A thermocouple spin maser

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It is demonstrated that if two spin systems maintained at different temperatures and characterized by different magnetic splittings are placed in an electromagnetic cavity common to both systems, sustained oscillations can arise in the combined system at a frequency equal to half of the detuning of the spin systems.

1. SCHEMATIC MASER DIAGRAM

The aim of this paper is to describe a new maser scheme, that is, a way of obtaining population inversion and emission. The suggested maser is a classical heat engine with a heater and cooler and resembles in structure an ordinary thermocouple, a fact reflected in the title of the paper.

Let us consider two spin systems S and I occupying regions of space that are spatially distinct. We assume that the spin of each is 1/2. Suppose that the spin system $S(I)$ contains $N_S(N_I)$ spins with a corresponding splitting $\omega_S(\omega_I)$. The temperatures of the systems are also assumed different: T_S and T_I, respectively. Since the systems are set far apart and there is no way in which they can exchange energy, the temperatures inequality can be maintained as long as desired. Next we introduce an interaction between the systems by placing them inside the coil of a common tank circuit, as depicted in Fig. 1. Spin flip in one spin system causes a current to appear in the circuit, and the induced magnetic field affects the spins of the other system. Obviously, an energy flux from the hot system to the cold sets in and tends to equalize the spin temperatures of S and I. The process can be interpreted as mutual spin flip in S and I; for instance, excitation of one of the spins in I is accompanied by the transition of one of the spins in S to the ground state. Let $T_S > T_I$, that is, the spins of S are cooling off and those of I are heating up. Hence, there are more spin flips accompanied by excitation of a spin in I and transition of a spin in S to the ground state per unit time than there are inverse processes. If $\omega_S > \omega_I$, mutual spin flip with excitation of a spin in I and deactivation of a spin in S is accompanied by an energy release equal to $\omega_S - \omega_I$. Since there are more such processes per unit time than there are inverse processes (i.e., processes in which energy $\omega_S - \omega_I$ is absorbed), the equalization of the temperatures of the two spin systems is accompanied by energy release. Each elementary mutual spin flip can be made resonant (from the viewpoint of energy conservation) by tuning the tank circuit in such a way that it absorbs the excess energy resonantly. We will see below that only two-photon excitation of the circuit is effective; hence, quantitatively the resonance condition can be written as $\omega_S - \omega_I = 2\omega$, with ω the natural frequency of the circuit. Thus, in our case equalization of the temperatures of S and I is accompanied by excitation of the tank circuit used to ensure interaction between the two systems.

The above process can be explained from another viewpoint. Let us assume, for the sake of simplicity, that $N_S = N_I = N$ and assign to each spin in S a spin in I (in an arbitrary manner). Then our two spin systems can be thought of as an ensemble of N complex "particles" each of which consists of a spin from S and the corresponding spin from I. The system of energy levels for such a particle and the level populations are shown in Fig. 2. The energy levels of the spins from S and I forming such a "particle" and the respective notation of the level populations are also shown. Obviously, if $\delta_1\sigma_2 > \delta_2\sigma_1$, population inversion is present in the first two excited states of our particle. It is easy to show that in the high-temperature approximation the population inversion condition has the form

$$\omega_I\beta_I > \omega_S\beta_S, \tag{1}$$

where $\beta = \hbar/kT$ is the inverse energy temperature of the spins. However, initial transitions between the two levels are forbidden because our particle consists of spins that belong to spatially distant samples. The presence of an interaction via the tank circuit (Fig. 1) allows such transitions to occur, and which creates conditions for maser emission.

We emphasize that the above interpretation based on a complex "particle" is not quite correct from the viewpoint of calculating the probabilities of the transitions of interest to us, because it allows for the interaction of each spin of the S species with only one spin belonging to I. A theory of the described spin maser is given below. We estimate also the probabilities of maser transitions and losses in the tank circuit. These calculations suggest that it is quite possible to achieve such emission or at least to discover an increase in the Q-factor of the tank circuit coupling the spin systems.

