Criterion for the observability of macroscopic quantum coherence

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The phenomenon of macroscopic quantum coherence is examined within the framework of a two-level system coupled to an Ohmic bath. A bound is obtained for the temperature above which the macroscopic variable cannot display the oscillatory behavior characteristic of quantum coherence. Different approximations for the dynamical behavior of the macroscopic variable in the low-dissipation limit are compared.

The purpose of this paper is to report on a criterion for how low the temperature must be in order to experimentally observe the phenomenon of macroscopic quantum coherence.[1] The sense in which the word "observe" is used here requires some explanation. The phenomenon is most likely to be seen (if at all) in an rf superconducting quantum interference device (SQUID) in a suitable external magnetic field[2] and Chakravarty and Leggett[3] have given a theory of it based on a model consisting of a two-level system (representing the two states of the macroscopic variable—the trapped flux in the case of the rf SQUID) coupled to a bath of oscillators (representing the environment).[4,5] The fundamental quantity of interest is the expectation value $P(t)$ of the flux at a time t, given that at $t=0$ it has a value corresponding to one of the two degenerate minima[6] of the potential energy, and the environment is in equilibrium with the flux held fixed at that value. It is found that unless the temperature and the dissipation arising from the coupling to the environment are both very low, $P(t)$ does not oscillate back and forth; instead, it relaxes monotonically to its equilibrium value. While a detailed experimental study of features such as the temperature dependence of the relaxation rate would provide some support for the model, an observation of oscillatory behavior would be much more dramatic and satisfying evidence for the superposition of macroscopically distinct states.[7,8] I obtain in this paper an upper bound on the temperature T^* for these oscillations to exist. This is a much more precise criterion than the order-of-magnitude estimate given in Ref. 3 and, since for currently fabricable SQUID's the temperatures at which oscillations occur are on the very verge of feasibility, it should be of value in an experimental search for them.

It should be noted at the outset that T^* does not demarcate (in the way that a phase boundary does) two regions of sharply differing behavior. The oscillations become progressively more damped as the temperature increases, and one may need temperatures two to three times below T^* for them to persist long enough. Further, T^* can only be related to $\Delta_{\rm eff}$, an effective tunneling frequency that will probably have to be found by trial and error in actuality, since it depends strongly on the amount of dissipation [see Eq. (12) below]. Within the resistively shunted-junction model of the rf SQUID, however, it can be related to the SQUID parameters fairly accurately,[9] and that should assist in narrowing the search considerably.

The approach of this paper follows that of Ref. 3 very closely. The model Hamiltonian is given by

$$H=\tfrac{1}{2}\hbar\Delta_0\sigma_x+\sum_\alpha\tfrac{1}{2}(p_\alpha^2/m_\alpha+m_\alpha\omega_\alpha^2x_\alpha^2)+\tfrac{1}{2}q_0\sigma_z\sum_\alpha c_\alpha x_\alpha\ , \tag{1}$$

where the σ's are Pauli matrices in the two-dimensional Hilbert space of the flux, Δ_0 is the bare tunneling frequency between the two states, q_0 is a measure of the flux difference between them, and the $\{x_\alpha,p_\alpha\}$ are the coordinates and momenta of a set of oscillators with masses $\{m_\alpha\}$ and frequencies $\{\omega_\alpha\}$.[5] The coupling constants c_α are constrained only by the spectral density $J(\omega)$, which is taken to be of the Ohmic form:

$$J(\omega)\equiv\frac{\pi}{2}\sum_\alpha(c_\alpha^2/m_\alpha\omega_\alpha)\delta(\omega-\omega_\alpha)=\eta\omega\exp(-\omega/\omega_c)\ , \tag{2}$$

where η is the friction coefficient, and ω_c is a cutoff frequency that is much larger than Δ_0 or $k_BT/\hbar$, but is much smaller than the classical small oscillation frequency in either well. It is convenient to introduce the dimensionless dissipation parameter α:

$$\alpha=\eta q_0^2/2\pi\hbar\ . \tag{3}$$

As shown in Ref. 3, $P(t)$ can be formally written as

$$P(t)=\sum_{n=0}^{\infty}(-\Delta_0^2)^n\int_0^t dt_{2n}\int_0^{t_{2n}}dt_{2n-1}\cdots\int_0^{t_2}dt_1F(t_1,t_2,\ldots,t_{2n})\ , \tag{4}$$

$$F=\exp\left[-\frac{q_0^2}{\pi\hbar}\sum_{j=1}^{n}S_j\right]2^{-n}\sum_{(\zeta_j=\pm1)}\exp\left[-\frac{q_0^2}{\pi\hbar}\sum_{\substack{j,k=1\\ j>k}}^{n}\Lambda_{jk}\zeta_j\zeta_k\right]\prod_{k=0}^{n-1}\cos\left[\frac{q_0^2}{\pi\hbar}\sum_{j=k+1}^{n}X_{jk}\right]\ . \tag{5}$$

