Is Macroscopic Quantum Coherence Incompatible with Macroscopic Realism? (*)

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(ricevuto il 19 Gennaio 1995)

Summary. — The proposal by Leggett and Leggett *et al.* (*Suppl. Prog. Theor. Phys.*, **69** (1980) 80; *Directions in Condensed Matter Physics*, edited by G. GRINSTEIN and G. MAZENKO (World Scientific, Singapore) 1986, p. 189; *Jpn. J. Appl. Phys.*, **26** (1987) 1986, *Suppl.* 26-3; *Phys. Rev. Lett.*, **54** (1985) 857) of using Macroscopic Quantum Coherence (MQC) in a SQUID as a test of the validity of Quantum Mechanics (QM) for macroscopic systems is considered. We note that if only Macroscopic Realism (MR) is assumed but the requirement that the flux measurement is non-invasive (NIM) is dropped, only the measurement of the charge would discriminate between QM and MR. This discrimination, however, depends critically on the experimental parameters. There is a region in which QM is consistent with MR, but the measurement is invasive as in QM. In this region the system is not fully macroscopic because the uncertainty relation between the flux and the conjugated charge is of the order of h.

PACS 03.65.Bz – Foundations, theory of measurement, miscellaneous theories.
PACS 74.50 – Proximity effects, tunneling phenomena and Josephson effects.
PACS 01.30.Cc – Conference proceedings.

1. – Introduction.

The essence of quantum mechanics (QM) is the superposition principle of states. If ψ_1, ψ_2 are two eigenstates of a variable G corresponding to the eigenvalues g_1, g_2, then

$$\psi = a_1 \psi_1 + a_2 \psi_2 \tag{1}$$

is a state in which the value of G is essentially undetermined until it acquires one of

(*) Paper presented at the International Conference «Mesoscopic Physics and Fundamental Problems in Quantum Mechanics», Rome, February 14-17, 1994.

its two possible values in the act of measurement. There is no doubt about the validity of eq. (1) and its interpretation for microscopic systems. The question however arises whether it is also valid for macroscopic bodies. This question is crucial for the issue of macroscopic realism. In fact, we are accustomed to believe that the variables of macroscopic bodies always have a definite value (even if unknown to us). This assumption contrasts with the quantum-mechanical statement that in the state (1) $\boldsymbol{G}$ is undetermined before measurement. How can we reconcile the universal validity of QM with our everyday experience?

To this question one can answer in the following way [1]. Consider the Wigner function $W(x, p)$ of a state $|\psi\rangle$ given by

$$W(x, p) = \int \exp[4\pi i p y/h] \langle x + y|\psi\rangle\langle\psi|x - y\rangle \, dy . \tag{2}$$

$W(x, p)$ is, of course, not positive-definite, and cannot therefore be interpreted as a probability. However, the mean value of a physical quantity $A(x, p)$ defined in terms of the operator $\boldsymbol{A}$ by means of

$$A(x, p) = \int \exp[-4\pi i p z/h] \langle x + z|\boldsymbol{A}|x - z\rangle \, dz \tag{3}$$

is given by the expression

$$\langle \boldsymbol{A} \rangle = \int W(x, p) A(x, p) \, dx \, dp \tag{4}$$

which closely parallels the classical expression for the mean value of the classical variable $A_{cl}(x, p)$ corresponding to $\boldsymbol{A}$:

$$\langle A_{cl} \rangle = \int f(x, p) A_{cl}(x, p) \, dx \, dp , \tag{5}$$

where $f(x, p)$ is the positive-definite classical distribution function in phase space corresponding to the quantum state ψ.

It is interesting to notice that for the quantum variables $\boldsymbol{x}$ and $\boldsymbol{p}$ the product of the uncertainties $\langle(\boldsymbol{x} - \langle\boldsymbol{x}\rangle)^2\rangle = \Delta x^2$ and $\langle(\boldsymbol{p} - \langle\boldsymbol{p}\rangle)^2\rangle = \Delta p^2$ computed by (3), (4) is always given by

$$\Delta x^2 \, \Delta p^2 = (\Delta x^2)_{cl} (\Delta p^2)_{cl} + O(h) , \tag{6}$$

where $(\Delta x^2)_{cl}$ and $(\Delta p^2)_{cl}$ are computed by means of (5) and $O(h)$ vanishes for $h \to 0$ [2]. A similar expression holds for any two conjugated variables $\boldsymbol{A}$ and $\boldsymbol{B}$.

