

# 3C3B

## The quantum mechanics of a macroscopic variable\*

In lecture 3A we discussed Josephson systems in a way which treated the flux threading a SQUID ring, or the phase difference across a Josephson junction, as a classical quantity. Thus, for example, there was no question of superposing states corresponding to different values of the flux. It is clear that if we have any hope of using any of these circuits as qubits, we will have to treat the flux  $\Phi$ , or the phase difference  $\Delta\phi$ , as **quantum-mechanical operators**.

How can we set about doing this? Let's start with the conceptually simplest case, that of the SQUID ring, and consider the equation of motion of the trapped flux  $\Phi(t)$ , for the moment neglecting the dissipative term due to the normal current:

$$Cd^2\Phi/dt^2 + I_c \sin(2\pi\Phi/\Phi_0) + (\Phi - \Phi_{ext})/L = 0$$

It is clear that this equation can be derived from a Lagrangian of the standard form T-V, where the « potential » energy V and « kinetic » energy T are given by

$$V(\Phi) = -E_J \cos(2\pi\Phi/\Phi_0) + (\Phi - \Phi_{ext})^2/2L \quad (\text{as previously: } E_J \equiv \Phi_0 I_c / 2\pi)$$

and

$$T(d\Phi/dt) = C(d\Phi/dt)^2/2$$

This is formally exactly analogous to the Lagrangian of a mechanical particle, with « mass » C, so it is tempting to apply the standard canonical quantization procedure by defining

$$p_\Phi \equiv \partial L / \partial (d\Phi/dt) = C(d\Phi/dt),$$

$$H \equiv p_\Phi (d\Phi/dt) - L = (p_\Phi^2/2C) + V(\Phi)$$

\*Parts of this lecture are based on A.J.L., in *Chance and Matter*, ed. J. Souletie et al., 1986.

So we have (classically)

$$H(\Phi, p_\Phi) = (p_\Phi^2 / 2C) + V(\Phi)$$

and now make the standard replacements

$$H \rightarrow -i\hbar \partial / \partial t, p_\Phi \rightarrow -i\hbar \partial / \partial \Phi$$

to obtain a TDSE for a « wave function »  $\Psi(\Phi)$  of the form

$$-i\hbar \partial \Psi(\Phi, t) / \partial t = -(\hbar^2 / 2C) \partial^2 \Psi / \partial \Phi^2 + V(\Phi) \Psi$$

Unfortunately, this may be too good to be true! After all,  $\Phi$  is a **collective** variable, and its classical equation of motion is itself derived using QM ideas; it is not a priori obvious that the canonical quantization procedure is legitimate. (« **Can you quantize the equations of mathematical economics?** »). The problem is even worse when we come to the phase difference  $\Delta\phi$ , since this cannot even be defined classically. So we need a more first-principles treatment. Let's try to do it first for the SQUID case:

Let's start by asking: for a given value of the trapped flux  $\Phi$ , what does the full many-body wave function look like? It is actually convenient to work in terms of the « molecular » function  $\chi(r_1, r_2, \sigma_1, \sigma_2)$  rather than the more conventional « pair wave function »  $F(r_1, r_2, \sigma_1, \sigma_2)$ ; the two functions differ\*\* only in their dependence on the relative coordinate, while we shall be interested only in the dependence on the COM coordinate  $R$ ; thus we write

$$\Psi_N(r_1 r_2 \dots r_N, \sigma_1 \sigma_2 \dots \sigma_N; \Phi) = \mathbb{N} \cdot \mathbb{N} \cdot \chi(r_1 r_2 \sigma_1 \sigma_2; \Phi) \chi(r_3 r_4 \sigma_3 \sigma_4; \Phi) \dots \chi(r_{N-1} r_N \sigma_{N-1} \sigma_N; \Phi) \quad \theta$$

where  $\Phi$  is for the moment a parameter. We write  $\chi(r_1 r_2 \sigma_1 \sigma_2; \Phi) \equiv \chi(\rho, \sigma_1 \sigma_2; R; \Phi)$  and write the COM coordinate  $R$  in terms of two irrelevant variables and its angle  $\theta$  around the ring.

\*We use the notation  $\chi$  for this quantity to avoid confusion with the phase.

\*\*For the singlet s-wave case of interest here.