Further,

$$S_j=P_{2j,2j-1}\ , \tag{6a}$$

$$\Lambda_{jk}=P_{2k,2j-1}+P_{2k-1,2j}-P_{2k,2j}-P_{2k-1,2j-1}\ , \tag{6b}$$

$$X_{jk}=R_{2j,2k+1}+R_{2j-1,2k}-R_{2j,2k}-R_{2j-1,2k+1}\ , \tag{6c}$$

where $P_{n,m}=Q_2(t_n-t_m)$, $R_{n,m}=Q_1(t_n-t_m)$, and the functions Q_1 and Q_2 are second integrals of the real and imaginary parts of the influence functional. For the spectral density (3), these take the form

$$Q_1(t)=\eta\tan^{-1}(\omega_ct)\ , \tag{7a}$$

$$Q_2(t)=\tfrac{1}{2}\eta\ln(1+\omega_c^2t^2)+\eta\ln\left[\frac{\beta\hbar}{\pi t}\right]\sinh\left[\frac{\pi t}{\beta\hbar}\right]\ , \tag{7b}$$

where $\beta=1/k_BT$, and it is understood that t_0 equals $-\infty$ in the above formulas.

The expression (1) can be thought of as a grand partition function of a system of interacting "blips," which are defined to be the segments $t_{2j-1}\leq t\leq t_{2j}$. (The remaining segments are called "sojourns."[3]) The quantity S_j is the self-energy of a blip, Λ_{jk} is the interaction between blips, and X_{jk} is a "blip-sojourn" phase factor. Following Ref. 3, we now assume that the only important configurations are those in which the blips are much narrower than the "sojourns." In that case one can neglect Λ_{jk} altogether, as well as all the phase factors X_{jk} except those with $k=j-1$, which can be approximated by $R_{2j,2j-1}$. The resulting approximation to $P(t)$, denoted $P_0(t)$, is then given by

$$P_0(t)=\sum_n(-1)^n\int_0^t dt_{2n}\int_0^{t_{2n}}dt_{2n-1}\cdots\int_0^{t_2}dt_1\prod_{j=1}^{n}f(t_{2j}-t_{2j-1})\ , \tag{8}$$

where

$$f(t)=\Delta_0^2\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp\left[-\frac{q_0^2}{\pi\hbar}Q_2(t)\right]\ . \tag{9}$$

It is advantageous to switch to the analogue of an isobaric ensemble via a Laplace transformation,[10] which converts Eq. (8) into a geometric series whose sum is

$$\tilde{P}_0(\lambda)=[\lambda+\tilde{f}(\lambda)]^{-1}\ . \tag{10}$$

Here, the tildes denote Laplace transforms, and λ is the transform variable. As $\lambda/\omega_c\to 0$, $\tilde{f}(\lambda)$ is asymptotically given by

$$\tilde{f}(\lambda)\sim\Delta_{\rm eff}^{2-2\alpha}(2\gamma)^{2\alpha-1}\Gamma(\alpha+\lambda/2\gamma)/\Gamma(1-\alpha+\lambda/2\gamma)\ , \tag{11}$$

where

$$\Delta_{\rm eff}=\Delta_0\left(\frac{\Delta_0}{\omega_c}\right)^{\alpha/(1-\alpha)}[\cos(\pi\alpha)\Gamma(1-2\alpha)]^{1/(2-2\alpha)}\ , \tag{12}$$

and $\gamma=\pi k_BT/\hbar$. By taking inverse Laplace transforms, one can[4] reproduce all the results of Ref. 3.

