# QUANTUM FLUCTUATIONS OF ELEMENTARY EXCITATIONS IN DISCRETE MEDIA

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Elementary excitations (electrons, holes, polaritons, excitons, plasmons, spin waves, etc.) on discrete substrates (e.g., polymer chains, surfaces, and lattices) may move coherently as quantum waves (e.g., Bloch waves), but also incoherently ("hopping") and may lose their phases due to their interaction with their substrate, for example, lattice vibrations. In the frame of Heisenberg equations for projection operators, these latter effects are often phenomenologically taken into account, which violates quantum mechanical consistency, however. To restore it, quantum mechanical fluctuating forces (noise sources) must be introduced, whose properties can be determined by a general theorem. With increasing miniaturization, in the nanotechnology of logical devices (including quantum computers) that use interacting elementary excitations, such fluctuations become important. This requires the determination of quantum noise sources in composite quantum systems. This is the main objective of my paper, dedicated to the memory of Ilya Prigogine.

## 1. Introduction

Thermodynamics impresses us again and again by its great generality. Its laws apply to all kinds of matter and all kinds of aggregations (provided the systems are in or close to thermal equilibrium). Thus it is no surprise that Ilya Prigogine, who was a master in thermodynamics and its applications to physical and chemical processes, used thermodynamics as a starting point for his explorations into the fascinating field of open systems with their ability to form dissipative structures. This is witnessed for instance by his books jointly with Glansdorff [2] as well as with Nicolis [5]. An excellent account of various approaches to the physics of open nonequilibrium systems can be found in the book by Babloyantz [1]. In fact, as it happens quite often in science, a new field may be explored from several starting positions. Thus in the field of nonequilibrium processes, my own approach was based on quantum field theory and quantum statistics. The present paper, that I dedicate to the memory of Ilya Prigogine, is a late outflow of my early steps in quantum statistics of systems away from thermal equilibrium. My paper is also motivated by


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the progress made in information technology, and here again especially in nanotechnology. So far, information processing is based on logical elements that use large numbers of elementary excitations such as electrons so that quantum fluctuations can be ignored, at least in many cases. With increasing miniaturization, however, the quantum domain becomes important and thus quantum fluctuations can no more be ignored. Therefore, my contribution tries to show how quantum fluctuations can be calculated in a unique way for all kinds of elementary excitations and their interactions that may be used in logical elements (devices).

## 2. Elementary excitations

The formalism I am going to develop in this paper is applicable to electrons, holes, excitons (Wannier, Frenkel), plasmons, spin waves, and so forth. They may be delocalized or localized, for example, at quantum dots. In the following, I will base the analysis on localized states from which running elementary excitations can be built up by means of suitable superpositions. In order to realize logical elements characterized by their truth table, one may start from rate equations for electron densities that are for instance of the typical form

$$\frac{dn}{dt} = p(n) - l(n), \tag{2.1}$$

where $p$ and $l$ represent gain and losses, respectively. A truth table for the logical operation "and" can be realized by

$$\frac{dn_r}{dt} = \alpha n_1 n_2 - \kappa n_r, \tag{2.2}$$

where $n_1$ and $n_2$ are incoming currents of the channels 1 and 2, and $n_r$ is the resulting occupation number in the outflow. Quite clearly, $n_r$ can be produced only if both $n_1$ and $n_2$ are unequal to zero. When we proceed to small particle numbers, quantum fluctuations will play an important role and the obvious question arises how we can replace the phenomenological rate equations (2.2) by fully quantum mechanical equations.

## 3. General approach

Here I will proceed in two steps. First, I will consider a single quantum system with levels $i = 1, \dots, N$, and later composite quantum systems. We describe its dynamics by means of projection operators $P_{ij}$ that project the system from state $j$ to state $i$. If we wish to use creation and annihilation operators for particles, we may represent $P_{ij}$ in the form $a_i^+ a_j$, where $a^+, a$ are the creation and annihilation operators, respectively. The use of $P$ is more general because it implies that we are dealing with elementary excitations, for instance, with polarons that are electrons surrounded by their ionic cloud. The same remark holds for other elementary excitations. If not otherwise stated, we have localized states in mind. In the following, we use the fundamental quantum mechanical property of projection operators

$$P_{ij} P_{lk} = \delta_{jl} P_{ik}. \tag{3.1}$$

Our approach will be based on the Heisenberg equations of motion that are in the form

