Comment on "Molecular gyroscopes and biological effects of weak extremely low-frequency magnetic fields"

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A mechanism whereby reaction rates may be influenced by weak alternating magnetic fields has been suggested by Binhi and Savin [Phys. Rev. E **65**, 051912 (2002)] to account for certain magnetobiological effects. It is proposed that the fields influence the probability of reaction of molecular rotators (gyroscopes) by inducing interference between eigenstates of angular momentum superposed in their wave functions. The predicted variation of reaction rate with the amplitude of the alternating field is found to be qualitatively consistent with observation. It is commented that the required interference occurs only in circumstances which are quite implausible, and that even if it were possible, the interference would not lead to a detectable magnetobiological effect.

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In a recent paper [1], Binhi and Savin (BS hereafter) suggest how biological reaction rates might be influenced by alternating magnetic fields with strength of the same order as the geomagnetic field, and frequency in the range 10–100 Hz. They consider an ensemble in which each molecule is constrained to rotate about a fixed axis in a protein cavity, and reacts with a fixed site on the cavity wall. It is shown that if the cavity is large enough, the rotational states have lifetimes of the order of 10^{-2} s at ordinary temperatures. The long lifetime allows such molecular rotators ("gyroscopes"), when created in a superposition of eigenstates of angular momentum, to exhibit quantum interference when subjected to a weak magnetic field. BS propose that the influence of this on the probability of reaction accounts for the biological effects of weak alternating magnetic fields, and obtain an expression for the field dependence of reaction rate, which agrees qualitatively with experimental evidence presented.

In this Comment, it is pointed out that the quantum interference is possible only in conditions which are most unlikely to exist in a biological system, and that even if the interference were to occur, it would not lead to a detectable magnetobiological effect (MBE).

The circumstances in which the quantum interference between rotational states might lead to a MBE have already been discussed by Adair [2] in an analysis of the ion parametric resonance (IPR) model, in which the states are those of an ion constrained by the walls of a spherically symmetric cavity. Adair identified several unrelated reasons why no detectable MBE is to be expected from the IPR mechanism in weak fields.

The BS proposal avoids some of the problems of the IPR models. Whereas the rotational states in the IPR model are likely to have lifetimes less than 10^{-10} s, those of the molecular rotators evidently can be sufficiently long lived to support interference in weak fields, at least in principle. The problem of correlating the phase of the interference (which is expected to vary randomly between rotators) with that of the applied alternating field is also avoided, by postulating a quadratic relation between reaction rate and probability density.

It is, however, practically impossible for the cavities demanded by the BS model to occur in biological systems. The necessary lifetimes require cavities of diameter 30 Å, empty except for the molecular rotator. Further, as in the IPR model, the cavities must have almost perfect axial symmetry if the required interference is to occur between the superposed eigenstates of angular momentum. If the rotators are subjected to the Lennard-Jones potentials quoted by BS, then the interference would be destroyed by a departure from symmetry of the order of 1 part in 10^8, as the eigenstates of angular momentum would no longer be stationary states. In the BS model, the active site on the cavity wall makes such a departure from symmetry seemingly inevitable.

Although it is clear from this that the BS model cannot be expected to represent a real biological system, it is still useful to enquire whether an ensemble of ideal rotators, as proposed by BS, would, in fact, exhibit a detectable MBE. This is discussed in the remainder of the Comment. It is found that the alternating field has an appreciable effect on the reaction rate only of rotators occupying a few low-lying rotational states, and then only if further restrictive conditions are met. As a result, any MBE is far smaller than could be detected.

The way in which the proposed MBE arises in an ensemble of rotators is now outlined, following BS. In the absence of field, quantization of angular momentum leads immediately to the rotator energy levels:

$$\varepsilon_m = m^2\hbar^2/2I, \quad m = 0, \pm 1, \ldots, \tag{1}$$

where $m\hbar$ is the angular momentum and I the moment of inertia. The wave function corresponding to angular momentum $m\hbar$ is expressed by

$$|m\rangle = e^{im\phi}e^{-(i/\hbar)\varepsilon_m t}, \tag{2}$$

where the intrinsic time dependence is included and a normalization factor omitted.