This means that when the quantum contribution is much smaller than the classical statistical uncertainty we are in the domain of classical statistical mechanics, namely we should attribute the uncertainty to ignorance of the actual values of $\boldsymbol{x}$ and $\boldsymbol{p}$ rather than to an essentially intrinsic quantum uncertainty. One should not say, as one does usually, that these variables do not have a value until they are measured, but only that they have a value (within the quantum uncertainty which is always present even if negligible compared with the classical one) unknown to us. This entails also that variables with a classical limit in a superposition of macroscopically different states of the form (1) have an unknown value corresponding *either* to ψ_1 *or* ψ_2 even before measurement. This means that the density matrix W associated to the superposition

(1) is practically equivalent to the corresponding statistical mixture

$$\underline{W} = |a_1|^2 \, |\psi_1\rangle\langle\psi_1| + |a_2|^2 \, |\psi_2\rangle\langle\psi_2| \, . \tag{7}$$

For these variables we can therefore speak of macroscopic realism. However, for variables whose uncertainties have a substantial quantum contribution, macroscopic realism fails to be valid.

2. – Flux tunnelling oscillations in a SQUID.

It is therefore extremely interesting to investigate whether the possibility exists of making a macroscopic system such that the coherence effects of the linear superposition (1) may be detected. One of the most promising devices in this perspective is provided by the flux tunnelling oscillations in a SQUID (Superconducting QUantum Interference Device) [3].

The SQUID, as is well known, is a superconducting ring interrupted by a Josephson junction (JJ). The magnetic flux Φ through the ring reverses its sign as the current (of the order of 10^{22} Cooper pairs) oscillates in the ring. The junction is a thin non-conducting barrier allowing the leakage of a current i_J. The SQUID is caracterized by a capacitance C and an inductance L. We neglect the resistance for the present considerations. The basic equations of the SQUID are the following.

If we denote by

$$\psi = \rho^{1/2} \exp[i\theta] \tag{8}$$

the common wave function of the Cooper pairs in the superconducting ring, from the expression of the current j,

$$j = (\rho/m)[(h/2\pi)\operatorname{grad}\theta - qA] \tag{9}$$

(A is the vector potential) we have

$$(h/2\pi)\,\Delta\theta = q\int \operatorname{rot} A \, \mathrm{d}S = q\Phi \, , \tag{10}$$

where $\Delta\theta$ is the phase difference on the two sides of the junction, because $j = 0$ inside the superconductor.

Furthermore, the current i_J through JJ is ($q = 2e$)

$$i_{eJ} = i_0 \sin\Delta\theta = i_0 \sin(4\pi e\Phi/h) \, , \tag{11}$$

where i_0 is the critical current.

It is straightforward now to write down the classical energy of the SQUID:

$$H = (1/2)CV^2 + (1/2)Li^2 + \int V i_J \, \mathrm{d}t \, , \tag{12}$$

namely, introducing the variable Φ ($V = \mathrm{d}\Phi/\mathrm{d}t$) and the elementary fluxon $\Phi_0 = h/2e$,

$$H_c = (1/2)C(\mathrm{d}\Phi/\mathrm{d}t)^2 + (1/2L)(\Phi - \Phi_{ext})^2 - (\Phi_0 i_0/2\pi)\cos(2\pi\Phi/\Phi_0) \, . \tag{13}$$

We notice that the momentum p_Φ conjugated to Φ is

$$p_\Phi = C\,\mathrm{d}\Phi/\mathrm{d}t = Q\,, \tag{14}$$

namely the charged Q stored in the SQUID.