2. THE HAMILTONIAN

To create a consistent theory of the spin maser described above we must quantize the tank circuit. In accordance with the general method of quantization, we must build the Hamiltonian function $H(p,q)$ of the tank circuit, that is, express the circuit energy $1/2(LJ^2 + CU^2)$ (here L is the inductance of the circuit, C its capacitance, J the

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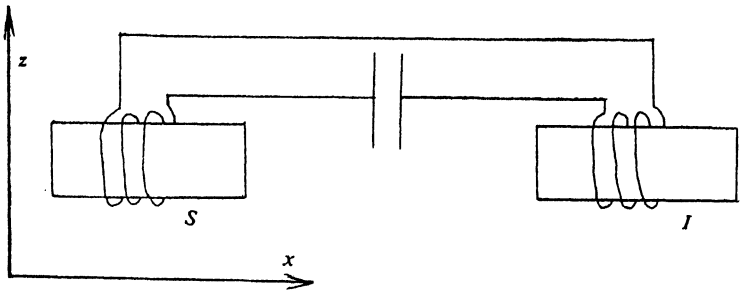

FIG. 1.

current in the circuit, and U the voltage) in terms of a generalized coordinate q and momentum p in such a way that the equations of motion for the circuit acquire the Hamiltonian form

$$\frac{\partial H}{\partial q}=-\dot{p}, \quad \frac{\partial H}{\partial p}=\dot{q}.$$

Clearly, the above can easily be achieved if we take the generalized momentum and coordinate in the form

$$p=\sqrt{L}J, \quad q=\sqrt{LC^2}U. \tag{2}$$

In this case the Hamiltonian of the circuit is $H=1/2(p^2+q^2\omega^2)$, where $\omega = 1/\sqrt{LC}$ is the circuit's natural frequency. In the quantum representation p and q are operators satisfying the commutation relation $[p,q]=-i\hbar$. By introducing the creation and annihilation operators for the excitation quanta in the circuit,

$$a=\frac{1}{\sqrt{2}}\left(\sqrt{\frac{\omega}{\hbar}}q+i\frac{p}{\sqrt{\hbar\omega}}\right), \quad a^+=\frac{1}{\sqrt{2}}\left(\sqrt{\frac{\omega}{\hbar}}q-i\frac{p}{\sqrt{\hbar\omega}}\right), \tag{3}$$

we reduce the circuit Hamiltonian to the standard form $H=1/2\hbar\omega(aa^+ +a^+a)$. To define the operator of the interaction of the circuit with the spin system we shall need below the current in the circuit expressed in terms of the creation and annihilation operators (3). Combining (2) and (3) we get

$$J=-i\sqrt{\frac{\hbar\omega}{2L}}(a-a^+). \tag{4}$$

Assume that the circuit coil encompasses an area equal to s and consists of m turns. If the coil is divided into two equal parts (Fig. 1), the magnetic field of the current flowing through one half is equal to that of the current flowing through the other and is determined by the formula $\mathscr{H}=LJ/sm$. Employing (4), we arrive at the following expression (in frequency units) for the Hamiltonian of the interaction of the circuit with the spin system:

$$H_i=\frac{g\beta\mathscr{H}}{\hbar}(S_x+I_x)=\gamma(a-a^+)(S_x+I_x), \tag{5}$$

where $\gamma = -i(g\beta/\hbar sm)\sqrt{\hbar\omega L/2}$, and S_x and I_x are the operators of the projections of the magnetic moments of S and I on the x axis (we assume that the coil axis is parallel to the x axis). If we suppose that the magnetic fields causing the initial splittings of the spin systems S and I are directed along the z axis, we get the following expression for the total Hamiltonian:

$$H=\omega_S S_z+\omega_I I_z+\frac{\omega}{2}(aa^+ +a^+a)+\gamma(a-a^+)(S_x+I_x).$$