$$\frac{dP_{ij}}{dt} = \frac{i}{\hbar}[H, P_{ij}] \equiv \frac{i}{\hbar}(HP_{ij} - P_{ij}H), \tag{3.2}$$

where $H$ represents the Hamiltonian. Most importantly in all practical applications, especially in nonequilibrium systems, the quantum system under consideration is coupled to reservoirs that give rise to damping and pumping and perhaps other incoherent effects. Thus it is absolutely necessary for a complete description to include these reservoirs. As can be shown, these reservoirs with their numerous variables can be eliminated, which gives rise to projection operator equations in the Heisenberg form but with additional terms:

$$\frac{dP_{ij}}{dt} = \frac{i}{\hbar}[H, P_{ij}] + L_{r,ij}. \tag{3.3}$$

The detailed derivation of the operator $L_{r,ij}$ may be tedious, but another approach has turned out to be successful. Namely, the damping and pumping terms, and so forth, can be introduced in a phenomenological manner as I will show by means of an example. The quantum statistical average over $P_{ii}$ can be interpreted as particle number at point $i$:

$$\bar{P}_{ii} = n_i. \tag{3.4}$$

Then in a phenomenological way, one may describe the hopping process of that particle along a chain with sites $i$ by means of the rate equations

$$\frac{dn_i}{dt} = -\gamma n_i + w(n_{i+1} + n_{i-1}). \tag{3.5}$$

This is, however, a quantum statistically averaged equation where the quantum fluctuations have been lost. Our main purpose will be to restore the quantum mechanical consistency as expressed by (3.1). Another example is provided by the coherent motion along a chain where the Hamiltonian can be described by

$$H = \sum_{lm} w_{lm} P_{lm}. \tag{3.6}$$

The Heisenberg equation of motion reads

$$\frac{dP_{ij}}{dt} = \frac{i}{\hbar}\left(\sum_{l} w_{li} P_{lj} - \sum_{m} w_{jm} P_{im}\right) + L_{r,ij}, \tag{3.7}$$

where we have used the property

$$[P_{lm}, P_{ij}] = \delta_{mi} P_{lj} - \delta_{jl} P_{im} \tag{3.8}$$

that derives from (3.1). The additional operator $L_{r,ij}$ stems from incoherent processes due to the interaction with reservoirs such as lattice vibrations. Taking only the nearest neighbour interaction in a linear chain into account, (3.7) can be evaluated as

$$\frac{dP_{ij}}{dt} = \frac{i}{\hbar}\left(w_{i+1,i}P_{i+1,j} + w_{i-1,i}P_{i-1,j} - w_{j,j+1}P_{i,j+1} - w_{j,j-1}P_{i,j-1}\right) + L_{r,ij}. \tag{3.9}$$

Again the incoherent processes can be incorporated in addition to the coherent processes determined by the Hamiltonian (3.6) by choosing

$$\bar{L}_{r,ii} = -2W\bar{P}_{ii} + W\bar{P}_{i+1,i+1} + W\bar{P}_{i-1,i-1} \quad \text{for } i = j, \tag{3.10}$$

$$\bar{L}_{r,ij} = -\gamma\bar{P}_{ij} \quad \text{for } i \neq j. \tag{3.11}$$

Equation (3.11) describes phase-destroying processes. In order to restore quantum mechanical consistency, we have to add fluctuating forces $\Gamma_{ij}$ so that the total Heisenberg equations acquire the form

$$\frac{dP_{ij}}{dt} = \frac{i}{\hbar}\left[H, P_{ij}\right] + \bar{L}_{r,ij} + \Gamma_{ij}(t), \tag{3.12}$$

where, however, in the second term on the right-hand side the averaged $\bar{P}$ is to be replaced by $P$. We now turn to the explicit determination of the fluctuating forces $\Gamma$.