We now transform the classical Hamiltonian (13) into a quantum Hamiltonian by replacing p_Φ with the operator $(h/2\pi i)\,\partial/\partial\Phi$. We thus have

$$\boldsymbol{H} = -((h/2\pi)^2/2C)\,\partial^2/\partial\Phi^2 + U(\Phi) \tag{15}$$

with

$$U(\Phi) = (1/2L)(\Phi - \Phi_{\mathrm{ext}})^2 - (\Phi_0 i_0/2\pi)\cos(2\pi\Phi/\Phi_0)\,. \tag{16}$$

The external flux Φ_{ext} may be chosen equal to $\Phi_0/2$. Then U becomes symmetrical around $\Phi = \Phi_0/2$, and, for suitably chosen values of L, i_0, and C, it has the shape of a double-well potential with the minima Φ_+, Φ_- such that

$$\Phi_+ + \Phi_- = \Phi_0\,, \qquad 0 < \delta\Phi = \Phi_+ - \Phi_- < \Phi_0\,. \tag{17}$$

Near each minimum the potential is approximately an harmonic-oscillator potential of frequency ω. On denoting by $\psi_\sigma(\Phi)$ (with $\sigma = \pm 1$) the ground-state wave functions of the two oscillators centred, respectively, at Φ_+, Φ_-, the Schrödinger equation

$$\boldsymbol{H}\Psi(\Phi, t) = i(h/2\pi)\,\partial\Psi(\Phi, t)/\partial t \tag{18}$$

admits solutions with initial value $\Psi_\sigma(\Phi, t_0) = \psi_\sigma(\Phi)$ of the form

$$\Psi_\sigma(\Phi, t) = \psi_\sigma(\Phi)\cos\Omega(t - t_0) - i\psi_{-\sigma}(\Phi)\sin\Omega(t - t_0)\,. \tag{19}$$

The frequency Ω may be calculated in terms of the potential parameters and is generally $\ll \omega$. The probabilities of finding at time t the flux Φ in the states $\psi_\sigma(\Phi)$, $\psi_{-\sigma}(\Phi)$ are therefore

$$P(\sigma, t; \sigma, t_0) = \cos^2\Omega(t - t_0)\,, \qquad P(-\sigma, t; \sigma, t_0) = \sin^2\Omega(t - t_0)\,. \tag{20}$$

3. – Macroscopic Quantum Coherence as a test of Quantum Mechanics for macroscopic systems.

Leggett and Garg have proposed [4] to use the oscillations of the magnetic flux trapped in a SQUID as a test of the validity of QM for macroscopic systems. More precisely, they argue that the predictions of QM are incompatible with the following two assumptions which should characterize the behaviour of a macroscopic system:

a) Macroscopic Realism (MR), namely that a macroscopic system will always be in either one or the other of two macroscopically distinct states;

b) Non-Invasive Measurability (NIM), namely that it is possible to determine the state of the system with arbitrarily small perturbation.

The proof goes as follows. Denote by σ_i the value (± 1) of Φ measured at time t_i. Then from *a*) one derives

$$\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 - \sigma_1\sigma_4 \leqslant 2\,. \tag{21}$$

By averaging on a statistical ensemble and introducing the two times correlations K_{ij}

$$K_{ij} = \langle \sigma_i \sigma_j \rangle , \tag{22}$$

one gets

$$K_{12} + K_{23} + K_{34} - K_{14} \leqslant 2 . \tag{23}$$

Assumption *b*) comes into play because if one wants to compare QM with MR one must assume that, by making flux measurements at t_1, t_2 or t_2, t_3 or t_3, t_4 or t_1, t_4 on *different* ensembles (since the QM predictions for K_{ij} are only valid if the evolution between t_i and t_j is not disturbed by intermediate measurements), the results would be the same *as if* the measurements were performed on a unique ensemble at all times.

On the other hand, eq. (20) shows that QM gives

$$K_{ij} = \sum_{\sigma} \sigma_i \sigma_j P(\sigma_i t_i;\, \sigma_j t_j) = \cos^2 \Omega(t_i - t_j) - \sin^2 \Omega(t_i - t_j) = \cos 2\Omega(t_i - t_j) . \tag{24}$$

This expression violates the Bell-type inequality (23) (*e.g.*, if we take $t_2 - t_1 = t_3 - t_2 = t_4 - t_3 = \pi/8\Omega$, the left-hand side is $2\sqrt{2}$). QM is therefore incompatible with MR + NIM.

