

Manifestation of quantum coherence upon recombination of radical ion pairs in weak magnetic fields. Systems with non-equivalent nuclei

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Abstract

Magnetsensitive radiofluorescence has been used to study the magnetic field effect at weak magnetic fields during geminate recombination of singlet radical ion pairs formed radiolytically in non-polar solutions. The existence of the local fluorescence maximum in zero field has been theoretically demonstrated and experimentally verified for radical pairs in which one of the partners contains a great number of non-equivalent magnetic nuclei and the local hyperfine fields of the other partner are negligibly small. In terms of a semiclassical approximation, a simple condition for the appearance of the effect has been obtained: $\Omega\tau^* \gg 1$, where Ω is the effective ESR spectrum width and τ^* is the lifetime of a spin-correlated pair.

1. Introduction

Static magnetic fields are known to have an effect on chemical reactions involving short-lived paramagnetic particles, i.e. radicals and radical ions [1,2], which are the intermediates in many chemical transformations. Spin and magnetic field effects in radical reactions occur due to singlet–triplet transitions in a pair of radicals that can recombine. In weak magnetic fields the singlet–triplet (S–T) evolution of a radical pair is mainly determined by the hyperfine

interaction (hfi) in radicals. When the hfi energy is comparable with the Zeeman one in the external magnetic field, the singlet state S mixes with all three triplet states (T_- , T_0 , T_+) of the radical pair. As the strength of the external magnetic field increases, the mixing efficiency decreases because the triplet T_+ and T_- states are no longer involved in S–T evolution. Thus, upon transition to strong fields one should expect that for the singlet precursor of the radical pair, for example, the decrease in the number of S–T conversion channels is sure to lead to an increase in the probability of recombination into the singlet product. The majority of available data is in fair agreement with this qualitative model.

The above mentioned qualitative pattern holds for short-lived radical pairs with $\mathcal{A}_{\text{eff}}\tau < 1$, where \mathcal{A}_{eff}

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is the effective hfi constant of pair radicals, τ is the pair lifetime [1]. The first detailed calculations carried out for simple systems [3–7] show that this scheme can fail for long-lived pairs due to level degeneracy resulting in the interference of different channels of S–T conversion. Thus, for example, in the radical pair with one magnetic nucleus ($\dot{R}\dots\dot{R}$) the probability of S–T transitions at long times is larger in a strong field than in zero field [3]. In this case the three interfering channels of S–T transitions in the weak field appear to be less efficient than one S– T_0 channel in the strong field due to the degeneracy of levels. The efficiency of S–T conversion does not decrease monotonically with increasing field strength but passes through a maximum in the fields of the order of the hyperfine one. As follows from calculations, the interference of different channels of S–T transitions must manifest itself in the recombination of simple radical pairs with equivalent nuclei [5,8] or a small number of nuclei [1]. For a radical pair containing a great number of non-equivalent nuclei in both of the partners the effect of interference is rather weak and vanishes in the semiclassical limit [9].

The degeneracy of levels and the resulting inversion of the sign of the magnetic field effect in weak fields have most clearly been observed in systems with equivalent nuclei [5]. A strong zero field fluorescence maximum attributed to the interference of the channels of S–T transitions was observed upon recombination of radical ion pairs containing C_6F_6 anions with a large hfi constant ($a(6F) = 134$ G).

Low-field peculiarities of the magnetic field effect have also been observed in the recombination of photochemically generated radical ion pairs in polar solutions [10,11] and radical pairs in micelles [12]. In the first case the pair partners contained a great number of non-equivalent nuclei and the peculiarities observed were not large. Therefore, the magnetic field modulation method appeared to be most suitable for their detection [10].

This Letter reports the experimental and theoretical study of the low-field features of the magnetic field effect for radical ion pairs with non-equivalent nuclei generated in non-polar solutions under ionizing radiation. Unlike photochemically generated ion radical pairs and radical pairs in micelles, in these systems the initial separation between pair partners is

large enough so that the exchange interaction can be considered unimportant. Therefore there is no need to consider an alternative reason for low-field features related to S–T transitions due to J -resonance [13].

It is demonstrated that for radical pairs with negligibly small hyperfine interactions in one of the pair partners, the low-field effects due to interference of S–T transition channels in zero magnetic field are observed, the other partner having arbitrary complex nuclear configuration.