The rotator is assumed to carry an effective charge q round a path of radius R. When the angular momentum is $m\hbar$, this is equivalent to a current $qm\hbar/2\pi I$ encircling an area πR^2, and thus to magnetic moment $qR^2m\hbar/2I$. In an axial magnetic field H, the energy then becomes

$$\varepsilon_m=\frac{\hbar^2}{2I}m^2-\frac{qR^2\hbar H}{2I}m, \tag{3}$$

lifting the degeneracy between $|m\rangle$ and $|-m\rangle$, but leaving their spatial wave functions unchanged.

Now suppose that at time $t=0$ a rotator is created in some superposition of states $|m\rangle$, and subjected to an axial magnetic field $H=H_{dc}+H_{ac}\sin\Omega t$, with an alternating component. It is sufficient to consider superpositions of two states, of the form

$$\Psi=c_m|m\rangle+c_{m'}|m'\rangle, \tag{4}$$

where $c_m=(1/\sqrt{2})e^{-i\theta/2}$, $c_{m'}=(1/\sqrt{2})e^{+i\theta/2}$, and θ specifies the relative phase of the contributions. With ε_m now varying on account of H_{ac}, the intrinsic time dependence of $|m\rangle$ is $\exp[-(i/\hbar)\int_0^t\varepsilon_m(t')dt']$, which can be written as

$$\exp\left[-i\left(\frac{\hbar}{2I}m^2t-m\omega_g t-m\omega_g\frac{h'}{\Omega}\sin\Omega t\right)\right]$$

with $\omega_g=qR^2H_{dc}/2I$ and $h'=H_{ac}/H_{dc}$. Probability $p(t)=\Psi^*(t,\Phi)\Psi(t,\Phi)$ of the rotator being found at time $t>0$ at position Φ of the active site is then

$$1+\cos\left\{(m-m')\Phi-\theta-\frac{\hbar}{2I}(m^2-m'^2)t+(m-m')\omega_g t+(m-m')\omega_g\frac{h'}{\Omega}\sin\Omega t\right\}, \tag{5}$$

where a normalizing factor is omitted. BS express $p(t)$ in terms of density matrices rather than wave functions, but the two formalisms are equivalent here and lead to identical results.

With $I=10^{-35}$ g cm^2, q being the electronic charge, and $R=10^{-7}$ cm, as suggested by BS, one has $\hbar/2I\approx10^7$ s^{-1} and $\omega_g\approx10$ s^{-1} when $H=100$ μT. As $|m|\approx870$ when $\varepsilon_m=k_BT$ at temperature $T=300$ K, $p(t)$ may oscillate with a frequency up to the microwave region. BS describe the response of the active site to variations in $p(t)$ by a sliding average, over time $2\tau\gg2I/\hbar$, whose smoothing effect ensures that such rapid oscillations can be disregarded. The smoothed $p(t)$, denoted by $p_\tau(t)$, is then equal to 1 except when $m'=-m$, in which case

$$p_\tau(t)=1+\cos\left\{2m\Phi-\theta+2m\omega_g t+2m\omega_g\frac{h'}{\Omega}\sin\Omega t\right\}, \tag{6}$$

provided that $2m\omega_g\tau\ll1$. A factor $e^{-\Gamma t}$ may be included to take account of the finite lifetime Γ^{-1} of the rotator.

The probability of the rotator reacting is some function of $p_\tau(t)$. For an ensemble of many rotators in a steady state, the reaction rate is proportional to the average of this probability, with respect to time and θ. This average will be denoted by S, with S_0 being its value in the absence of H_{ac}. Following BS, $\rho=1-S_0/S$ is used as a measure of any MBE.

Suppose first that the reaction probability depends linearly on $p_\tau(t)$. A MBE may then arise whenever $\Omega=2m\omega_g/n$, with n being an integer. In that situation, the argument of the cosine in Eq. (6) increases nonuniformly with t, but in the same way in each cycle of $\sin\Omega t$, and the time average of $p_\tau(t)$ differs from 1 to an extent dependent on h' and θ.