Thus, the many-body wave function  $\Psi_N$  is schematically given by

$$\Psi_N = \mathbb{N} \cdot \mathbb{S} \cdot \prod \chi(\zeta : \theta : \Phi)$$

where  $\zeta$  is a shorthand for all the irrelevant variables. Now, the phase  $\phi(r)$  of the « molecular » wave function  $\chi(r)$  is the same as that of the pair function  $F(r)$ , which as we have seen obeys (on any path deep in the bulk ring) the relation

$$\nabla \phi(r) = 2eA(r) / \hbar$$

Since the dependence on  $r$  comes only through the angle  $\theta$  and  $A(r)$  can be taken equal to  $\Phi / 2\pi r$ , this gives the  $\theta$ -dependence

$$\phi(\theta) = (\Phi / \Phi_0) \theta$$

so that

$$\chi(\zeta : \theta : \Phi) = \chi(\zeta) \exp i(\Phi / \Phi_0) \theta \equiv \chi(\zeta) \exp i(\Phi / \Phi_0) (\theta_1 + \theta_2)$$

where  $\theta_1, \theta_2$  are the angles of the two electrons of the pair and  $\chi(\zeta)$  is independent of  $\Phi$ . Thus,

$$\Psi_N(r_1 r_2 \dots r_N : \Phi) = \prod_i [\exp(i/2)(\Phi / \Phi_0) \theta_i] \cdot \Psi'_N(\zeta)$$

where the function  $\Psi'_N(\zeta)$  is independent of  $\Phi$ . So we reach the fundamental conclusion that **the flux-dependence of the many-body wave function (in the bulk ring) lies entirely in the factor**

$$\prod_i [\exp(i/2)(\Phi / \Phi_0) \theta_i]$$

So far, the flux  $\Phi$  has been treated entirely as a c-number parameter. Now we need to go further.....

## Converting the flux to an operator

Let us introduce for convenience the notation

$$\Psi_N(r_1 r_2 \dots r_N; \Phi) = (\exp(i/2)(\Phi / \Phi_0) \cdot \sum_i \theta_i) \Psi' \equiv |\Phi\rangle$$

This is a perfectly respectable many-body wave function; it may be regarded as an eigenstate of the variable  $\Phi$ , just as in ordinary single-particle QM one defines an eigenstate  $|x\rangle$  of the coordinate variable  $x$ . And just as in that case, one may form a superposition of eigenstates corresponding to different values of  $\Phi$  :

$$|\Psi_N\rangle = \int a(\Phi) |\Phi\rangle d\Phi$$

or explicitly

$$\Psi_N(r_1 r_2 \dots r_N) = \int d\Phi a(\Phi) \Psi_N(r_1 r_2 \dots r_N; \Phi)$$

where  $a(\Phi)$  is a complex amplitude function. This is a perfectly good many-body wave function (**principle of superposition!**); all we need is a shorthand notation for it. In analogy with the standard notation  $\psi(x)$  in single-particle QM for the amplitude with which the position eigenstate  $|x\rangle$  is represented in the general quantum state  $| \rangle$ , it seems natural to adopt the change of notation  $a(\Phi) \rightarrow \psi(\Phi)$  so that a general state of the many-body system is represented as

$$| \rangle \equiv \int d\Phi \psi(\Phi) |\Phi\rangle$$

or more concisely just by the wave function  $\psi(\Phi)$ . From now on we shall treat  $\psi(\Phi)$  just like any other Schrodinger wave function.

## Identification of the « momentum » conjugate to $\Phi$

In order for the Schroedinger equation  $-i\hbar\partial\psi(\Phi)/\partial t = H\psi(\Phi)$  to be nontrivial, we have to find a « kinetic energy » term which depends on the momentum conjugate to  $\Phi$ , and therefore have to identify this quantity.

We first enquire what it looks like when expressed in terms of the original single-electron coordinates. For this purpose it is convenient to choose a definite origin of the angular coordinate  $\theta$ , let us say at the point on the ring opposite the junction. Now, in ordinary single particle QM the state  $|\psi\rangle$  specified by the wave function  $\partial\psi/\partial x$  is explicitly  $|\psi\rangle \equiv \int dx (\partial\psi/\partial x) |x\rangle$ , i.e. the amplitude (but not the ket vector  $|x\rangle$ ) is differentiated. Similarly in our case, we expect the wave function  $\partial\psi(\Phi)/\partial\Phi$  to be given explicitly by the expression

$$\partial\psi(\Phi)/\partial\Phi \equiv \int (\partial\psi/\partial\Phi) |\Phi\rangle d\Phi$$