### 4. Haken-Weidlich theorem [3, 4]

We denote quantum statistical averages by square brackets. We assume that, for instance, the following averaged equations are given phenomenologically or partly phenomenologically and partly from first principles:

$$\frac{d\langle P_{ij}\rangle}{dt} = \sum_{kl}\langle M_{ij,kl}P_{kl}\rangle, \tag{4.1}$$

where the elements $M$ do not depend on $P$, but may depend on variables of other quantum systems. As one may show, the solutions to (4.1) do not obey the quantum mechanical consistency relations (3.1). To restore quantum mechanical consistency, we introduce the equation

$$\frac{dP_{ij}}{dt} = \sum_{kl} M_{ijkl}P_{kl} + \Gamma_{ij}(t). \tag{4.2}$$

We assume that the averages vanish:

$$\langle\Gamma_{ij}(t)\rangle = 0, \tag{4.3}$$

and that the fluctuating forces are $\delta$-correlated in time:

$$\langle\Gamma_{ij}(t)\Gamma_{kl}(t')\rangle = G_{ij,kl}\delta(t-t'). \tag{4.4}$$

This is the only assumption to be made in the present context. In many cases, it is fulfilled if for instance the reservoirs are broadband or the relaxation time of the fluctuating forces is short compared to that of all other processes in the system. The Haken-Weidlich theorem states that the strength of the fluctuating forces is uniquely determined by

$$G_{ij,kl} = \sum_{mn} \langle (\delta_{jk} M_{il,mn} - \delta_{nl} M_{ij,mk} - \delta_{mi} M_{kl,jn}) P_{mn} \rangle. \tag{4.5}$$

As a comparison with Section 3, for example (3.3), $M$ may be decomposed into

$$M_{ij,kl} = M^{(1)}_{ij,kl} + M^{(2)}_{ij,kl}, \tag{4.6}$$

where $M^{(1)}$ stems from $i/\hbar[H, P_{ij}]$. As can be shown, the terms $M^{(1)}$ cancel each other so that it is sufficient to determine the strengths of the fluctuating forces by using $M^{(2)}$ instead of $M$ in (4.5). We illustrate our result by means of an example that is self-explanatory:

$$\begin{gathered}
\frac{d\langle P_{ij}\rangle}{dt} = -\gamma_{ij}\langle P_{ij}\rangle, \quad i \neq j, \\
M_{ijkl} = -\gamma_{ij}\delta_{ik}\delta_{jl}, \quad i \neq j, \\
\frac{d\langle P_{ii}\rangle}{dt} = -2W\langle P_{ii}\rangle + W\langle P_{i+1,i+1}\rangle + W\langle P_{i-1,i-1}\rangle, \quad i = j, \\
M_{ii,ii} = -2W, \qquad M_{ii,i+1,i+1} = W, \qquad M_{ii,i-1,i-1} = W.
\end{gathered} \tag{4.7}$$

## 5. Composite quantum systems

Logical elements are realized by means of the interaction or transformations of different quantum systems as can be seen, for example, from (2.2). We must observe, however, that such relations can be translated into quantum mechanics in several ways depending on the experimental setup. For instance, the particle numbers can be translated into particle number operators according to

$$n_l^j \longrightarrow P_{1,1}^j, \tag{5.1}$$

but they can also be translated into probability amplitudes according to

$$n^j \longrightarrow b_j, \tag{5.2}$$

where $b_j$ is an annihilation operator of a particle of the kind $j$. In the latter case, the interaction stems from the Hamiltonian of the form

$$H = g b_r^+ b_1 b_2 + g^* b_2^+ b_1^+ b_r, \tag{5.3}$$

and the annihilation operators must be translated into projection operators according to

$$b_j \longrightarrow P_{0,1}^j. \tag{5.4}$$

The details of these translations will be published elsewhere. Here, however, we want to concentrate on the central issue, namely, how to generalize the Haken-Weidlich theorem to composite quantum systems. This requires the introduction of the appropriate multiplication rules of projection operators. First, we adopt the already known rule

$$P^1_{ij}P^1_{kl} = \delta_{jk}P^1_{il}, \tag{5.5}$$

where the upper index $l$ refers to the specific subsystem. Similarly we have

$$P^2_{ij}P^2_{kl} = \delta_{jk}P^2_{il}. \tag{5.6}$$

However, what is new is the relation for the composite system given by

$$P^1_{ij}P^2_{kl} = P^0_{ik,jl}. \tag{5.7}$$

From (5.5), (5.6), and (5.7), we may deduce the following multiplication rules:

$$P^1_{ij}P^0_{i'k',j'l'} \equiv P^1_{ij}P^1_{i',j'}P^2_{k'l'} = \delta_{ji'}P^0_{ik',j'l'}, \tag{5.8}$$

$$P^2_{ij}P^0_{i'k',j'l'} = P^2_{ij}P^1_{i'j'}P^2_{k'l'} = \delta_{jk'}P^0_{i'i,j'l'}, \tag{5.9}$$

$$P^0_{ij,kl}P^0_{i'j',k'l'} = P^1_{ik}P^2_{jl}P^1_{i'k'}P^2_{j'l'} = \delta_{ki'}\delta_{lj}P^0_{ijk'l'}. \tag{5.10}$$

