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Distributed pumped dipole systems do not admit true Bose condensations

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Abstract. Biological interest attaches to systems of coupled electric dipoles with pumping applied to the phonon modes. In certain cases known as Fröhlich systems the master equation for pumped phonon models in general is known to admit Bose condensations. It is shown, in contrast, that for the biological systems of interest a Bose condensation does not occur (though this does not rule out a generalized condensation).

1. General setting

Considerable interest in theoretical biology has been focussed on non-equilibrium systems of coupled oscillators which are claimed to form Bose condensations and so offer the possibility of establishing long-range quantum coherence at room temperature. It has been postulated that this mechanism could form the basis for consciousness (Marshall 1989) or could even constitute a 'second nervous system' (Rowlands 1983).

The basic mathematical model is as follows. We consider a heat bath B (the general cellular environment), a system S consisting of oscillators with frequencies $\omega_0, \dots, \omega_N$ (identified with the normal modes of a system of electrically coupled polar molecules such as membrane proteins), and a source of energy (or 'pump') P coupled to the system (identified with, for example, the membrane energy transfer mechanisms involved in the propagation of a nervous action potential).

A number of authors (Fröhlich 1968, Sewell 1986) have proposed for this system the master equation

$$\dot{n}_k = s_k - a_k(n_k - \mathrm{e}^{-\omega_k\beta}(n_k + 1)) - \sum_i b_{ik}(n_k(n_i + 1) - \mathrm{e}^{(\omega_i - \omega_k)\beta} n_i(n_k + 1)) \tag{1}$$

where n_k is the expectation value of the number operator for the kth mode of the system, ω_k is its frequency, β is the inverse temperature, s_k represents the rate of pumping to the mode, a_k represents the coupling to the heat bath and b_{ik} the coupling between different (first-order) modes due to nonlinearities in the classical Hamiltonian. This equation has been derived using conventional approximations by Wu and Austin (1978). The case of a Frölich system has been discussed rigorously by Duffield (1988b), who shows that the continuum limit of this equation can be derived exactly. The formation of Bose condensations in the master equation has been demonstrated in special cases by Sewell (1986), Fröhlich (1968) and Duffield (1988a).

The concept of a Bose condensation is related to the limiting form of the equilibrium solution to the master equation in the limit as the number of modes becomes infinite. Thus

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we are in effect dealing with a sequence of systems, parametrized by N, the total number of modes. We suppose that there exists a smooth density function $\rho(\omega)$ such that

$$\frac{1}{N}\begin{pmatrix}\text{number of modes with energies}\\ \text{between } \hbar\omega_1 \text{ and } \hbar\omega_2\end{pmatrix} \rightarrow \int_{\omega_1}^{\omega_2} \rho(\omega)\,\mathrm{d}\omega$$

as $N \rightarrow \infty$. We write $\mathbf{d}\omega$ for $\rho(\omega)\,\mathrm{d}\omega$, noting that a large part of what follows will also be valid in the case where $\mathbf{d}\omega$ is a general measure. We write $\hbar\omega_0$ and $\hbar\omega_1$ for the limiting values of the lowest and highest energies and suppose also that, for $\omega_{i_N} \rightarrow \omega$, $\omega_{j_N} \rightarrow \omega'$

$$\begin{aligned} &N b_{i_N j_N} \rightarrow b'(\omega', \omega) \\ &a_{i_N} \rightarrow a(\omega) \\ &s_{i_N} \rightarrow s(\omega) \end{aligned} \tag{2a}$$

where b', a, s are smooth functions.

A sequence of systems at some inverse temperature β will then be said to have an uncondensed state if the equilibrium solution tends to a smooth function n; i.e. $n_{i_N} \rightarrow n(\omega)$ in the above notation, for all i_N tending to some ω. A Bose condensation, on the other hand, is said to occur if as $N \rightarrow \infty$

$$n_0/N \rightarrow \bar{n}_0 \tag{2b}$$

a non-zero limit, while

$$\int_{\omega_0}^{\omega_1} n(\omega)\,\mathbf{d}\omega < \infty. \tag{2c}$$

If there is neither an uncondensed state nor a Bose condensation we shall refer to the situation as a generalized condensation (following Girardeau 1960, see also van den Berg *et al* 1986).