Energy transfer between the spin systems is ensured by the interaction Hamiltonian (5), which can be replaced by a simpler effective operator obtained by the following reasoning. Assume that $\omega_I<\omega_S$ and $\omega_S-\omega_I \ll 1/2(\omega_S+\omega_I)\equiv\bar{\omega}$. We describe the state of the system by the wave function $|n,I,S\rangle$, where n is the number of photons in the tank circuit, and S_z and I_z are the projections of the total magnetic moments of S and I on the z axis (we are not interested in the other quantum numbers). Then the probability of mutual spin flip accompanied by circuit excitation,

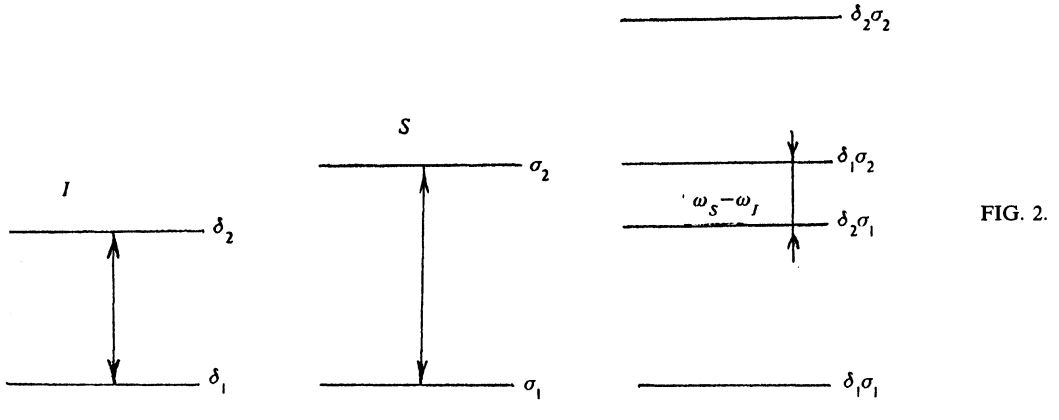

FIG. 2.

$$|n,I,S\rangle \to |n+2,I+1,S-1\rangle,$$

is determined in second-order perturbation theory by compound matrix elements for which, using the above inequalities, we can write the following approximate equality:

$$-(\omega+\omega_I)^{-1}\langle n+2,I+1,S-1|H_i|n+1,I+1,S\rangle \times\langle n+1,I+1,S|H_i|n,I,S\rangle-(\omega+\omega_S)^{-1} \times\langle n+2,I+1,S-1|H_i|n+1,I,S-1\rangle \times\langle n+1,I,S-1|H_i|n,I,S\rangle\simeq-\frac{\gamma^2}{2\bar{\omega}}\sqrt{(n+2)(n+1)}.$$

Clearly, the operator $-(\gamma^2/2\bar{\omega})S^-I^+a^+a^+$, where $S^\pm=S_x\pm iS_y$ and $I^\pm=I_x\pm iI_y$, yields in first-order perturbation theory the same transition probability as the exact operator (5) does in second-order theory. Taking into account also the inverse process, we get the effective interaction Hamiltonian in the form

$$H_{\text{eff}}=-\frac{\gamma^2}{2\bar{\omega}}(S^+I^-aa+S^-I^+a^+a^+). \tag{6}$$

In Sec. 3 we will use this operator to derive a kinetic equation for the diagonal elements of the tank circuit density matrix.