This possibility of $p_\tau(t)$ departing from 1 was noted by Binhi [3], but dismissed as being of no physical significance as in experiments, condition $\Omega=2m\omega_g/n\Omega$ is never satisfied exactly. Its dismissal is, however, mistaken: the response is broadened by the inverse lifetime Γ of the rotators, which, in effect, makes ω_g uncertain, and a MBE results if the rotators have some preferred value of $2m\Phi-\theta$. This MBE appears to be predicted by Eq. (14) of Ref. [1], if the lack of any specific mention of Φ and θ is taken to imply that $2m\Phi-\theta=0$. However, as discussed in Ref. [3], the equation is intended to apply only when $|2m\omega_g-n\Omega|\gg\Gamma$. As $p_\tau(t)$ then behaves, during successive cycles of $\sin\Omega t$, as though θ had changed by an amount incommensurate with 2π, averaging with respect to time becomes equivalent to averaging also with respect to random θ. As is expected, if θ are distributed randomly, the average is then 1, and no MBE arises.

To obtain a MBE with random θ, BS assume a probability of reaction proportional to $p_\tau^2(t)$, and suppose also that $2m\omega_g\tau$ is of the order of 1. These restricted circumstances can hardly be of frequent occurrence: a quadratic dependence of the probability on $p_\tau(t)$ would usually be accompanied by a (possibly much larger) linear term, and it would be a surprising coincidence if τ were roughly the same as $(2m\omega_g)^{-1}$. The estimates of ρ made below, on the basis of these assumptions, are thus the upper limit of what might be possible in the already idealized situation being considered.

The way in which a MBE then arises can be seen by considering the effect of smoothing and squaring Eq. (6) for $p_\tau(t)$. With no extra smoothing one has $S=\frac{3}{2}$, after averaging with respect to θ and t. The smoothing reduces the amplitude of the cosine term, but because the periodicity of $p_\tau(t)$ is modulated at frequency Ω, the reduction (and therefore S) depends on h', leading to a MBE.

Allowance for random θ may again be made by avoiding the singularities (broadened by Γ) which in occur $p_\tau^2(t)$ when $\Omega=2m\omega_g/n$ or $\Omega=4m\omega_g/n$. This leads to

$$S=1+\frac{1}{2}\sum_{n=-\infty}^{\infty}\frac{1}{1+(2m\omega_g+n\Omega)^2\tau^2}J_n^2\left(h'\frac{2m\omega_g}{\Omega}\right), \tag{7}$$

when, as is now assumed, $\Gamma\tau \ll 1$. Rather than a sliding average, which leads to problems when $\Gamma\tau$ is large, the smoothing has been assumed to be governed by $\dot{p}_\tau = (p - p_\tau)/\tau$, as in relaxation with time constant τ.

Except for the treatment of smoothing, Eq. (7) is close to that for S given by BS, the appropriate density matrix elements being $\sigma_{mm} = \sigma_{m'm'} = |\sigma_{mm'}| = \frac{1}{2}$. However, it should be noted that the diagonal elements, not being associated with any time dependence, contribute the square of their sum, here $(\sigma_{mm} + \sigma_{m'm'})^2$, whence the initial term 1 in Eq. (7).

The behavior of S, as a function of h', depends on $2m\omega_g\tau$ and $\Omega/2m\omega_g$. When $2m\omega_g\tau$ is small, S falls monotonically with h', and approaches 1 asymptotically. With larger $2m\omega_g\tau$, oscillatory behavior develops, which is most evident when $2m\omega_g$ is close to Ω, when it first appears for $2m\omega_g\tau \approx 1$. When $2m\omega_g\tau$ is greater than 2, S rises from near 1 when $h' = 0$, to a maximum when $h' \approx 2$, followed by a succession of maxima of decreasing amplitude. This behavior, which provides the MBE which BS compared with experiment, arises because the smoothing causes the sum in Eq. (7) to be dominated by the term $n = -1$.

The maximum of S/S_0 is greatest when $2m\omega_g\tau \gg 1$ and $\Omega = 2m\omega_g$. One then has

$$\rho = 1 - \frac{1}{1 + \frac{1}{2}J_1^2(h')}, \tag{8}$$

with maximum value 0.145. This, however, is approached only for Ω within τ^{-1} of $2m\omega_g$. More realistic MBE is found with $2m\omega_g\tau \approx 5$, which gives maximum ρ about 0.13 when $\Omega/2m\omega_g = 1$, but greater than 0.07 for all $\Omega/2m\omega_g$ between 0.6 and 1.2.