2. Condition for a condensation

First, we examine the necessary conditions for a Bose condensation actually occurring. The result derived (equation (8) below) is well known, but the proof does not seem to have appeared in print before. We suppose the existence of a Bose condensation, as specified by (2*b*), (2*c*).

Setting $k = 0$ in (1), defining $b'_{ik} = N b_{ik}$ and equating $\dot{n}_0$ to 0 gives

$$\begin{aligned} 0 = s_0 + a_0 \mathrm{e}^{-\omega_0\beta} + \frac{1}{N}\sum_{i>0} b'_{i0} \mathrm{e}^{(\omega_i-\omega_0)\beta} n_i + n_0 a_0 (\mathrm{e}^{-\omega_0\beta} - 1) \\ - \frac{1}{N}\sum_{i>0} b'_{i0} n_0 \left((n_i + 1) - \mathrm{e}^{(\omega_i-\omega_0)\beta} n_i\right). \end{aligned} \tag{3}$$

As $N \rightarrow \infty$ the first three terms tend to limits, by assumption (cf (2)). Thus dividing (3) by N and taking this limit eliminates these terms, leaving

$$0 = \bar{n}_0 \left(a(\omega_0)(\mathrm{e}^{-\omega_0\beta} - 1) - \int_{\omega_0}^{\omega_1} b'(\omega_0, \omega) n(\omega)(1 - \mathrm{e}^{(\omega-\omega_0)\beta})\,\mathbf{d}\omega - \int_{\omega_0}^{\omega_1} b'(\omega_0, \omega)\,\mathbf{d}\omega \right). \tag{4}$$

Defining

$$b(\omega,\omega') = b'(\omega,\omega')e^{\omega'\beta}$$
$$k(\omega) = s(\omega) + a(\omega)e^{-\beta\omega}$$
$$v(\omega) = \int_{\omega_0}^{\omega_1} b(\omega,\omega')e^{-\beta\omega'}\,d\omega' + a(\omega)(1-e^{-\omega\beta})$$

we write this as

$$\int_{\omega_0}^{\omega_1} b(\omega_0,\omega')n(\omega')(e^{-\beta\omega'} - e^{-\beta\omega_0})\,d\omega' + v(\omega_0) = 0. \tag{5}$$

Now take the continuum limit (2a) in the master equation (1) for equilibrium, namely $\dot{n}_k = 0$, and solve for $n(\omega)$ as

$$n(\omega) = \frac{k(\omega) + \int_{\omega_0}^{\omega_1} b(\omega,\omega')n(\omega')\,d\omega' e^{-\beta\omega} + b(\omega,\omega_0)\bar{n}_0 e^{-\beta\omega}}{\int_{\omega_0}^{\omega_1} b(\omega,\omega')n(\omega')(e^{-\beta\omega'} - e^{-\beta\omega})\,d\omega' + b(\omega,\omega_0)\bar{n}_0(e^{-\beta\omega_0} - e^{-\beta\omega}) + v(\omega)}. \tag{6}$$

Subtracting the left-hand side of (5) from the denominator of (6) gives

$$v(\omega) - v(\omega_0) + \int_{\omega_0}^{\omega_1} n(\omega')\left[b(\omega_0,\omega')(e^{-\beta\omega_0} - e^{-\beta\omega'}) - b(\omega,\omega')(e^{-\beta\omega} - e^{-\beta\omega'})\right]d\omega'$$
$$+ b(\omega,\omega_0)\bar{n}_0(e^{-\beta\omega_0} - e^{-\beta\omega}) \tag{7}$$

whose modulus is easily seen to be bounded above by $K(\omega - \omega_0)$ for some K. The numerator of (6) is clearly positive, and so for convergence of $\int_{\omega_0}^{\omega_1} n(\omega)\,d\omega$ we require

$$\int_{\omega_0}^{\omega_1} \frac{d\omega}{\omega - \omega_0} < \infty \tag{8}$$

the usual result in Bose condensations, as is stressed by, for example, Blatt (1964) and assumed by both Sewell (1986) and Fröhlich (1968).