The approximation of neglecting interblip interactions is not quite as arbitrary as it seems, provided one does not want $P(t)$ for very long times.[11] This is because $Q_2(t)$ grows with t and thus suppresses long blips via the S_j factors. Further, the aproximation improves with increasing temperature, and if we can show it to be good at $T=0$, we will have justified it for all $T>0$. We can do this fairly convincingly everywhere except in the range $\frac{1}{2}<\alpha<1$, but since $P(t)$ oscillates only if $\alpha<\frac{1}{2}$, this shortcoming will not matter for the purpose of this paper. Since the interactions can be of either sign (i.e., $\zeta_j\zeta_k$ can equal $+1$ or -1), their contribution vanishes as α^2 as $\alpha\to 0$, and it can be argued[4] that it also vanishes as $(1-2\alpha)$ as $\alpha\to\frac{1}{2}$. A somewhat more quantitative assessment can be made by including only the *nearest-neighbor* interblip interactions. These can be treated via a transfer matrix whose eigenvalues and eigenvectors can be found numerically.[12] The resulting approximation to $P(t)$, denoted $P_1(t)$, has the following structure:

$$P_1(t)=\sum_{m=1}^{\infty}A_m(\alpha)P_0(t;\Delta_m)+\left[1-\sum_{m=1}^{\infty}A_m\right], \tag{13}$$

$$\Delta_m=\Delta_{\rm eff}[e_m(\alpha)]^{1/2(1-\alpha)}\ . \tag{14}$$

Here, $P_0(t;\Delta_m)$ is given by Eq. (24) of Ref. 3, with $A(\alpha)$ set to unity, $\Delta P(t)$ set to zero, and $\Delta_{\rm eff}$ replaced by Δ_m. The first two eigenvalues $e_m(\alpha)$ and related amplitudes $A_m(\alpha)$ for $m=1,2$ are shown in Table I for selected values of α. Note that A_2 is never greater than about 5%, and that it vanishes both as $\alpha\to 0$ and as $\alpha\to\frac{1}{2}$. We do not show the A_m's and e_m's for $m\geq 2$, since they are much smaller and their contribution is entirely negligible.[13] The corrections to $P_1(t)$ vanish as $(1-2\alpha)^2$ as $\alpha\to\frac{1}{2}$.[4]

Since $\Delta_1\gg\Delta_2,\Delta_3,\ldots$, the terms with $m\geq 2$ in Eq. (13) dominate the behavior of $P(t)$ at very long times. By these times, however, $P(t)$ is very close to zero, and if one is interested primarily in looking for oscillatory behavior, it suffices to retain only the first term in Eq. (13). The result is the same as would be obtained by inverting Eq. (10) (at $T=0$), except for minor corrections to $\Delta_{\rm eff}$ and the overall amplitude of $P(t)$. In light of the earlier discussion, we can expect Eqs. (10) and (11) to provide an even better approximation for $T>0$.

The upper bound $T^*(\alpha)$ is now obtained by noting that for $\alpha<\frac{1}{2}$ and $T=0$, $\tilde{P}_0(\lambda)$ has a pair of complex-conjugate poles on the circle $|\lambda|=\Delta_{\rm eff}$, and a branch point at $\lambda=0$. The poles lead to the oscillatory part of $P(t)$ and the branch point leads to the incoherent part $P_{\rm inc}$ defined in Eq. (24) of Ref. 3. As the temperature is increased, the branch cut degenerates into a set of poles on the negative real λ axis, with an uneven spacing that grows roughly linearly with T.

TABLE I. Eigenvalues and associated amplitudes for the nearest-neighbor interblip transfer matrix for selected values of α [see Eqs. (13) and (14)].

α	e_1	A_1	e_2	A_2
0.1	1.012	0.988	0.00525	0.00913
0.2	1.039	0.962	0.0218	0.0283
0.25	1.052	0.950	0.0350	0.0390
0.3	1.06	0.94	0.0525	0.048
0.4	1.06	0.94	0.0105	0.053
0.45	1.05	0.95	0.0145	0.040
0.495	1.01	0.99	0.0195	0.006

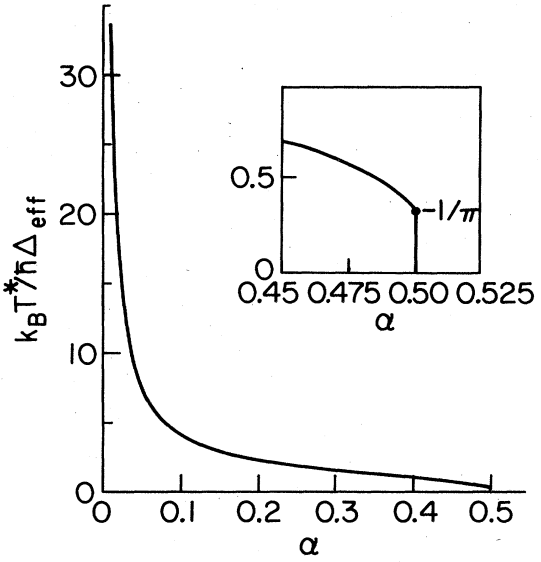

FIG. 1. The upper bound $T^*(\alpha)$ on the temperature above which $P(t)$ cannot show oscillatory behavior.