For the following, we need a concise notation so that we introduce the following abbreviations: $P^K_{\underset{\sim}{i},\underset{\sim}{j}}$ for $K = 1$, $\underset{\sim}{i} = 1$, and $\underset{\sim}{j} = j$; for $K = 2$, $\underset{\sim}{i} = 1$, and $\underset{\sim}{j} = j$; and for $K = 0$, $\underset{\sim}{i} = i_1 i_2$, and $\underset{\sim}{j} = j_1 j_2$. With its help, we can cast the relations (5.5), (5.6), (5.7), (5.8), (5.9), and (5.10) in the concise form

$$P^K_{\underset{\sim}{i},\underset{\sim}{j}}P^L_{\underset{\sim}{i}',\underset{\sim}{j}'} = h^{KLV}_{\underset{\sim}{i},\underset{\sim}{j};\underset{\sim}{i}',\underset{\sim}{j}';\underset{\sim}{i}'',\underset{\sim}{j}''} \cdot P^V_{\underset{\sim}{i}''\underset{\sim}{j}''}, \tag{5.11}$$

where, for instance, if $(K,L) = 1,1$, $h^{111}_{ij,i'j',i''j''} = \delta_{ji'}\delta_{i''i}\delta_{j'j''}$ holds. The basic idea is now similar to that of Section 4. We assume that the averaged equations

$$\frac{d}{dt}\left\langle P^K_{\underset{\sim}{i},\underset{\sim}{j}}\right\rangle = \left\langle \sum_{\underset{\sim}{k},\underset{\sim}{l},L} M^{KL}_{\underset{\sim}{i}\underset{\sim}{j},\underset{\sim}{k}\underset{\sim}{l}}P^L_{\underset{\sim}{k}\underset{\sim}{l}}\right\rangle, \tag{5.12}$$

that may be either based on Hamiltonians and phenomenologically added incoherent terms, or containing only incoherent terms, are given. We want to convert these equations into quantum mechanically consistent equations by adding fluctuating forces

$$\frac{d}{dt}P^K_{\underset{\sim}{i},\underset{\sim}{j}} = \sum_{\underset{\sim}{k},\underset{\sim}{l},L} M^{KL}_{\underset{\sim}{i}\underset{\sim}{j},\underset{\sim}{k}\underset{\sim}{l}}P^L_{\underset{\sim}{k}\underset{\sim}{l}} + \Gamma^L_{\underset{\sim}{i}\underset{\sim}{j}}. \tag{5.13}$$

We lump the projection operators together to a state vector

$$A = \begin{pmatrix} P^{(1)} \\ P^{(2)} \\ P^{(0)} \end{pmatrix} \tag{5.14}$$

that has to obey equations that we write in the form

$$\frac{dA}{dt} = MA + \Gamma. \tag{5.15}$$

The formal solution of (5.15) reads

$$A = \int^{t} G(t,\tau)\Gamma(\tau)d\tau + A_h, \tag{5.16}$$

where $G$ is the Green's function with the property

$$G(t,t) = E \tag{5.17}$$

and $A_h$ a solution to the homogeneous equation (5.15). We consider

$$\langle \tilde{A}BA \rangle = \left\langle \left( \int^{t} \tilde{\Gamma}(\tau)\tilde{G}(t,\tau)d\tau + \tilde{A}_h \right) B \left( \int^{t} G(t,\tau')\Gamma(\tau')d\tau' + A_h \right) \right\rangle, \tag{5.18}$$

where the tilde refers to the transposed matrix or transposed vector $\tilde{A}, \tilde{B}$, and so forth. We have introduced a matrix $B$ in the form

$$B = \begin{pmatrix} B^{11} & B^{12} & B^{10} \\ B^{21} & B^{22} & B^{20} \\ B^{01} & B^{02} & B^{00} \end{pmatrix}, \tag{5.19}$$

where each submatrix is further labelled by means of indices $I = \underset{\sim}{i}, \underset{\sim}{j}$, where eventually we will choose only one nonvanishing element. Because of (5.11), we obtain for the left-hand side of (5.15)

$$\langle P_I^K B_{IJ}^{KL} P_J^L \rangle = B_{IJ}^{KL} \langle P_I^K P_J^L \rangle = B_{IJ}^{KL} h_{I,I',I''}^{KLV} \langle P_{I''}^V \rangle. \tag{5.20}$$