4. – Macroscopic Quantum Coherence and MR.

It may be, however, interesting to investigate whether a separate test of MR would be possible without assuming NIM. An experimental proposal to test NIM independently has in fact been recently proposed [5] and is currently in preparation. In fact, NIM is independent of RM and one may well conceive a theory in which the system will always have either one or the other of the two values of the flux, but the time evolution of the relevant probabilities will start again from the new initial condition corresponding to the measured value of Φ whenever a measurement is performed, as in QM.

A macrorealistic model of this type can be constructed by describing the system by means of the density matrix

$$\underline{W}(t) = \psi_\sigma(\Phi)\psi_\sigma^*(\Phi)\cos^2 \Omega(t - t_0) + \psi_{-\sigma}(\Phi)\psi_{-\sigma}^*(\Phi)\sin^2 \Omega(t - t_0) \tag{25}$$

obtained from the density matrix $W(t)$ of the pure state (19) by dropping the off-diagonal terms. Expression (25) describes in fact a statistical mixture, in which the flux is *either* in one *or* in the other of these two states, representing the previously discussed classical limit of the quantum density matrix when both $\psi_\sigma(\Phi)$ and $\psi_{-\sigma}(\Phi)$ are macroscopically different. In fact, when the distance between the two wells becomes macroscopic, the overlap of $\psi_\sigma(\Phi)$ and $\psi_{-\sigma}(\Phi)$ vanishes exponentially [6]. The same thing happens for the off-diagonal contributions to the mean value of any observable with a classical limit.

It is then clear that the predictions of the MR model for the flux measurements are identical to those of QM because both $\underline{W}(t)$ and $W(t)$ give the same probabilities (20) of finding the flux in either the state $\psi_\sigma(\Phi)$ or $\psi_{-\sigma}(\Phi)$ at time t. It is therefore also clear that no experiment in which only the flux is measured can distinguish between this MR model and QM.

Only if one measures the variable Q conjugated to Φ can one test therefore the validity of the superposition principle for the macroscopic flux coherent oscillations in the double well. In fact, since

$$Q = (h/2\pi i)\,\partial/\partial\Phi\,, \tag{26}$$

one obtains, for the wave function $\Theta(Q, t)$ in Q-space

$$\Theta_\sigma(Q, t) = (h)^{-1/2}\int \Psi_\sigma(\Phi, t)\exp[-2\pi i Q\Phi/h]\,\mathrm{d}\Phi\,. \tag{27}$$

By using (19) and taking into account that the ground-state oscillator wave functions $\psi_\sigma(\Phi)$ are given by

$$\psi_{\pm 1}(\Phi) = (\beta/\pi)^{1/4}\exp[-\beta(\Phi - \Phi_\pm)^2/2]\,, \qquad \beta = 2\pi C\omega/h\,, \tag{28}$$

we obtain the probability $P_\sigma(Q, t) = |\Theta_\sigma(Q, t)|^2$ of finding the value Q of the charge at time t,

$$P_\sigma(Q, t) = 2(\pi/\beta h^2)^{1/2}\exp[-4\pi^2 Q^2/\beta h^2]\{1 + \sigma\sin 2\Omega(t - t_0)\sin[2\pi Q\,\delta\Phi/h]\}\,. \tag{29}$$

The oscillating interference term is characteristic of QM. In the MR model (25) this term is missing. It is therefore possible, at least in principle, to discriminate between QM and MR by measuring the variable Q. The easiest thing to do might be to determine the sign of Q. Then the probability $P_\sigma(Q > 0)$ is given by

$$P_\sigma(Q > 0, t) = (1/2)\{1 + \sigma\exp[-\beta(\delta\Phi)^2/4]\sin 2\Omega(t - t_0)\}\,. \tag{30}$$

The coefficient of the oscillating term, however, depends critically on the actual values of the experimental parameters. If one takes the values $C \approx 2\cdot 10^{-13}\,\mathrm{F}$, $\omega \approx \approx 3\cdot 10^9\,\mathrm{Hz}$, $\delta\Phi \approx \Phi_0/2$ from the available experimental proposals [5, 7], the absolute value of the argument of the exponential is of the order of one. This means that an increase of these parameters of a factor of some units is sufficient to reduce drastically the visibility of the quantum interference effect. If this happens QM is consistent with MR because there is no observable difference between the quantum-mechanical density matrix $W(t)$ and the density matrix $\underline{W}(t)$ of the corresponding mixture.

