential behavior can be revealed when we take just the  $\dagger$  sign solution (4; 23), which we write

$$\bar{\rho}_a^\dagger = e^{iF(t)}\rho_0, \bar{\rho}_b^\dagger = e^{iF(t)}\rho_0, \quad (4; 41)$$

where now

$$F(t) = \int_0^t g_1\bar{Q}(\tau)d\tau \quad (4; 42)$$

$$\text{and } \bar{Q}(\tau) = S_0^2, \text{ with } S_0 \text{ real, arbitrary.} \quad (4; 43)$$

Note that we have put  $\varphi = 0$  in a self-consistent manner. By use of (4; 27), (4; 28) we find the unperturbed solutions as

$$\bar{S}_g^\dagger = e^{iU}S_0, \bar{S}_e^\dagger = e^{iU}S_0 \text{ and} \quad (4; 44)$$

$$U = \int_0^t g_1e^{-2\gamma\tau}\rho_0^2d\tau.$$

Now we study the impact of the perturbations  $\alpha g_2$ . We insert (4; 37) and (4; 38) in (4; 32) and (4; 33) and compare terms linear in  $g_2$ . Thus we obtain

$$\varepsilon_a^\dagger = ig_1\bar{Q}\varepsilon_b^\dagger + ig_1\bar{\rho}_b^\dagger q + i\bar{\rho}_b^\dagger e^{-iK}B, \quad (4; 46)$$

$$\varepsilon_b^\dagger = ig_1\bar{Q}\varepsilon_a^\dagger + ig_1\bar{\rho}_a^\dagger q^* + i\bar{\rho}_a^\dagger e^{iK}B^\dagger. \quad (4; 47)$$

To treat these equations further, we have to derive an explicit expression for  $q$ . To this end, we insert (4; 39) in (4; 38) and obtain

$$\tilde{Q} \approx \bar{Q} + \eta_e\bar{S}_g^\dagger + \bar{S}_e\eta_g^\dagger = \bar{Q} + q, \quad (4; 48)$$

which fixes  $q$ .

Clearly, now we need equations for  $\eta_e, \eta_g^\dagger$ . To derive these equations we insert (4; 39), (4; 40) in (4; 35) and (4; 36) to obtain, in an obvious way:

$$\dot{\eta}_g^\dagger = ig_1\bar{G}\eta_e^\dagger + ig_1g\bar{S}_e^\dagger, \quad (4; 49)$$

$$\dot{\eta}_e^\dagger = ig_1\bar{G}\eta_g^\dagger + ig_1g^*\bar{S}_g^\dagger. \quad (4; 50)$$

To derive an explicit expression for  $g$ , we insert (4; 37) in (4; 38) and obtain

$$G = e^{-2\gamma t}(\bar{\rho}_a^\dagger\bar{\rho}_b + \varepsilon_a^\dagger\bar{\rho}_b + \varepsilon_b\bar{\rho}_a^\dagger) + \text{h.a.} \quad (4; 51)$$

so that

$$g = e^{-2\gamma t}(\varepsilon_a^\dagger\bar{\rho}_b + \varepsilon_b\bar{\rho}_a^\dagger). \quad (4; 52)$$

By means of (4; 46), (4; 47) with (4; 48) and of (4; 49), (4; 50) with (4; 52), we are in a position to write down the complete set of equations. They read

$$\begin{aligned} \dot{\varepsilon}_a^\dagger &= ig_1 S_0^2 \varepsilon_b^\dagger + ig_1 \rho_0 e^{iF} (\eta_e e^{iU} S_0 + \eta_g^\dagger e^{-iU} S_0) + \\ &ig_2 e^{iF} \rho_0 e^{-iK} B, \end{aligned} \quad (4; 53)$$

$$\begin{aligned} \dot{\varepsilon}_b^\dagger &= ig_1 S_0^2 \varepsilon_a^\dagger + ig_1 \rho_0 e^{iF} (\eta_e^\dagger S_0 e^{-iU} + \eta_g e^{iU} S_0) + \\ &ig_2 \rho_0 e^{iF} e^{iK} B^\dagger, \end{aligned} \quad (4; 54)$$

$$\dot{\eta}_g^\dagger = ig_1 e^{-2\gamma t} (\rho_0^2 \eta_e^\dagger + \rho_0 e^{-iF} \varepsilon_a^\dagger + \rho_0 e^{iF} \varepsilon_b), \quad (4; 55)$$

$$\dot{\eta}_e^\dagger = ig_1 e^{-2\gamma t} (\rho_0^2 \eta_g^\dagger + \rho_0 e^{iF} \varepsilon_a + \rho_0 e^{-iF} \varepsilon_b^\dagger). \quad (4; 56)$$