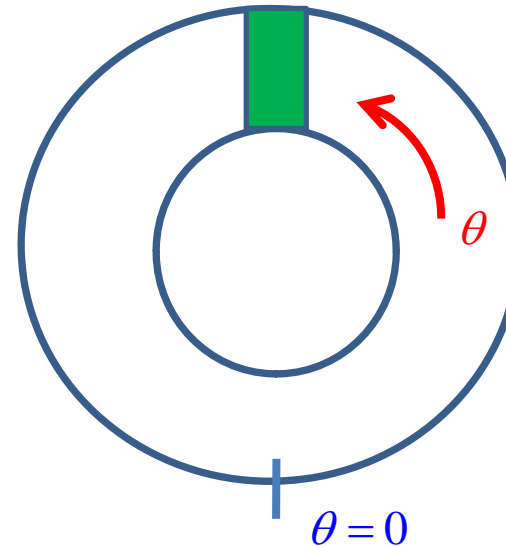
However, we can now integrate this expression by parts: assuming that the amplitude tends to zero for  $\Phi \rightarrow \pm\infty$  as must be true for any physically reasonable state, this gives

$$\partial\psi(\Phi)/\partial\Phi \equiv -\int \psi(\Phi) (\partial/\partial\Phi) |\Phi\rangle d\Phi = (-i/2\Phi_0) \sum_i \theta_i \int \psi(\Phi) |\Phi\rangle d\Phi \equiv (-i/2\Phi_0) (\sum_i \theta_i) \psi(\Phi)$$

where we used the fact that

$$|\Phi\rangle \equiv (\exp i(\Phi/\Phi_0) \sum_i \theta_i) \times |\zeta\rangle$$

with  $|\zeta\rangle$  independent of  $\Phi$



## Identification of the canonical momentum (cont.)

We just demonstrated that

$$\partial\psi(\Phi)/\partial\Phi = (-i/2\Phi_0)(\sum_i\theta_i)\psi(\Phi)$$

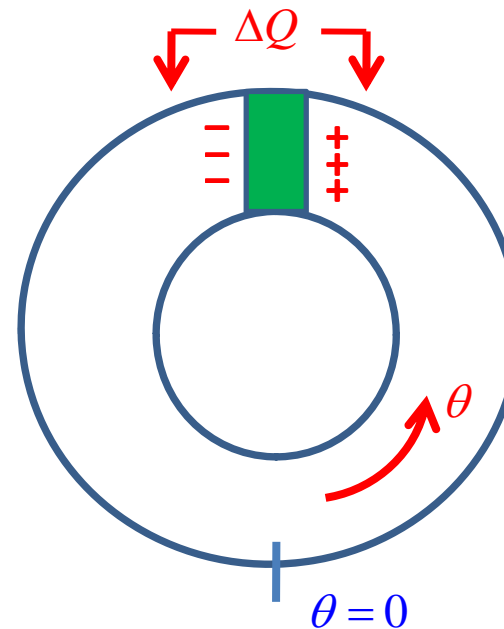
It follows that the momentum operator canonically conjugate to  $\Phi$ ,  $p_\Phi \equiv -i\hbar(\partial/\partial\Phi)$ , is to be identified with the expression

$$p_\Phi = -e(\sum_i\theta_i/2\pi)$$

This is an interesting result; it shows that the momentum conjugate to  $\Phi$  is not strictly speaking the charge imbalance across the junction (which is what one would have inferred from the « naive » argument based on canonical quantization) but rather the weighted distribution of charge around the ring. However, we now use a physical consideration: under the conditions normally found in real-life SQUIDs, the capacitance of the junction is much greater than the distributed (« geometrical ») capacitance of the bulk ring (which is what we implicitly assumed when deriving the classical equation of motion). Under these conditions, any charge imbalance will pile up on the « plates » of the junction, corresponding to  $\theta_i = \pm\pi$  in the above formula, so that  $p_\Phi$  is indeed the charge imbalance  $Q$  and we can write the commutation relation

$$[Q, \Phi] = -i\hbar$$

(which is often assumed in the literature without going through the above painstaking argument). It is clear that the capacitance energy associated with this charge build-up is  $Q^2/2C$ , so we finally reach the Schrodinger equation deduced earlier by canonically quantizing the classical equation of energy conservation:



So, finally, the correct Schroedinger equation governing the behavior of the flux in a SQUID ring (in the approximation of the neglect of any dissipation due to normal current in the junction) is

$$-i\hbar\partial\psi(\Phi,t)/\partial t = -\hbar^2/2C)\partial^2\psi/\partial\Phi^2 + V(\Phi)\psi(\Phi)$$

where  $V(\Phi)$  is the « potential energy » derived earlier :

$$V(\Phi) (\equiv E(\Phi) = (\Phi / -\Phi_{ext})^2 / 2L - E_J \cos(2\pi\Phi / \Phi_0))$$

$$(E_J \equiv I_C \Phi_0 / 2\pi)$$

We can now proceed to calculate various properties exactly as we would for a mechanical particle moving in the potential  $V$ . E.g. we can apply the usual formulae for tunnelling of the flux out of a metastable well:

$$P = const. \exp - 2A$$

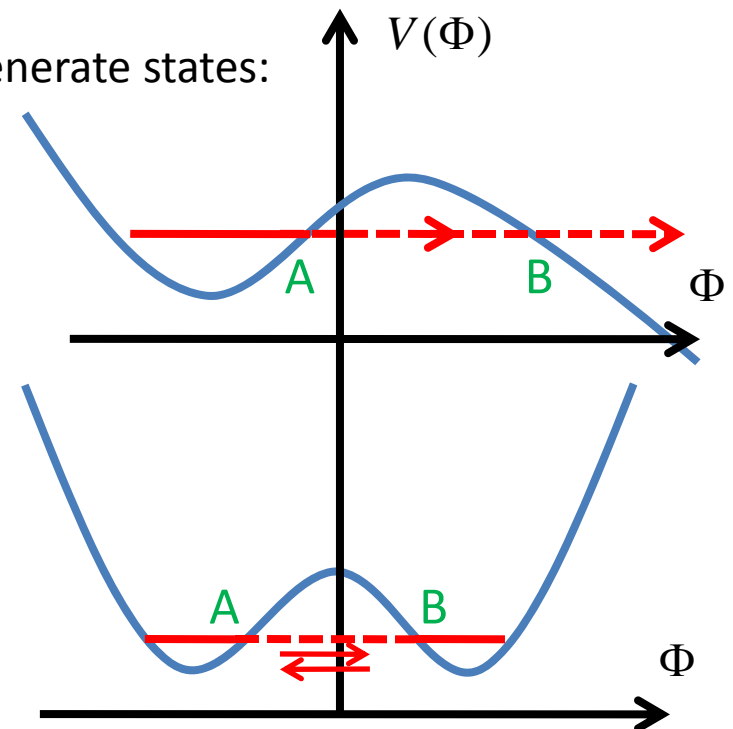
and for the tunnelling splitting between two nearly degenerate states:

$$\Delta = const. \exp - A$$

where in each case  $A$  is the appropriate WKB exponent:

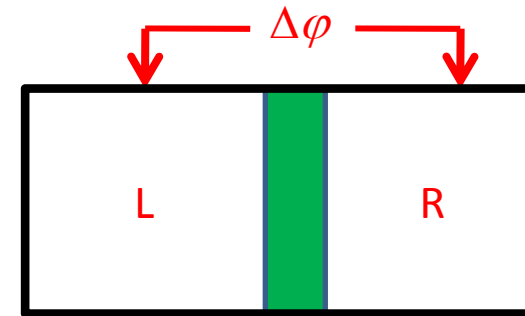
$$A \equiv \int (2CV(\Phi))^{1/2} d\Phi / \hbar$$

where the integral is taken in each case between the two classical turning points determined by  $E = V(\Phi)$  (see figure). Note that both  $P$  and  $\Delta$  decrease exponentially with the junction capacitance  $C$ , so that to get appreciable quantum effects one needs  $C$  to be small. (but not so small that it is overwhelmed by the distributed capacitance!)



## Quantum mechanics of a Cooper-pair box (CPB)

The QM of a J.J. sandwiched between two isolated bulk superconductors is in some ways simpler than that of a SQUID, provided one is happy to treat the phase drop  $\Delta\phi$  of the Cooper-pair wave function across the junction as an operator, despite the fact that it is itself of QM origin.



Consider the paired many-body wave function

$$\Psi_N(r_1 r_2 \dots r_N : \Delta\phi) \equiv \mathbb{N} \cdot \mathcal{S} \cdot \chi(r_1, r_2, \sigma_1, \sigma_2 : \Delta\phi) \cdot \chi(r_3 r_4 \dots) \dots$$

where as in the SQUID case  $\chi(r_1 r_2 \sigma_1 \sigma_2)$  is the « molecular » wave function. Again we focus on the COM variable  $r$ , and write this time (cf. lecture 3A)

$$\chi(r) = a\psi_L(r) + b\psi_R(r) \equiv |a| \exp(i\Delta\phi/2)\psi_L(r) + |b| \exp(-i\Delta\phi/2)\psi_R(r)$$

where  $\psi_{L,R}(r)$  are COM wave functions localized on the left (right) of the junction. Thus we have schematically (ignoring normalization and antisymmetrization)

$$\Psi_N(r_1 r_2 \dots r_N) = (|a| \exp(i\Delta\phi/2)\psi_L + |b| \exp(-i\Delta\phi/2)\psi_R)^{N/2} \equiv |\Delta\phi\rangle$$

where  $N$  is the total number of electrons in the device. We now consider, as in the SQUID case, the possibility of a many-body wave function which is a linear superposition of states of different  $\Delta\phi$ :

$$|\rangle = \int d(\Delta\phi) \psi(\Delta\phi) |\Delta\phi\rangle \rightarrow \psi(\Delta\phi)$$