2. Experimental

Magnetic field effects under X-radiation were recorded in stationary conditions as described in Ref. [14]. The sample, containing about 1 ml of solution in a quartz cuvette, was put into the magnetic field of a Bruker ER-200D ESR spectrometer equipped with an X-ray tube for sample irradiation and a PMT with a quartz light guide for fluorescence detection. No microwave pumping was applied. Fluorescence was monitored through a light filter ($\lambda < 360$ nm). The PMT signal was fed to a phase-sensitive detector. The scanned magnetic field was modulated by a small alternating one at the 12.5 kHz reference frequency of the phase-sensitive detector. This technique seems to be more convenient as compared to direct recording of fluorescence without modulation due to its lower sensitivity to temperature drift and higher signal-to-noise ratio. The residual magnetic field of the magnet was compensated by additional coils to provide the reverse shift of the field. This allowed us to scan the magnetic field in the range from -50 to $+4000$ G.

The sample temperature was varied by blowing cold nitrogen through the spectrometer cavity. The temperature was kept to within 1 K. Prior to the experiment, the samples were degassed to about 10^{-3} Torr by repeated freeze–pump–thaw cycles.

To improve the signal-to-noise ratio, the scans were repeated, the data were accumulated in the memory of the multichannel ORTEC 6240B analyzer and then processed on a personal computer.

Squalane (99%, Fluka), used as a solvent, was purified by passing through a column with activated silica gel. The purity was tested by UV-absorption in the range 215–225 nm [15]. N,N,N',N'-tetramethyl-

paraphenylenediamine (TMPD), N,N-dimethylaniline (DMA), paraxylene, toluene, tetramethylbenzene (durene), naphthalene- h_8 , naphthalene- d_8 , naphthalene- F_8 and biphenyl- F_{10} were used as hole and electron acceptors. The hfi constants of their ions (except for biphenyl- F_{10}) are given in Table 1. TMPD (98%, Aldrich), durene (> 99%, Fluka) were used without further purification. Dimethylaniline, paraxylene and toluene were purified by distillation.

3. Theory

Generally, the ensemble spin state of a radical pair is described by the density matrix $\rho(t)$. The state of the spins of unpaired electrons changes with time because of their interaction with the external magnetic field H and the hyperfine interaction with magnetic nuclei. The populations of the singlet and triplet states of the radical pair by the time of recombination can be found by solving the equation ($\hbar \equiv 1$)

$$\partial\rho/\partial t = -i[\hat{\mathcal{H}}, \rho]. \quad (1)$$

Assuming $g_1 \approx g_2 \equiv g$ the spin-Hamiltonian $\hat{\mathcal{H}}$ can be written as

$$\hat{\mathcal{H}} = g\beta H(S_{1z} + S_{2z}) + \sum_i a_i S_1 \cdot I_{1i} + \sum_j a_j S_2 \cdot I_{2j}, \quad (2)$$

where the first term is the Zeeman energy of electrons in the external magnetic field, and the second and third ones describe hfi in pair radicals [1]. For the system containing only equivalent nuclei in each of the pair partners, Eq. (1) can be solved analytically [5]. Systems with non-equivalent nuclei can be analyzed numerically. However, it is actually impossible to solve accurately the equation for the density matrix of the radical pair containing a great number of magnetic nuclei in weak fields even with the help of a computer [16]. Therefore, a semiclassical approach allowing one to calculate the dynamics of singlet–triplet transitions in any magnetic field neglecting the detailed structure of pair radicals was proposed to study the magnetic field effects in such systems [17,18]. The method has already been used to demonstrate that the effect of the interference of