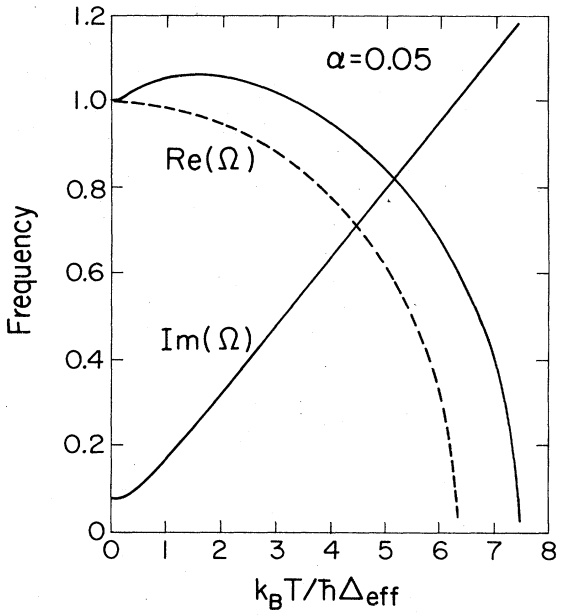

FIG. 2. Real and imaginary parts of the complex frequency Ω for $P_{NMR}(t)$ (broken line) and $P_{osc}(t)$ (solid line). Since the two imaginary parts are too close to resolve on this figure, only that for P_{osc} is shown. The unit of frequency is Δ_{eff}.

(Note that there is no pole at $\lambda=0$.) The complex-conjugate pair of poles moves towards the negative real axis, eventually hits it, and then moves along it in opposite directions. If we now define $T^*(\alpha)$ to be the temperature at which these two poles coincide, it is clear that for $T > T^*(\alpha)$, $P(t)$ is given by a sum of decaying exponentials, and cannot show oscillatory behavior. It is straightforward to show that

$$2\gamma^* \equiv \frac{2\pi kT^*(\alpha)}{\hbar\Delta_{eff}} = \left[-\frac{1}{u^*}\frac{\Gamma(\alpha+u^*)}{\Gamma(1-\alpha+u^*)} \right]^{1/(2-2\alpha)} , \quad (15)$$

where u^* is the real, negative solution to the equation

$$u^*[\psi(\alpha+u^*)-\psi(1-\alpha+u^*)]=1 , \quad (16)$$

where ψ is the digamma function. The results of solving Eqs. (15) and (16) numerically are shown in Fig. 1. As $\alpha \to 0$, the solutions for γ^* and λ^* are given by

$$\gamma^*/\Delta_{eff}(\alpha) \approx \alpha^{-1} - \ln\alpha + O(\alpha\ln\alpha) , \quad (17a)$$

$$\lambda^*/\Delta_{eff}(\alpha) \approx -1 + \alpha\ln\alpha + O(\alpha^2\ln\alpha) . \quad (17b)$$

Similarly, as $\alpha \to \frac{1}{2}$,

$$\gamma^*/\Delta_{eff}(\alpha) \approx 1 + 4(\tfrac{1}{2}-\alpha)^{1/2} + O(1-2\alpha) , \quad (18a)$$

$$\lambda^*/\Delta_{eff}(\alpha) \approx -1 - 2(\tfrac{1}{2}-\alpha)^{1/2} + O(1-2\alpha) . \quad (18b)$$

I conclude this paper with a comparison of two approximate treatments of the very low α region (less than 0.1, say). This region is likely to be the most relevant to the experimental observation of oscillations in $P(t)$ for two reasons. First, in absolute terms, T^* drops even more precipitously with increasing α than Fig. 1 would suggest, because of the α dependence of Δ_{eff}. Second, even at $T=0$, the oscillatory part of $P(t)$ has a Q factor of $\frac{1}{2}\cot[\pi\alpha/2(1-\alpha)]$, which also decreases rapidly with increasing α.

The first approximation [denoted $P_{NMR}(t)$] is obtained by doing perturbation theory in α. One can write down a set of Bloch-like equations for the "spin" components $\langle\sigma_i(t)\rangle$, which lead to the following equation for P_{NMR}:

$$\ddot{P}_{NMR} + T_2^{-1}\dot{P}_{NMR} + \Delta_0^2 P_{NMR} = 0 , \quad (19)$$

with

$$T_2^{-1} = \pi\alpha\Delta_0\coth(\hbar\Delta_0/2k_BT) . \quad (20)$$

The second approximation [denoted $P_{osc}(t)$] is obtained by inverting $\tilde{P}_0(\lambda)$, and retaining only the contributions from the complex-conjugate poles for $T \leq T^*$, or the two real poles into which they transform for $T > T^*$.[14] The neglected terms can be shown to be order α for $T=0$, and of order α^3 for $T \gtrsim T^*$.