3. Biological models

We now move on to show that the above condition is in fact not fulfilled for the systems of interest in biology, so that at best there is a generalized condensation rather than a true Bose condensation.

We consider for simplicity a system consisting of a three-dimensional distribution of polarizable dipoles, each thought of as an elastically coupled pair of charged massive particles constrained to move along an axis that is fixed for each dipole. Thus one can introduce $\boldsymbol{k}$ (a function of position) for the direction of the dipoles, $\nu\boldsymbol{k}$ the polarization per unit volume, Ω the oscillation frequency of an isolated dipole, and ν_0 the volume polarization that would be produced if all the dipoles were in the equilibrium state for an isolated dipole. Then the oscillator equation for a single dipole, in the harmonic approximation (neglecting for the time being nonlinear terms, though these will be crucial for the Fröhlich mechanism) is

$$\frac{d^2\nu}{dt^2} = \Omega^2[p\boldsymbol{k}\cdot\boldsymbol{E} - (\nu - \nu_0)]$$

where p is a constant related to the dielectric constant. The electric field $\boldsymbol{E}$ is given by

$$\boldsymbol{E} = \boldsymbol{E}_0 + \boldsymbol{E}_1 + \boldsymbol{E}_2$$
$$\nabla \cdot \boldsymbol{E}_1 = -(\boldsymbol{k} \cdot \nabla)\nu$$
$$\boldsymbol{E}_2 = \gamma \nu \boldsymbol{l}$$

in which $\boldsymbol{E}_0$ is the externally imposed field, $\boldsymbol{E}_1$ is the field due to the averaged effect of the dipoles some distance from the source, and $\boldsymbol{E}_2$ is a correction-field to take account of near neighbours. $\boldsymbol{l}$ is a fixed vector field determined by the geometry of the local distribution of the dipoles. (For details of the theory here, see Burfoot 1967.)

The equations are linear and so we can subtract off the static equilibrium solution for a given external $\boldsymbol{E}_0$. If a $'$ denotes the difference between a quantity and its equilibrium value, and we put $\boldsymbol{E}_1' = -\nabla\phi$, then

$$\frac{\mathrm{d}^2\nu'}{\mathrm{d}t^2} = \Omega^2[p\boldsymbol{k} \cdot \{-\nabla\phi + \gamma\nu'\boldsymbol{l}\} - \nu'] \tag{9}$$

$$-\nabla^2\phi = -(\boldsymbol{k} \cdot \nabla)\nu' \tag{10}$$

If we Fourier analyse with respect to time t and take the mode with frequency ω, retaining the same letters for the Fourier mode amplitudes, then from (9)

$$\nu' = \frac{\Omega^2 p\boldsymbol{k} \cdot \nabla\phi}{\omega^2 - \Omega^2(1 - p\gamma\boldsymbol{k} \cdot \boldsymbol{l})}$$

so that (10) gives

$$\nabla^2\phi = A(\boldsymbol{k} \cdot \nabla)^2\phi$$

with

$$A = \Omega^2 p/(\omega^2 - \Omega^2(1 - p\gamma\boldsymbol{k} \cdot \boldsymbol{l})). \tag{11}$$

Passing to a spatial Fourier analysis and taking the component proportional to $\exp(\mathrm{i}(lx + my + nz))$ gives, in the special case where all the parameters are spatially constant and $\boldsymbol{k}$ is along the z-axis,

$$l^2 + m^2 = n^2(A - 1). \tag{12}$$

If the dipoles are arranged on sheets, which is the situation we have in mind for representing layers of membranes in living matter, then we would expect γ to be negative; the condition that $A > 1$ (from the last equation) then gives a range of possible values of ω with a ground state at $A = +\infty$ having a frequency

$$\omega_0 = \Omega(1 - \gamma p\boldsymbol{k} \cdot \boldsymbol{l})^{1/2}$$

and an upper limit at $A = 1$ with frequency

$$\omega_1 = \Omega(1 + p[1 - \gamma\boldsymbol{k} \cdot \boldsymbol{l}])^{1/2}.$$