Table 1
hfi parameters and effective spectrum width of ion radicals

Ion radical of acceptor	hfi parameters (G)		Ω^a (G)	Ref.
(naphthalene- F_8) $^{\cdot-}$	4F	28.1	50.1	[22]
	4F	21.6		
(DMA) $^{\cdot+}$	2N	10	27.1	[23]
	6H(CH ₃)	12		
	3H(CH)	5		
(TMPD) $^{\cdot+}$	2N	7.05	20.4	[23]
	12H(CH ₃)	6.77		
	4H(CH)	1.99		
(toluene) $^{\cdot+}$	3H(CH ₃)	20	25	[24]
	H(CH)	12.5		
(paraxylene) $^{\cdot+}$	6H(CH ₃)	18.3	32	[24]
	4H(CH)	3.0		
(durene) $^{\cdot+}$	12H(CH ₃)	11.5	28.2	[14]
(naphthalene- h_8) $^{\cdot+}$	4H	7.4	10.8	[25]
	4H	1.87		
(naphthalene- h_8) $^{\cdot-}$	4H	4.93	7.44	[25]
	4H	1.83		

$$^a \Omega = \sqrt{\frac{2}{3}} \sum a_i^2 I_i(I_i + 1)$$

S–T transition channels disappears for the radical pair with a great number of magnetic nuclei in each of the partners, i.e. when both of the partners can be described semiclassically [9].

Consider now a radical pair, undergoing geminate recombination with exponential decay kinetics in the ensemble, in which one of the radicals has no hfi (a narrow partner). For the yield of singlet products, G_S , in the external magnetic field H one obtains

$$G_S = \tau^{-1} \int_0^\infty \rho_{SS}(t) \exp(-t/\tau) dt. \quad (3)$$

For a pair of non-interacting radicals the population of the singlet state $\rho_{SS}(t)$ can be deduced from the equation of motion for each spin separately

$$\rho_{SS}(t) = Sp\left\{\left[\frac{1}{4} - S_1(t) \cdot S_2(t)\right] \rho(0)\right\}, \quad (4)$$

where the trace is taken over all nuclear states. The result reads

$$G_S(\omega_0, \tau_0) = \frac{1}{4} + R(\omega_0, \tau_0), \quad (5)$$

where the dimensionless parameters ω_0 and τ_0 are the external magnetic field H and the pair lifetime τ reduced to the effective ESR spectrum width of the broad partner Ω ,

$$\omega_0 = H/\Omega, \quad \tau_0 = \Omega\tau. \quad (6)$$

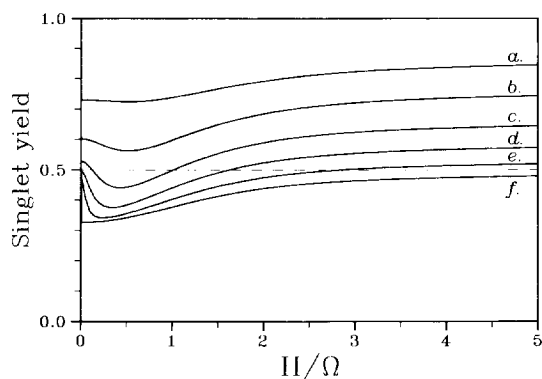


Fig. 1. The dependence of singlet products yield on external magnetic field calculated in the semiclassical approximation for different pair lifetimes $\tau_0 = \Omega\tau$: (a) 1; (b) 2; (c) 4; (d) 8; (e) 20; (f) ∞ . The radical pair originates in the singlet state and exponentially decays with time τ due to recombination. The hfi in one of the pair partners are zero; the effective spectrum width of the second partner is Ω .

Here $\Omega = \sqrt{\frac{2}{3} \sum a_i^2 I_i(I_i + 1)}$, and the function $R(\omega_0, \tau_0)$ is obtained by averaging over all nuclear configurations of the broad pair partner,

$$R(\omega_0, \tau_0) = \pi^{-3/2} \int_0^\infty 2\pi r dr \times \int_{-\infty}^\infty Q(r, \omega_z) \exp(-\omega_z^2 - r^2) d\omega_z \quad (7)$$

The analytical expression for $Q(r, \omega_z)$ is given in Appendix A. When deducing (5) it was taken into

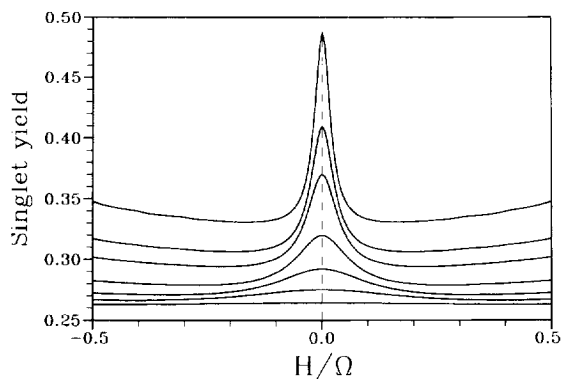


Fig. 2. The calculated singlet products yield in the region of weak magnetic field for the given pair lifetime $\tau_0 = 50$ and different relaxation times. From top to bottom: $\Omega T_{1,2} = 10000, 100, 50, 20, 10, 5, 2$.

account that the pairs originate in the singlet state and the hfi constants in one of the partners are zero ($a_j = 0$).