We are confronted with the task of solving the four coupled equations (4; 53) - (4; 56), with *time-dependent* coefficients, for the variables  $\varepsilon_a^\dagger$ ,  $\varepsilon_b^\dagger$ ,  $\eta_e^\dagger$ ,  $\eta_g^\dagger$  and their complex conjugates. These equations can be solved on a computer. For our present purpose it suffices to discuss the solution in quite good an approximation. To the end we assume that  $S_0 \approx \rho_0$  of order unity,  $g_1 > 0$  large and  $\gamma$  small. We discuss equations (4; 53) and (4; 54) in the spirit of the rotating wave approximation, well known, e.g., in spin resonance. Because of the form of  $F(t)$  and  $U(t)$ , in equations (4; 53) and (4; 54) we may neglect the rapidly oscillating terms  $e^{i(F+U)}$  (large  $g_1!$ ) against the slowly varying terms  $e^{i(F-U)}$  (because  $S_0 \approx \rho_0$  and  $\gamma$  small). Equations (4; 53) and (4; 54) thus reduce to

$$\dot{\varepsilon}_a^\dagger = ig_1 S_0^2 \varepsilon_b^\dagger + ig_1 \rho_0 e^{i(F-U)} \eta_g^\dagger S_0 + ig_2 e^{iF} \rho_0 e^{-iK} B, \quad (4; 57)$$

$$\dot{\varepsilon}_b^\dagger = ig_1 S_0^2 \varepsilon_a^\dagger + ig_1 \rho_0 e^{i(F-U)} \eta_a^\dagger S_0 + ig_2 e^{iF} \rho_0 e^{iK} B^\dagger \quad (4; 58)$$

We discuss the solutions to (4; 55) - (4; 58) in the spirit of a self-consistency approach. In a first step, in each of the equations (4; 55) - (4; 58) we interpret the l.h.s. and the *first* term on the r.h.s. as homogeneous part and the rest on the r.h.s. as inhomogeneity.

According to the theory of ordinary differential equations, a particular solution to (4; 57) and (4; 58) is given by

$$\begin{aligned} \left. \begin{aligned} \varepsilon_a^\dagger \\ \varepsilon_b^\dagger \end{aligned} \right\} &= e^{iF(t)} \int_0^t e^{-iF(\tau)} \frac{1}{2} (I_a(\tau) + I_b(\tau)) d\tau \\ &\pm e^{-iF(t)} \int_0^t e^{iF(\tau)} \frac{1}{2} (I_a(\tau) - I_b(\tau)) d\tau \end{aligned} \quad (4; 59)$$

where, up to an unimportant term,  $I_a$  and  $I_b$  are given by

$$I_a(\tau) = ig_2 e^{iF(\tau)} \rho_0 e^{-iK} B(\tau) \quad (4; 60)$$

$$I_b(\tau) = ig_2 e^{iF(\tau)} \rho_0 e^{iK} B^\dagger(\tau). \quad (4; 61)$$

For further discussion of (4; 59), we need the explicit form of  $B$ ,  $B^\dagger$  which follows from equation (4; 31). Again, we need only a typical solution (4; 31). Inserting (4; 19) in the r.h.s. of (4; 31) we obtain in leading approximation

$$\dot{B}^\dagger = i \sum_l g'_2 e^{-iK} e^{-2\gamma t} \bar{\rho}_b^\dagger \bar{\rho}_a - \gamma_B B^\dagger, \quad (4; 62)$$

where, according to (4; 41),  $\bar{\rho}_b^\dagger \bar{\rho}_a$  is time-independent. The wanted solution reads

$$B^\dagger = i e^{-iK} C \frac{1}{\gamma_B - \gamma} (e^{-\gamma t} - e^{-\gamma_B t}), \quad (4; 63)$$

where

$$C = \sum_l g'_2 \bar{\rho}_b^\dagger \bar{\rho}_a \quad (4; 64)$$

is a real, positive constant.

Now, and finally, we are in a position to discuss the solution (4; 59), again in the spirit of a rotating wave approximation. Inserting  $B$  and  $B^\dagger$  in (4; 60) and (4; 61) yields

$$I_a(\tau) = g_2 C \rho_0 e^{iF(\tau)} \frac{1}{\gamma_B - \gamma} (e^{-\gamma \tau} - e^{-\gamma_B \tau}), \quad (4; 65)$$

and

$$\begin{aligned} I_b(\tau) &= -g_2 C \rho_0 e^{iF(\tau)} \frac{1}{\gamma_B - \gamma} (e^{-\gamma \tau} - e^{-\gamma_B \tau}) \\ &= -I_a(\tau). \end{aligned} \quad (4; 66)$$

While, clearly, the first integral in (4; 59) vanishes because of (4; 66), the second becomes very small in the limit  $g_1$  large because of the exponential function

$$e^{2iF(\tau)} \quad (4; 67)$$

in the integrand.

In conclusion we may state that in the leading approximation  $\varepsilon_a^\dagger$  and  $\varepsilon_b^\dagger$  are vanishing small, i.e. the coupling of the robot to the field has practically no impact on the original quantum wave. In how things change when  $g_2$  becomes of the same order or even larger than  $g_1$  must be left unanswered.

## V. CONCLUSION

In our paper we have presented fully quantum mechanical equations based on a version of quantum field theory that allows us to take into account the effects of the molecular environment leading to damping, energy transfer and fluctuating forces representing both thermal and, still more important, quantum noise. Our equations can be interpreted as a quantum mechanical analogue to classical nonlinear stochastic differential equations of the (generalized) Langevin-type

As we have shown, our approach provides us with new insights which go beyond a purely classical treatment. For instance we obtain not only "grass fire" solutions but also quantum waves. Our approach includes the study of cooperative effects among mobile molecular robots. By means of a support of the substrate molecules, e.g. by semi-conductor devices (i.e. by a hybrid system), the behavioral patterns of the mobile robots can be influenced.

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