There is one tricky point, now, which has no analog in the SQUID case: because the topology is no longer « multiply connected », values of  $\Delta\phi$  which differ by  $2n\pi$  must be identified.



## QM of a Cooper-pair box (cont.)

We now consider the question of the « momentum » canonically conjugate to the phase drop  $\Delta\phi$  across the junction. We recall that we had (with  $\psi_{L,R}$  real and  $(\psi_L, \psi_R) \equiv 0$ )

$$\Psi_N(r_1, r_2, \dots, r_N; \Delta\phi) = (|a| \exp(i\Delta\phi/2) \psi_L + |b| \exp(-i\Delta\phi/2) \psi_R)^{N/2} \equiv |\Delta\phi\rangle$$

Now consider the quantity  $\partial\psi(\Delta\phi)/\partial(\Delta\phi)$ . We assume that as in the SQUID case we can integrate by parts, so we need to work out the effect of this operator on the ket  $|\Delta\phi\rangle$ . We see that this is to multiply by  $iN/2$  and by a factor  $\varpi_- / \varpi_+$ , where  $\varpi_{\pm} \equiv |a| \psi_L \exp(i\Delta\phi/2) \pm |b| \psi_R \exp(-i\Delta\phi/2)$ . If the pair wave function is normalized, then since  $(\psi_L, \psi_R) \equiv 0$  this factor is just  $|a|^2 \psi_L^2 - |b|^2 \psi_R^2$ . Thus,

$$\partial\psi(\Delta\phi)/\partial(\Delta\phi) = -i(N/2)(|a|^2 \psi_L^2 - |b|^2 \psi_R^2) \psi(\Delta\phi) \equiv -i\Delta N \cdot \psi(\Delta\phi)$$

where  $\Delta N$  is the number of particles displaced across the junction (relative to the expectation value in the groundstate). Hence, the variable conjugate to  $\Delta\phi$  is  $\Delta N$ :

$$[\Delta N, \Delta\phi] = -i$$

Note that we would also get this relation in the SQUID case, since  $\Delta\phi$  is uniquely related to the flux and  $\Delta N$  to the displaced charge  $Q$ .

Finally, since the capacitance (« kinetic ») energy is  $(2e)^2(\Delta N)^2/2C$ , the Schrodinger eqn. for a Cooper-pair box is

$$-i\hbar\partial\psi(\Delta\phi, t)/\partial t = (-E_C)\partial^2\psi/\partial(\Delta\phi)^2 + V(\Delta\phi)\psi(\Delta\phi)$$

where  $E_C \equiv (2e)^2/2C$  is the « capacitance energy per pair », and where we must recall that  $\Delta\phi$  is defined only modulo  $2\pi$ . However, we shall often find it more convenient when discussing Cooper-pair box qubits to use the conjugate representation, and so write out explicitly the (rather simple) form of the Hamiltonian in terms of  $\Delta N$  and  $\Delta\phi$ :

$$H = E_C(\Delta N)^2 - E_J \cos(\Delta\phi)$$

As we shall see, the general nature of the eigenstates is very sensitive to the ratio  $E_C/E_J$

## External bias on a CPB

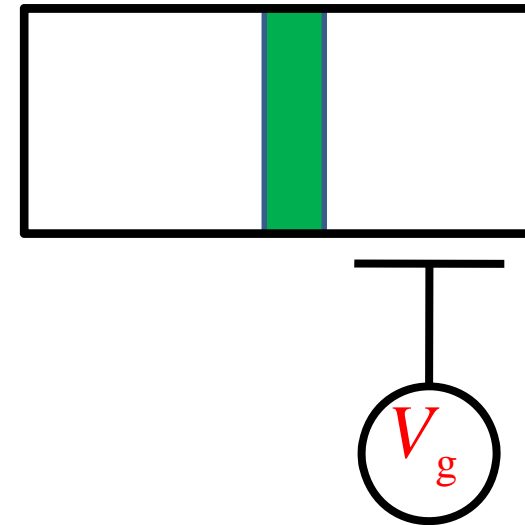
One further point which is of great practical importance in the context of the use of the CPB as a qubit is the possibility of applying a (dc or ac) external bias  $V_g$  by means of a « gate ». The effect of this is to add to the  $\Delta N$  -dependent term a contribution