In this approach the only parameter characterizing the inherent structure of the pair is the effective spectrum width of the broad partner, and the yield of singlet products is described by a function of the dimensionless variables H/Ω and $\Omega\tau$. Fig. 1 shows the yield of singlet products calculated from formula (5), versus magnetic field for the different pair lifetimes. As follows from the plot, a sharp maximum arises in zero field with increasing recombination time, which points to the existence of the interference of S–T transition channels in the system under study. A quantitative condition for the appearance of the interference maximum can be written as

$$\Omega\tau \gg 1, \quad (8)$$

which qualitatively means multiple evolution of the spin system during the pair lifetime.

Formulae (4) and (5) neglect the influence of relaxation on the spin system dynamics. Assuming that longitudinal and cross relaxation times coincide ($T_1 = T_2$) in the vicinity of zero field, expression (4) can readily be modified,

$$\rho_{SS}(t) = Sp\left\{\left[\frac{1}{4} - S_1(t) \cdot S_2(t) \exp(-t/T_{1,2})\right] \rho(0)\right\}. \quad (9)$$

Hence, one obtains

$$G_S(\omega_0, \tau, T_{1,2}) = \frac{1}{4} + (\tau^*/\tau)R(\omega_0, \Omega\tau^*), \quad (10)$$

where τ^* is the lifetime of a spin-correlated pair: $(\tau^*)^{-1} = \tau^{-1} + T_{1,2}^{-1}$.

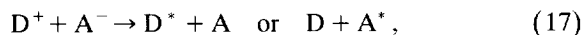
Fig. 2 shows the theoretical curves of the yield of singlet products in the vicinity of zero field for different relaxation times and a fixed pair lifetime. As the relaxation time shortens, the interference peak broadens and vanishes. Under conditions of fast relaxation ($\tau^*/\tau \rightarrow 0$), the yield of singlet products tends to $\frac{1}{4}$. Thus, taking into account the relaxation in the system, the criterion for interference maximum appearance (8) is modified,

$$\Omega\tau^* \gg 1, \quad (11)$$

which means the prevailing influence of spin dynamics (Ω) over stochastic processes (τ^*).

4. Results and discussion

The formation of radical ion pairs in hydrocarbon solutions under ionizing radiation and their recombination with the generation of excited molecules are described by the scheme [19]



Here S is the solvent molecule, D and A are the hole and electron acceptors, respectively. The primary pairs S^+/e^- mainly arise in the singlet state. The yield of fluorescing recombination products depends on the singlet–triplet evolution in radical pairs, and the multiplicity of the forming excited products A^* , D^* corresponds to the spin multiplicity of the pair by the time of recombination.

As follows from theoretical considerations, the interference effects must be pronounced in the recombination of radical pairs in which the hfi in one of the partners are negligibly small. The reactions of the recombination of electron and solvent holes (when their hfi are small or averaged down by fast charge transfer) with the corresponding counter-ions (reactions (15), (16)) meet these requirements. As is known, the spectra of the optically detected ESR (OD ESR) of solvent holes often appear to be narrow single lines at room temperature [20]. By choosing the acceptor type (either hole or electron), one can selectively observe the radical ion pairs either of (15) or (16) type.