3. THE KINETIC EQUATION

Let us think of the tank circuit as a dynamic system connected to a complex thermostat, two spin systems maintained at different temperatures. The only kinetic coefficients that remain finite under the action of the operator H_{eff} [Eq. (6)], which reflects the dynamics of the circuit, are those corresponding to two-photon transitions. Hence, the equation for the diagonal elements of the density matrix (the populations of the oscillation states of the circuit) has the form

$$\dot{\rho}_n=W_{n+2\to n}\rho_{n+2}+W_{n-2\to n}\rho_{n-2}-W_{n\to n+2}\rho_n -W_{n\to n-2}\rho_n, \tag{7}$$

where the kinetic coefficients are given by the following formula:[1]

$$W_{nn'}=2\pi\sum_{ff'}\rho_f\langle fn|H_{\text{eff}}|f'n'\rangle\langle f'n'|H_{\text{eff}}|fn\rangle\delta \times(\omega_f+\omega_n-\omega_{f'}-\omega_{n'}). \tag{8}$$

Here ρ_f is the density matrix of the thermostat, with f the set of quantum numbers characterizing the state of the thermostat. In our case the thermostat's density matrix is separable, $\rho_f=\rho_S\rho_I$, where ρ_S and ρ_I are the equilibrium density matrices of the spin systems, which depend on the inverse temperatures β_S and β_I, respectively. Substituting (6) into (8) and applying standard transformations,[1] we obtain

$$W_{n\to n+2}=\left(\frac{\gamma^2}{2\bar{\omega}}\right)^2(n+1)(n+2)\int_{-\infty}^{+\infty}dte^{-2i\omega t} \times\langle S^+S^-(t)\rangle_{\rho_S}\langle I^-I^+(t)\rangle_{\rho_I},$$
$$W_{n\to n-2}=\left(\frac{\gamma^2}{2\bar{\omega}}\right)^2n(n-1)\int_{-\infty}^{+\infty}dte^{2i\omega t} \times\langle S^-S^+(t)\rangle_{\rho_S}\langle I^+I^-(t)\rangle_{\rho_I}, \tag{9}$$

where

$$S^\pm(t)=\exp(-i\omega_SS_zt)S^\pm\exp(i\omega_SS_zt),$$
$$I^\pm(t)=\exp(-i\omega_II_zt)I^\pm\exp(i\omega_II_zt),$$

and the notation $\langle\ \rangle_{\rho_S}(\langle\ \rangle_{\rho_I})$ stands for averaging with the density matrix $\rho_S(\rho_I)$. The correlation functions in Eq. (9) are related to the EPR spectrum of the spin systems[1] and can be derived explicitly. For instance, we can calculate $\langle S^+S^-(t)\rangle_{\rho_S}$ using the following chain of equalities:

$$\langle S^+S^-(t)\rangle_{\rho_S}=\exp(i\omega_St)\langle S^+S^-\rangle_{\rho_S} =N_S\exp(i\omega_St)\langle S_1^+S_1^-\rangle_{\rho_S} =\frac{\exp(i\omega_St)N_s\exp(-\beta_S\omega_S/2)}{\exp(-\beta_S\omega_S/2)+\exp(\beta_S\omega_S/2)}.$$

Here the operators S_1^+ and S_1^- refer to any spin (say, the first) of the S species.

Now let us turn to the high-temperature approximation and allow for the finite width of an EPR line, which is characterized by a phase relaxation time T_{2S} (for spins belonging to the I species this time is denoted by T_{2I}). We obtain

$$\langle S^+S^-(t)\rangle_{\rho_S}=\frac{N_S}{2}\exp\left[i\omega_St-\frac{|t|}{T_{2S}}\right]\left(1-\frac{\beta_S\omega_S}{2}\right).$$

Calculating the other correlation functions in a similar manner and introducing the notation $\beta_I\omega_I-\beta_S\omega_S\equiv\Delta$ and $T_{2S}^{-1}+T_{2I}^{-1}=T_2^{-1}$, we finally arrive at the following:

$$W_{n\to n+2}=\left(\frac{\gamma^2}{2\bar{\omega}}\right)^2(n+1)(n+2)\frac{N_IN_S}{4}(2+\Delta) \times\frac{T_2}{1+(\omega_S-\omega_I-2\omega)^2T_2^2},$$
$$W_{n\to n-2}=\left(\frac{\gamma^2}{2\bar{\omega}}\right)^2n(n-1)\frac{N_IN_S}{4}(2-\Delta) \times\frac{T_2}{1+(\omega_S-\omega_I-2\omega)^2T_2^2}. \tag{10}$$