$-(2e)V_g(t)\Delta N$ , so that the full Hamiltonian is now

$$H = E_C(\Delta N)^2 - 2eV_g(t)\Delta N - E_J \cos(\Delta\phi)$$

In other words, the « origin » (reference level) with respect to which  $\Delta N$  is measured is now

shifted. As we shall see when we come to the use of the CPB as a qubit, the crucial point is that the new « reference level »  $eV_g / E_C \equiv CV_g / 2e$ , does not have to be integral. (This result is sometimes presented, somewhat misleadingly, as equivalent to a fractional « external charge » on the box).



## QM of a current-biased junction (CBJ):

This system differs from the Cooper-pair box (CPB) only in that it is not isolated but receives an externally input current  $I_{ext}(t)$ . We can thus take over much of the lore from the CPB, including the fundamental commutation relation

$$[\Delta N, \Delta \phi] = -i$$

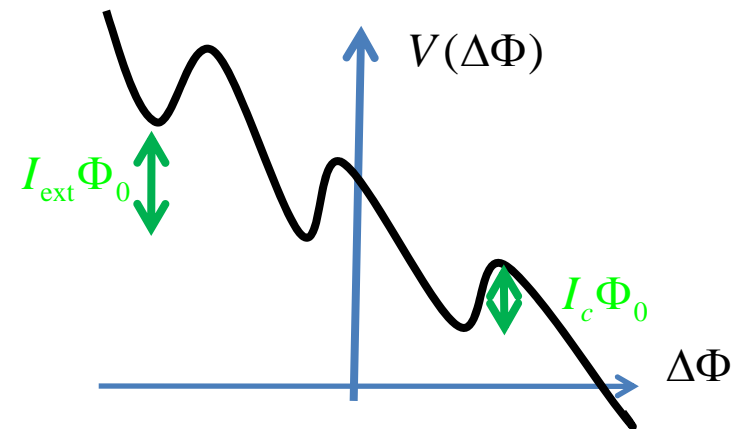
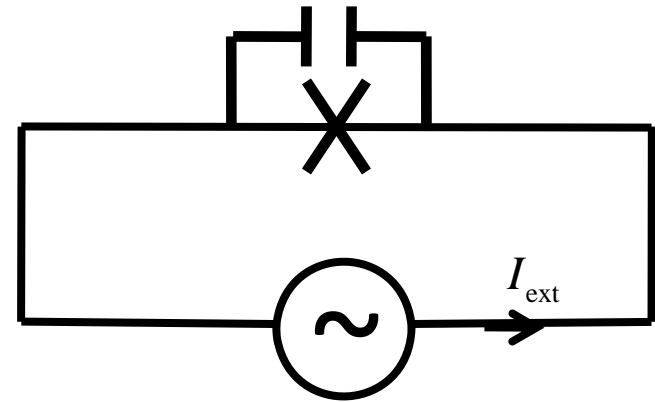
provided that  $\Delta N$  is interpreted as the time integral of the pairs actually crossing the junction. However, there is a slight problem with the Hamiltonian: at the classical level we need to be able to recover the continuity equation of the current, namely

$$C(dV/dt) + I_c \sin \Delta \phi = I_{ext}(t)$$

It may be verified that this is achieved by including in the Lagrangian, and thus in the Hamiltonian, an extra « potential » term  $-I_{ext}(t)(\Phi_0/2\pi)\Delta\phi$ . When combined with the periodic Josephson term this gives the famous « washboard potential » shown in the figure. However, there is a conceptual problem, in that evidently values of  $\Delta\phi$  differing by  $2n\pi$  are no longer identified. We shall take the view that this should cause no problems provided that one is never interested in quantum motion between such points, as we shall see is the case in the qubit application. Then the Schrodinger equation for a CBJ is the same as that for a CPB with the extra term:

$$-i\hbar \partial \psi(\Delta\phi, t) / \partial t = -(-E_c) \partial^2 \psi / \partial (\Delta\phi)^2 + V(\Delta\phi, t) \psi(\Delta\phi),$$

$$V(\Delta\phi) \equiv -E_J \cos \Delta\phi - I_{ext}(t) \Delta\phi$$



## The QM of a macrovariable: effects of dissipation

All the considerations we have mentioned so far concerning the QM of a macroscopic variable such as the flux in a SQUID or the phase difference in a CPB ignore a fundamental difficulty: In all these cases, the « true » classical equation of motion is not of conservative form but contains a **dissipative** term, e.g. in the SQUID case the term  $(d\Phi/dt)/R$ . In the presence of such a term the « naive » quantization procedure fails, and it is also not clear how to incorporate its effects into the more first-principles treatment.