Fig. 3 demonstrates the experimental curves of the dependence of the fluorescence intensity of squalane solutions of different acceptors on the magnetic field. Substances with a low ionization potential and negative affinity for electrons (e.g. TMPD) were chosen as hole acceptors. Since the ionization potential of fluorinated compounds is, as a rule, higher than that of squalane, perfluoronaphthalene and perfluorobiphenyl were taken as electron acceptors. Substances that can capture both solvent holes and electrons were avoided. Therefore, each experi-

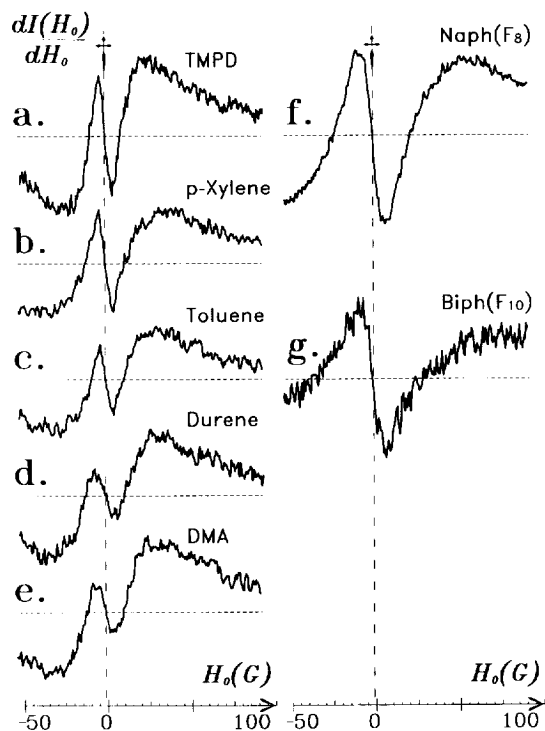


Fig. 3. The field dependences of the fluorescence intensity of squalane solutions of different electron and hole acceptors at 20°C presented as the first derivatives: (a) 10^{-3} M TMPD; (b) 2.5×10^{-3} M paraxylene (0°C); (c) 2.5×10^{-3} M toluene (0°C); (d) 1.5×10^{-3} M durene; (e) 2.2×10^{-3} M DMA; (f) 5×10^{-3} M naphthalene- F_8 ; (g) 10^{-3} M biphenyl- F_{10} .

mentally observed magnetic field effect originates from reactions of only one type. Curves (a)–(e) correspond to pairs of (acceptor) $^+/e^-$ type, curves (f)–(g) to pairs of (acceptor) $^-/S^+$ type. All the curves shown in Fig. 3 display inversion in zero field. This phenomenon was first observed in the solution of hexafluorobenzene in squalane and was explained as the result of interference of S–T transition channels [5]. The similarity of the curves allows the effects observed to be referred to the same mechanism.

As has been believed, a minor inversion is to be observed for radical pairs with a few groups of equivalent nuclei [5] and the inversion amplitude exponentially decreases with increasing number of non-equivalent magnetic nuclei in the system [11]. However, as follows from Table 1, nuclear equivalence is far from being a necessary condition for the

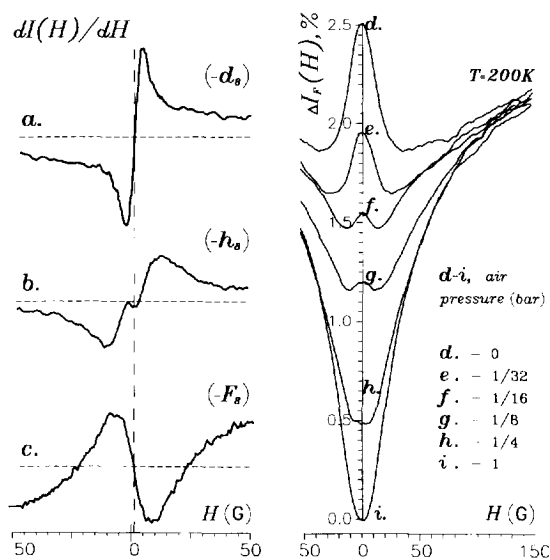


Fig. 4. (a)–(c) The field dependences of the fluorescence intensity of 10^{-3} M naphthalene solution and its substituted analogues in squalane at 293 K given as the first derivative: (a) naphthalene- $-d_8$, (b) naphthalene- $-h_8$, (c) naphthalene- $-F_8$; (d)–(i) fluorescence intensity of 5×10^{-2} M naphthalene- $-h_8$ solution in squalane at 200 K. Oxygen concentration is varied by air leak-in: (d) degassed sample, (e) $\frac{1}{32}$ bar, (f) $\frac{1}{16}$ bar, (g) $\frac{1}{8}$ bar, (h) $\frac{1}{4}$ bar, (i) 1 bar. For convenience the curves are shifted relative to the vertical axis.

appearance of inversion in such systems. As is evident from semiclassical considerations, the second moment of the wide partner Ω is the determining parameter. Indeed, perfluorobiphenyl and perfluoronaphthalene, the large anion spectrum widths of which are due to the strong hfi with fluorine nuclei, demonstrate the largest inversion of the field dependence (Figs. 3f–3g). At the same time, the effect for durene, containing twelve equivalent protons, is weaker than for TMPD.