We can easily show that the distribution of the density-matrix diagonal elements satisfying the equation

$$\frac{\rho_{n+2}}{\rho_n}=\frac{W_{n\to n+2}}{W_{n+2\to 2}}=\frac{2+\Delta}{2-\Delta}\equiv q$$

is time-independent for Eq. (7) with the kinetic coefficients (10). Clearly, these formulas can be used to express all the diagonal elements in terms of ρ_0 and ρ_1 as follows:

$$\rho_{n+2}=q\rho_n.$$

The normalization condition for the diagonal elements yields

$$\rho_0\sum_{k=0}^{\infty}q^k+\rho_1\sum_{k=0}^{\infty}q^k=\frac{\rho_0+\rho_1}{1-q}=1,$$

and, hence,

$$\rho_0+\rho_1=1-q.$$

We see that for $q<1$ there is a time-independent distribution of the level populations in the oscillatory circuit in contact with two spin thermostats. For $q\leqslant 1$ all level populations vanish, which corresponds to an unlimited increase in the amplitude of circuit oscillations, or excitation. Clearly, the condition $q>1$ is equivalent to (1). Nowhere in the above calculation have we allowed for the finiteness of the circuit's Q-factor, which must be done to estimate the possibility of the described effect. Section 4 is devoted to this aspect.

4. DAMPING IN THE QUANTIZED OSCILLATORY CIRCUIT

All along we have assumed that the circuit interacts only with the two spin thermostats but, obviously, the circuit also interacts with "its own" thermostat, the thermal vibrations in the metal from which the coil and capacitor are made. This latter interaction leads to damping of natural oscillations in the circuit. All macroscopic properties of the circuit can be correctly described if we take the operator of the interaction of the circuit with the circuit thermostat proper in the form

$$H_t=\phi(a+a^+). \tag{11}$$

Here the operator ϕ depends on the degrees of freedom of the circuit thermostat proper. The structure of (11) suggests that H_t leads only to single-photon transitions, with the result that the kinetic equation for the density-matrix diagonal elements is

$$\dot\rho_n=-\rho_n(V_{n\to n+1}+V_{n\to n-1})+\rho_{n+1}V_{n+1\to n}+\rho_{n-1}V_{n-1\to n}, \tag{12}$$

with the kinetic coefficients given by the following formulas:[1]

$$V_{n\to n+1}=\langle\phi\phi(\tau)\rangle_\omega(n+1),\quad V_{n\to n-1}=\langle\phi\phi(\tau)\rangle_{-\omega}n.$$

Here $\langle\phi\phi(\tau)\rangle_\omega$ is the spectral density of the correlation function of ϕ at the transition frequency, that is, at the frequency of circuit oscillations. Averaging is done with the equilibrium matrix density of the circuit thermostat proper, whose inverse temperature is denoted by β. The spectral density must obey the detailed-balance principle

$$\frac{V_{n\to n+1}}{V_{n+1\to n}}=\frac{\langle\phi\phi(\tau)\rangle_\omega}{\langle\phi\phi(\tau)\rangle_{-\omega}}=e^{-\beta\omega}.$$

This leads to the following expressions for the kinetic coefficients:

$$V_{n\to n+1}=K(n+1),\quad V_{n\to n-1}=Ke^{\beta\omega}n.$$

Here $K\equiv\langle\phi\phi(\tau)\rangle_\omega$.