A point which is not at first sight related is one which for long inhibited the serious contemplation of macroscopic superconducting systems as qubits, namely the suspicion that once one is dealing (as one must in such a case) with quantum superpositions of states which are by some reasonable common-sense criterion « macroscopically distinct », then the phenomenon of **decoherence** (entanglement with the environment) will automatically turn the reduced density matrix of the system into a mixture, which would be useless for quantum computing.

Very fortunately, it turns out that one can kill both of these birds with one stone: once one finds a consistent way of modifying the QM description of the dynamics of a macrovariable so as to take into account the effects represented in the classical equation of motion by the dissipative term, this will automatically allow us to compute the magnitude of the decoherence which we may expect in the quantum dynamics; moreover, crudely speaking, the smaller the classical dissipation the smaller the quantum decoherence. (**subject to some reservations**). In fact, a possible procedure may be stated as follows:

1. Set up a model which allows calculation of both the classical dissipation and the quantum decoherence.
2. Use experimental knowledge of the classical dissipation to determine the parameters of the model.
3. Now use the model to calculate the quantum decoherence.

## The oscillator-bath model

A general principle which is by now almost universally accepted is that the dissipation in the classical equation of motion does not come out of thin air but is the result of the interaction of the system (S) with its environment (E). Note that « environment » means just about anything other than S which may interact with S. In some cases the environment may be approximately described classically but its state may be unknown in detail (this is the case, for example, with the electromagnetic 60 Hz background); such a situation can lead to decoherence, since in calculating the physically meaningful density matrix of S one has to average over the unknown state of E. If one has a good statistical description of the state of E, it is reasonably clear how to do so, so this case (« classical » environment) does not need further discussion at this point; I return to it in lecture 4A.

A more common case is where the environment has to be itself described by QM, and thus can become entangled with the system. This is particularly likely to happen when (part of) E consists of internal degrees of freedom of the physical system itself, which are not included in our definition of « S ». (For example, if S is the macroscopic DOF represented by the flux in a SQUID ring, then part of E would be constituted by the nuclear spins of the solid metal in question. In the rest of this lecture I will concentrate on this case (« quantum environment »).

A « model » which has been found particularly fruitful in the discussion of the dissipation and decoherence due to a quantum environment is the « oscillator-bath model », which treats E as equivalent to a set of simple linear harmonic oscillators with a coupling to S which is linear in the oscillator coordinates. However, despite its name, it is important to realize that this description is more than an arbitrary « model »; it can in fact be given a very convincing justification as a quite general description of an arbitrary quantum environment E, **provided** (and this is crucial!) **that any one degree of freedom of E is only « weakly » perturbed by the S-E interaction.** (Cf. 19th-century « oscillator » model of atoms (pre-laser!))

## Details of the oscillator-bath model

For the purposes of this discussion let's consider a general macroscopic variable  $q$  of the system  $S$  with associated canonical momentum  $p$ . In the absence of any coupling to  $E$  we can write the Hamiltonian of the system as

$$H \equiv H_S = H(p, q)$$

We now add to this expression three terms:

(a) The Hamiltonian of the isolated environment, written in terms of the oscillator coordinates  $x_\alpha$ , canonical momenta  $p_\alpha$  and masses  $m_\alpha$  (actually it is possible to set all the  $m_\alpha$  equal to unity, but it may help one's intuition to keep them)

$$H_E = \sum_\alpha (p_\alpha^2 / 2m_\alpha) + (m_\alpha \omega_\alpha^2 x_\alpha^2)$$

It will be implicitly assumed that the oscillator frequencies  $\omega_\alpha$  are sufficiently closely spaced that they may be regarded as forming a continuum.

(b) The system-environment coupling: the most general form which is linear in the coordinates and momenta is (apart from a constant)

$$H_{S-E} = \sum_\alpha (F_\alpha(p, q)x_\alpha + G_\alpha(p, q)p_\alpha)$$

but one can argue that under « reasonable » conditions (time-reversal invariance of the S-E interaction, etc.) we can always choose our oscillator « coordinates » so that the term in  $G$  vanishes and that in  $F$  depends only on  $q$ , so

$$H_{S-E} = \sum_\alpha F_\alpha(q)x_\alpha \quad (*)$$

(However, it may sometimes be convenient to keep the more general form).