To evaluate the density of modes as a function of ω, we impose a cut-off at a high wavenumber, so that

$$k^2 + l^2 + n^2 \leqslant K^2 \tag{13}$$

(the value of K being determined by the point at which the continuum model breaks down) together with periodic box boundary conditions requiring l, m and n to be integer multiples of small constants. The form of the density is insensitive to the details of the cut-off. The number of modes $\mathrm{d}N$ with frequencies between ω and $\omega + \mathrm{d}\omega$ is then proportional to the volume of (l, m, n)-space between the surfaces defined by (12) with A and $A + \mathrm{d}A$ given by (11), and bounded by (13). This is easily evaluated to be

$$\mathrm{d}N \propto \frac{\omega \mathrm{d}\omega}{\sqrt{\omega^2 - \omega_0^2}}.$$

We see immediately that, in sharp contrast to the usual situation for superfluidity or superconductivity, the density of modes does not go to zero as the ground state is approached, but in fact diverges to infinity! In other words, the necessary condition (8) is not fulfilled. The basic reason for the breakdown is the shifting of the ground state to a high frequency, so that the ω^3 factor for the volume of wavenumber space in three dimensions (which is responsible for the validity of (8) for superconductivity) no longer helps to reduce the state density to zero near the ground state. It is very likely, therefore, that equation (8) will not hold for more realistic models, incorporating, for example, quadrupole layers reflecting the actual double-layer structure of lipid membranes.

4. Conclusions

We have shown that for the systems considered in biology one cannot assume the Fröhlich mechanism for a Bose condensation. It is still possible that for large pumping rates there is a generalized condensation, in which the ground state does not dominate. This is borne out by simulations, which suggest that there is almost invariably a clustering of the energy in a group of low-energy states. The exact nature of this will depend on the particular parameters of the model.

The implications for theories of consciousness (Marshall 1989) are particularly severe, since these have depended on the qualitative difference between a Bose condensation and an ordinary distribution of states; a generalized condensation, on the other hand, differs only in degree from an ordinary distribution. Again, only a detailed estimate of the numerical size of the effect will determine whether this distinction really matters.

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References

Blatt J M 1964 *Theory of Superconductivity* (New York: Academic)
Burfoot J C 1967 *Ferroelectrics* (Englewood Cliffs, NJ: Prentice Hall)
Duffield N G 1988a Global stability of condensation in the continuum limit for Fröhlich's pumped phonon system *J. Phys. A: Math. Gen.* **21** 625–41

Duffield N G 1988b The continuum limit of dissipative dyamics in H. Fröhlich's pumped phonon system *Helv. Phys. Acta* **61** 363–78

Fröhlich H 1968 Long-range coherence and energy storage in biological systems *Int. J. Quantum Chem.* **2** 641–9

Girardeau M 1960 Relationship between systems of impenetrable bosons and fermions in one dimension *J. Math. Phys.* **1** 516–523

Marshall I 1989 Consciousness and Bose–Einstein condensates *New Ideas in Psychol.* **7** 73–83

Rowlands S 1983 Coherent excitations in blood *Coherent Excitations in Biological Systems* ed H Fröhlich and F Kremer, pp 145–61

Sewell G L 1986 *Quantum Theory of Collective Phenomena* (Oxford: Oxford University Press)

van den Berg M, Lewis T J and Pule J V 1986 A general theory of Bose–Einstein condensation *Helv. Phys. Acta* **59** 1271–88

Wu T M and Austin S 1978 Bose–Einstein condensation in biological systems *J. Theor. Biol.* **71** 209–14