Equation (18) of Ref. [1] differs from Eq. (8) in omitting the factor $\frac{1}{2}$ from the denominator. The difference is a result of the contribution to S of the diagonal elements of the density matrix having been taken as σ_{00}^2, where $|0\rangle$ is introduced to provide a contribution independent of H_{ac}. However, that is not necessary: the diagonal elements σ_{mm} and $\sigma_{m'm'}$, wrongly omitted in Ref. [1], already make a contribution $(\sigma_{mm} + \sigma_{m'm'})^2$ which is independent of H_{ac}.

It is evident that even in this ideal situation, and when the superposition is of the two low-lying states most closely matched to Ω, the MBE arising from quantum interference is rather weak, with ρ being of the order of 0.1 (denoted by ρ_0 below). With $\Omega/2\pi \approx 50$ Hz and ω_g as estimated above, $2m\omega_g \approx \Omega$ when $|m| \approx 15$, and ρ arises mainly from rotators having $|m|$ between perhaps 10 and 25.

As rotators in other states have $p_\tau^2(t)$ close to 1, they make field-independent contributions to S [4], whose effect is to reduce ρ. To estimate the likely value of ρ, one needs to know how the rotators are created in superpositions of states. The most effective way would be for them to be suddenly set free to rotate, with no immediate change in wave function, after being subjected to a potential in which they occupy stationary states having wave functions Ψ suitably localized with respect to ϕ. It is not difficult to see that if Ψ is restricted (improbably) to a range 2π of ϕ, then half the original stationary states are the required superpositions of $|m\rangle$ and $|-m\rangle$ (the others are superpositions of several such pairs, which make smaller contributions to ρ). If the stationary states are occupied as in thermal equilibrium before the rotator is created, then the probability that it will appear in one which contributes significantly to ρ is about 0.02, so that $\rho \approx 0.02\rho_0 \approx 2\times 10^{-3}$. It is most unlikely that a MBE would be detectable in this situation, despite its already having been idealized in so many ways [5].

Still lower estimates of ρ result if, as is more likely, Ψ is initially restricted to a smaller range of ϕ, as all the stationary states then become superpositions of several pairs of states $|m\rangle$ and $|-m\rangle$, and occupation p_m of each $|m\rangle$ is less than $\frac{1}{2}$. As the contribution of $|m\rangle$ to ρ is proportional to p_m^2, the effect is to multiply ρ by a factor of the order of $2p_m$ if all the m lie within the contributing range, and of the order of $4p_m^2$ if most lie outside it. In terms of the density matrix, the field-dependent contributions to S depend on $|\sigma_{mm'}|^2 = p_m p_{m'}$, but the squared sum of the diagonal elements, which provides the constant term, necessarily remains 1. In the (not necessarily extreme) case where Ψ occupies a range of ϕ of the order of $2\pi/m_T$, where $m_T \approx 870$ is the value of m for which $\varepsilon_m = k_B T$, then approximately m_T pairs of states are superposed, and ρ is reduced to about 10^{-7}.

It is clear from this that even if rotators were available with adequate lifetimes and surroundings of perfect axial symmetry, and had probability of reaction dependent only on $p_\tau^2(t)$ and smoothing time constant τ matched to $(2m\omega_g)^{-1}$, the mechanism proposed by BS would not lead to any detectable MBE in weak alternating fields.

[1] V.N. Binhi and A.V. Savin, Phys. Rev. E **65**, 051912 (2002).

[2] R.K. Adair, Bioelectromagnetics (N.Y.) **19**, 181 (1998).

[3] V.N. Binhi, *Magnetobiology: Underlying Physical Problems* (Academic Press, London, 2002).

[4] There would be no field-independent contributions to S if the probability of reaction were proportional to $(p_\tau - 1)^2$ rather than to p_τ^2. That would be equivalent to the omission of diagonal elements of the density matrix from the expression for S given by BS; the extent to which they are present is not entirely clear. It is not obvious how a dependence on $(p_\tau - 1)^2$ (or, for that matter, one purely on p_τ^2) could arise.

[5] While living systems are never exactly in equilibrium, it is not credible that they support the selective population of levels having energy of the order of $10^{-4}k_B T$, which is needed if the MBE is to be observable.