5. – The uncertainty relation for Q and Φ.

It might be possible therefore that the experiments yield results which are consistent with MR (absence of interference terms) but incompatible with NIM (measurements are always invasive). To understand how this may happen, it is useful to work out the uncertainty relations between Φ and Q in the state (3). One finds

$$(\Delta\Phi)^2 = 1/2\beta + (\delta\Phi)^2\cos^2\Omega(t - t_0)\sin^2\Omega(t - t_0)\,, \tag{31}$$

$$(\Delta Q)^2 = (h/2\pi)^2\beta/2 - \langle Q\rangle^2 \approx (h/2\pi)^2\beta/2 \tag{32}$$

because $\langle Q\rangle^2$ is negligible compared to $\langle Q^2\rangle$ when the overlap between $\psi_\sigma(\Phi)$ and $\psi_{-\sigma}(\Phi)$ is small. One has therefore

$$(\Delta\Phi)^2(\Delta Q)^2 = (h/2\pi)^2/4 + (h/2\pi)^2(\beta/2)(\delta\Phi)^2\cos^2\Omega(t - t_0)\sin^2\Omega(t - t_0)\,. \tag{33}$$

The first term is clearly the minimum quantum indeterminacy. The second term oscillates between zero and $\lambda(h/2\pi)^2$ with

$$\lambda = h\pi C\omega/16e^2 \approx (1/4)\,\pi^2 \tag{34}$$

for the values of the experiment parameters chosen above.

In conclusion,

$$h/4\pi \leqslant \Delta\Phi\,\Delta Q < \approx h/4\,. \tag{35}$$

The value of the uncertainty relation is therefore still of the order of h. This indicates that, in spite of the presence of a macroscopic number of Cooper pairs in the current, the relevant variables Q and Φ are still quantum variables.

This explains why NIM might be violated without violation of MR. It should be noted, in fact, that, while the interference term in (30) vanishes exponentially with increasing $\beta(\delta\Phi)^2$, the maximum uncertainty increases as $\beta^{1/2}\,\delta\Phi$. This means that the transition from the quantum to the classical domain goes through an intermediate region in which the interference term vanishes, while the uncertainty product is still of the order of h. It is not surprising, therefore, that in this region QM may be compatible with MR but not with NIM (the measurement is invasive when the uncertainty is of the order of the intrinsic minimum quantum uncertainty) [1]. Only when the uncertainty becomes large compared to the minimum quantum uncertainty, the transition to the classical domain will be completed [2].

Let us summarize our conclusions. The first test of the quantum-mechanical behaviour of the flux oscillations in an r.f.-SQUID is the measurement of the flux sign. This may be done in principle using a d.c.-SQUID [8]. If the probability $P(\pm\sigma, t_1; \sigma, t_0)$ of finding the value σ (or $-\sigma$) at time t_1 with the r.f.-SQUID prepared in the state σ at time t_0 is given by eq. (20) one concludes, as shown in ref. [4], that at least one of the two conditions, NIM and MR, is violated. The second test consists in performing a second measurement (with the same initial preparation σ at t_0) of the flux sign at time $t_2\,(t_2 > t_1)$ on the two samples with the values σ and $-\sigma$ obtained at t_1. If the probability of finding the value σ at t_2 depends only on the values found at t_1 and not on the value prepared at t_0, then NIM is violated. Finally, if the charge at time $t_1 > t_0$ is measured and the probability of obtaining the result $Q > 0$ (or $Q < 0$) agrees with eq. (30), then MR is violated and quantum mechanics applies. This set of measurements would therefore clarify the details of the transition between the quantum and the classical region for macroscopic bodies.

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