Combining these relations with Eq. (12), we arrive at the following equation for the average number of photons in the circuit:

$$\frac{d}{dt}\sum_n n\rho_n\equiv\frac{d}{dt}\langle n\rangle=\frac{\langle n\rangle_{\rm eq}-\langle n\rangle}{\langle n\rangle_{\rm eq}/K},$$

where $\langle n\rangle_{\rm eq}=(e^{\beta\omega}-1)^{-1}$ is the Bose–Einstein function. We see that the average number of photons tends to an equilibrium value with a characteristic relaxation time $T=\langle n\rangle_{\rm eq}/K$, which is simply the time of energy decay in the circuit and is related to the circuit's Q-factor by the well-known formula

$$Q=\omega T.$$

Thus, the kinetic coefficients can be expressed in terms of easily observable circuit characteristics:

$$V_{n\to n+1}=\frac{\langle n\rangle_{\rm eq}(n+1)}{T},\quad V_{n\to n-1}=e^{\beta\omega}\frac{\langle n\rangle_{\rm eq}n}{T}. \tag{13}$$

In the next section we compare these probabilities of transitions leading to damping with (10).

5. ESTIMATES

Let us now consider that part of the kinetic coefficients (10) that is independent of the photon number,

$$W=\left(\frac{\gamma^2}{2\bar\omega}\right)^2\frac{N_IN_S}{4}T_2$$

(we assume that the circuit is in resonance, that is, $\omega_S-\omega_I=2\omega$), and the similar part for (15),

$$V=\frac{\langle n\rangle_{\rm eq}}{T}.$$

Let us fix the parameters entering into these quantities at the following (quite realistic) values: the circuit frequency $\omega=3\times10^8\ {\rm s}^{-1}$, the circuit temperature 100 K (the corresponding value of $\langle n\rangle_{\rm eq}$), the Q-factor $Q=100$, the inductance of the circuit coil $L=10^{-6}$ H, the coil's cross-sectional area $s=10^{-4}\ {\rm m}^2$, the number of turns in the coil $m=10$, the spin numbers in the two systems $N_I=N_S=10^{20}$, the average splitting $\bar\omega=3\times10^9\ {\rm s}^{-1}$, and the phase relaxation time $T_2=10^{-6}$ s. Calculations yield $W\approx10^8\ {\rm s}^{-1}$ and $V\approx10^{11}\ {\rm s}^{-1}$, that is, the losses are one thousand times greater than the gain. It is clear, however, that loss factors increase like the first power of the number of photons and gain factors like the second, which means that at sufficiently high excitation the gain exceeds the losses. For instance, at 100 K the average number of photons in the circuit is roughly 10^5. With such photon numbers the gain factors considerably exceed the loss factors.

Note that the loss factors increase like the first power of the number of photons in the circuit because the adopted operator for the interaction of the circuit with the circuit

thermostat proper contains only the first powers of the operators a and a^+ (in other words, the interaction operator is single-photon). Clearly, the operator representing the total interaction of the circuit with its thermostat can contain higher degrees of a and a^+ and describe higher-order processes. The respective kinetic coefficients will increase like higher powers of the excitation number. But is it sufficient to allow only for single-photon processes? The author believes that such an assumption is valid as long as the level of circuit excitation is so low that the circuit can be described fairly accurately by a linear differential equation (i.e., using the classical language) and free oscillations decay according to an exponential law. If we allow for multiphoton processes, it becomes impossible to obtain a closed equation for $\langle n \rangle$, and the kinetics of relaxation of the circuit to an equilibrium state becomes nonexponential. On the other hand, experience has shown that for real excitation levels the kinetics of decay of free oscillations in a circuit proves to be exponential with a high degree of accuracy. This suggests that at real excitation levels, allowing only for single-photon relaxation processes is justified.

The above ideas make it possible to hope that, if not masing, at least an increase in the Q-factor of the coupling circuit can be expected to manifest itself in experiments. A possible way to achieve this is to apply the ordinary technique used in observing NMR (EPR), which allows spotting extremely minute changes in the Q-factor of the tank circuits (cavities).

[1] I. V. Aleksandrov, *The Theory of Magnetic Relaxation*, Nauka, Moscow (1975), p. 33 [in Russian].

Translated by Eugene Yankovsky

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