The above mentioned criterion for the observation of inversion at zero field can be verified experimentally. As follows from formula (11), the inversion depth is determined by two independent parameters the first of which (Ω) is the inner characteristic of the spin system and the other (τ^*) depends on the molecular dynamics of the pair.

Figs. 4a–4c show the fluorescence yield in the vicinity of the zero field for the solutions of $-d_8$, $-h_8$, $-F_8$ -substituted naphthalene molecules in squalane recorded under the same conditions. Since the naph-

thalene molecules are the acceptors of both the holes and electrons, their concentration was taken quite low (10^{-3} M) to suppress the channel of reaction (15) involving naphthalene radical-cations. Thus, the observed signals arise mainly from recombination of naphthalene radical-anions with matrix holes (reaction (16)). Since the hyperfine coupling constants of the hydrogen, deuterium and fluorine nuclei are quite different, the spectrum width can be varied using the chemically substituted acceptor molecules. For the $-d$, $-h$, and $-F$ -substituted acceptors the spectrum widths correspond to

$$\Omega_d : \Omega_h : \Omega_F = 0.25 : 1 : 6.74. \quad (18)$$

According to formula (11), the inversion depth increases with spectrum width.

Since the oxygen molecule is paramagnetic, the existence of oxygen in the sample shortens the relaxation time and, as a result, the lifetime of spin-correlated pairs τ^* . Figs. 4d–4i demonstrate the experimental curves of the fluorescence yield in the vicinity of zero field for 5×10^{-2} M naphthalene- $-h_8$ solution in squalane at 200 K and different oxygen concentrations. The latter was varied by air leak-in into the sample. In the absence of oxygen, a pronounced maximum is observed in the zero field (Fig. 4d) which decreases and vanishes with added air (figs. 4e–4i). Thus, the decrease in the correlated pair lifetime disturbs the process of the coherent mixing of S and T levels. In these experiments the luminescence is likely to arise from the recombination of naphthalene radical cations with solvated electrons (reaction (15)). Employing the optically detected ESR (OD ESR) technique [21] the yield of this reaction in squalane has been shown to increase with decreasing temperature and to exhibit a characteristic maximum in the range of 200 K. The temperature dependence of inversion amplitude has been demonstrated to be similar which testifies in favour of such a reference.

Thus, it has been theoretically demonstrated and experimentally verified that for a radical pair in which the hfi in one of the partners are negligibly small, there is a local fluorescence maximum in zero field. This phenomenon originates from the interference of the S–T transition channels in weak magnetic fields and can be observed under condition $\Omega\tau^* \gg 1$.

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Appendix

The kernel of the integral expression for the function $R(\omega_0, \tau_0)$ is of the form

$$\begin{aligned}
 Q(r, w_z) &= \frac{1}{4} \left[\frac{(\omega_0 + \omega_z)^2}{r^2 + (\omega_0 + \omega_z)^2} \right. \\
 &+ \frac{\frac{1}{2}(1+k)^2}{1 + \left[\omega_0 - \sqrt{r^2 + (\omega_0 + \omega_z)^2} \right]^2 \tau_0^2} \\
 &+ \frac{\frac{1}{2}(1-k)^2}{1 + \left[\omega_0 - \sqrt{r^2 + (\omega_0 + \omega_z)^2} \right]^2 \tau_0^2} \\
 &+ \frac{r^2}{r^2 + (\omega_0 + \omega_z)^2} \\
 &\left. \times \left(\frac{1}{1 + \omega_0^2 \tau_0^2} + \frac{1}{1 + (\omega_0 + \omega_z)^2 \tau_0^2 + r^2 \tau_0^2} \right) \right], \quad (19)
 \end{aligned}$$

where

$$k = \frac{\omega_0 + \omega_z}{\sqrt{r^2 + (\omega_0 + \omega_z)^2}}.$$

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