Plainly, $P_{osc}(t)$ satisfies the equation of motion of a damped harmonic oscillator, which will in general differ from Eq. (19). It is clear that the perturbative approach misses the frequency renormalization effect, but one might wonder how well it does even if this is put in by hand, i.e., Δ_0 is replaced by Δ_{eff} everywhere in Eqs. (19) and (20). Figure 2 shows the real and imaginary parts of the complex frequency associated with both $P_{NMR}(t)$ and $P_{osc}(t)$ as a function of T for $\alpha=0.05$. It is amusing that while the damping rate is virtually the same for the two approximations, the true oscillation frequency [which should be very close to that of $P_{osc}(t)$] is higher than that indicated by $P_{NMR}(t)$.

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[1]A. J. Leggett, in *Proceedings of NATO Advanced Study Institute on Percolation, Localization, and Superconductivity,* edited by A. Goldman and S. Wolf (Plenum, New York, 1984).

[2]See, for example, R. de Bryun Oubouter, in *Proceedings of the International Symposium on the Foundations of Quantum Mechanics in the Light of New Technology,* edited by S. Kamefuchi (Physical Society of Japan, Tokyo, 1984).

[3]S. Chakravarty and A. J. Leggett, Phys. Rev. Lett. **52**, 5 (1984).

[4]A comprehensive study of the macroscopic quantum coherence problem is given in A. J. Leggett, S. Chakravarty, A. Dorsey, M. P. A. Fisher, Anupam Garg, and W. Zwerger (unpublished).

[5]A thorough discussion of the use of a set of oscillators for describing the environment of a quantum system is given in A. O. Cladeira and A. J. Leggett, Ann. Phys. (N.Y.) **149**, 374 (1983).

[6]If the trapped flux due to the applied magnetic field is not precisely half a flux quantum, then the minima are nondegenerate, and observing oscillations in $P(t)$ is even more problematical.

[7]A somewhat quantitative formulation of when two states can be regarded as *macroscopically* distinct is given in A. J. Leggett, Prog. Theor. Phys. **69**, 80 (1980).

[8]Such an observation would not, of course, *prove* that superpositions of macroscopically distinct states exist. It is possible, however, to obtain criteria that allow one to rule out the hypothesis that the macroscopic system *is* always in one state or another. See A. J. Leggett and Anupam Garg, Phys. Rev. Lett. **54**, 857 (1985).

[9]A. Dorsey, M. P. A. Fisher, M. Wartak, and A. J. Leggett (unpublished).

[10]This method has also been used by H. Grabert and U. Weiss, Phys. Rev. Lett. **54**, 1605 (1985); M. P. A. Fisher and A. Dorsey, *ibid.* **54**, 1609 (1985), in very similar problems.

[11]Equations (10) and (11) also involve an approximation to $P(t)$ for very short times, of order ω_c^{-1}.

[12]We continue to approximate X_{jk} by $\delta_{j,k-1}R_{2j,2j-1}$, and $Q_1(t)$ by $\eta\pi/2$, and to neglect the 1 in comparison to $(\omega_c t)^2$ in Eq. (7b). These approximations affect $P(t)$ only for $t \lesssim \omega_c^{-1}$.

[13]Since $P_0(t) \to 0$ as $t \to \infty$, it would appear that $P_1(\infty)$ does not vanish due to the last term in Eq. (13). My numerical evidence indicates, however, that $\sum A_m = 1$, and I suspect that this is so, although I do not have a proof.

[14]The approximation P_{NMR} is obtained, e.g., by R. A. Harris and R. Silbey, J. Chem. Phys. **78**, 7330 (1983). The same authors [J. Chem. Phys. **80**, 2615 (1984)], use a variational approach to obtain an equation for $P(t)$ of the same form as Eq. (19). While this method gives the oscillation frequency and damping rate reasonably accurately for small α and T, it misses perforce the incoherent part $P_{\mathrm{inc}}(t)$. It also indicates that for $T=0$, oscillations in $P(t)$ persist up to $\alpha = 2/\pi$ as opposed to the true result $\alpha = \frac{1}{2}$. [The latter conclusion is supported by an essentially exact treatment of the behavior of $P(t)$ on the line $\alpha = \frac{1}{2}$ contained in Ref. 4.]