(c) A « counter-term » to prevent the « dissipative » mechanism from also shifting the effective potential in which the system moves: for the form (\*) this is

$$H_{count} = \sum_\alpha F_\alpha^2(q) / m_\alpha \omega_\alpha^2$$

Thus we have for the Hamiltonian of the « universe »(S+E) the expression

$$H = H_S(p, q) + H_E + H_{S-E} + H_{count}(q)$$

where the second term depends only on the variables of E while the third couples the coordinates of S and E. This Hamiltonian should be valid for both classical and quantum purposes.

Let's start by trying to calculate the classical equation of motion. To do this, we simply write down the coupled equations for the coordinates of S and E which follow from the above Hamiltonian and eliminate the coordinates of E; because of the quadratic (linear) form of the second (third) terms this can be done analytically, and results in an equation (in general of integrodifferential form) for the system coordinate  $q$ . Now, in many cases of practical importance one knows from experiment that the dissipative term in the classical equation of motion has a « simple ohmic » structure, i.e. it is of the form  $\eta(dq/dt)$  where  $\eta$  is a phenomenological friction coefficient (e.g. in the SQUID case it is  $1/R$  where  $R$  is the resistance shunting the junction). A sufficient condition for the equation of motion to take this form is that the coupling function  $F_\alpha(q)$  in the S-E interaction term has the simple form  $qC_\alpha$ , with the « coupling spectral density »

$$J(\omega) \equiv (\pi/2) \sum_\alpha (C_\alpha^2 / m_\alpha \omega_\alpha) \delta(\omega - \omega_\alpha)$$

given by the simple form

$$J(\omega) = \eta\omega$$

(The question of whether this is a necessary condition is a lot more tricky).

(Note: many of the points raised on this and the last slide are discussed in more detail in the following references:

A.O. Caldeira and A.J.L., Ann. Phys. (NY) 149, 374 (1983), especially appendix C

A.J.L., Phys. Rev. B30, 1208 (1984)

« », in Chance and Matter, ed. J. Souletie et al., 1986

Let's try to summarize the result of the above discussion. For a system S interacting with **any** environment E such that any one degree of freedom of E is only « weakly » perturbed, and is adequate to take the Hamiltonian of the « universe » to be a sum of

- (a) the original system Hamiltonian  $H = H_S(p, q)$
- (b) an oscillator-bath Hamiltonian  $H_E(p_\alpha, x_\alpha)$  representing E
- (c) an interaction term of the general form

$$H_{S-E} = \sum_{\alpha} (F_{\alpha}(p, q)x_{\alpha} + G_{\alpha}(p, q)p_{\alpha})$$

- (d) a « counterterm »

$$H_{count}(p, q)$$

which depends on the system variables and on the parameters of the bath (but not on the bath coordinates or momenta), and whose role is to correct for any « unwanted » effects of the S-E coupling such as unphysical renormalization of the potential felt by S. Note that for any « universe » Hamiltonian of this type, the environment degrees of freedom can be integrated out analytically and a closed equation thus obtained for the dynamics of S (though in the general case its form may be very messy, cf. C.+L., Ann. Phys., appendix C).

In the case where the dissipation in the classical equation of motion of q is of simple « ohmic » nature, the description simplifies considerably: then  $H_{S-E}$  takes the simple form

$$H_{S-E} = q \sum_{\alpha} C_{\alpha} x_{\alpha}$$

with the constraint

$$J(\omega) \equiv (\pi/2) \sum_{\alpha} (C_{\alpha}^2 / m_{\alpha} \omega_{\alpha}) \delta(\omega - \omega_{\alpha}) = \eta \omega$$

and the counterterm given by

$$H_{count}(p, q) = q^2 \sum_{\alpha} C_{\alpha}^2 / 2m_{\alpha} \omega_{\alpha}^2$$



The point of all this work is that once we have the effective « universe » Hamiltonian, we can go ahead and integrate out the environmental degrees of freedom not just for the classical dynamics but also for various **quantum** problems. For example, it is possible to express the effects of an ohmically dissipative environment on the quantum tunneling of a macrovariable out of a metastable well (« MQT ») uniquely in terms of the phenomenological dissipation coefficient  $\eta$ . We shall meet some other applications in lecture 4A.

However, one caveat is necessary: as we shall see in lecture 4A, an important contribution to the decoherence rate in a qubit may be the so-called « phase noise », which essentially arises from zero-frequency excitation of the environment. Such noise may not be easy to infer directly from the (nonzero-frequency) classical dynamics and may have to be treated separately. However, the scheme described in this lecture provides a firm conceptual basis for this treatment.