Taking the derivative with respect to time, we then obtain for the left-hand side of (5.18) the relation

$$\frac{d}{dt} \langle P_I^K B_{IJ}^{KL} P_J^L \rangle = B_{IJ}^{KL} h_{I,I',I''}^{KLV} \sum_{J,W} \langle M_{I''J}^{VW} P_J^W \rangle. \tag{5.21}$$

After differentiation, the right-hand side (5.18) contains the terms

$$\left\langle \tilde{\Gamma}(t) B \left( \int_0^t G(t,\tau)\Gamma(\tau)d\tau + A_h \right) \right\rangle, \tag{5.22}$$

$$\left\langle \left( \int_0^t \tilde{\Gamma}(\tau)\tilde{G}(t,\tau)d\tau + \tilde{A}_h \right) B\Gamma(\tau) \right\rangle, \tag{5.23}$$

$$\langle \tilde{A}\tilde{M}BA \rangle, \tag{5.24}$$

$$\langle \tilde{A}\tilde{B}MA \rangle. \tag{5.25}$$

A simple analysis and using a single element of $B$ transforms (5.22) into $B_{IJ}^{KL} 1/2 G_{IJ}^{KL}$ and the same expression results from (5.23). The expression (5.25) can easily be transformed into

$$B_{IJ}^{KL}\left\langle P_I^K \sum_{NU} M_{JN}^{LU} P_N^U \right\rangle = B_{IJ}^{KL} \sum_{NU} h_{INJ'}^{KUV} \langle M_{JN}^{LU} P_{J'}^{V} \rangle. \tag{5.26}$$

Similarly, the expression $\langle (MA)^T B_{IJ}^{KL} P_J^L \rangle$ that stems from (5.24) can be transformed into

$$B_{IJ}^{KL} \sum_{I',V'} \langle M_{IJ'}^{KV'} P_{J''}^{W} \rangle h_{J'JJ''}^{V'LW}. \tag{5.27}$$

Collecting all expressions and choosing only one matrix element $B$ with its specific indices, we obtain our final result

$$\begin{aligned} G_{IJ}^{KL} = h_{I,I',I'''}^{KLV} \sum_{JW} \langle M_{I''J}^{VW} P_J^W \rangle - \sum_{NU} h_{INJ'}^{KUV} \langle M_{JN}^{LU} P_{J'}^{V} \rangle \\ - \sum_{J',V'} h_{J'JJ''}^{V'LW} \langle M_{IJ'}^{KV'} P_{J''}^{W} \rangle. \end{aligned} \tag{5.28}$$

This is the desired extension of the theorem of Section 4 to a composite quantum system.

## 6. Conclusion and outlook

Some general remarks about the applicability of our above formalism may be in order. The projection operators correspond, at least in general, to physical observables, such as occupation numbers, (complex) amplitudes, and so forth. With their help, we may calculate correlation functions of the form

$$\langle P_{I,J}^{V}(t) P_{I',J'}^{V'}(t') \rangle \tag{6.1}$$

or

$$\langle (P_{I,J}^{V}(t) - \langle P_{I,J}^{V}(t) \rangle)(P_{I',J'}^{V'}(t') - \langle P_{I',J'}^{V'}(t') \rangle) \rangle. \tag{6.2}$$

In particular, the latter form (6.2) enables us to determine the contribution of the fluctuations. We may thus determine the error made by a quantum device, for example, by a logical gate. The formalism is rather general in that it does not only apply to elementary excitations, but also to general collective states provided that they can be characterized by quantum numbers and that their generalized Heisenberg equations are known.

A final remark should be made. As our above formalism reveals, Hamiltonian quantum systems are noise free. Only when they are coupled to reservoirs that cause incoherent processes, fluctuations become manifest. Explicit examples on specific logical elements will be published elsewhere.

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