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Josephson equations for an electron in the presence of a barrier

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Résumé. — A partir de l'équation de Schrödinger on exprime les équations de Josephson pour un électron en présence d'une barrière de potentiel. Pour cela on étudie, en fonction de la hauteur de la barrière, l'évolution temporelle de la phase de la fonction d'onde. Cette évolution (qui est déterminée par le mouvement des vortex associés au gradient de la phase) conduit, dans le cas de barrières très hautes, à une oscillation monochromatique du courant (effet Josephson alternatif).

Abstract. — The Josephson equations for a single electron in the presence of a potential barrier are derived from the Schrödinger equation. To this end the time evolution of the phase of the wavefunction as a function of the barrier height is investigated. The evolution of the phase function (which is determined by the motion of phase gradient vortices) leads to a monochromatic current oscillation (ac-Josephson effect) in the limit of very high barriers.

Introduction.

The dynamical behaviour of particles in quantum mechanics may be quite different from classical behaviour. This is related to the fact that in quantum mechanics the position and the velocity cannot be chosen independent of each other. The former is related to the modulus and the latter to the gradient of the phase of a complex space-dependent function $\psi(x) = |\psi(x)| \exp[i \eta(x)]$. The phase and the modulus are related in a characteristic way, and each state is represented by a characteristic phase structure [1]. These structures are composed of one or several phase gradient vortices around phase singularities situated on $(n-2)$-dimensional nodal (hyper-)lines of the modulus of the wave function $\psi(x)$, where $x$ denotes the position in the $n$-dimensional configuration space.

In the presence of a homogeneous electric field the wave functions usually change with time. Recently general laws have been established for the adiabatic change of the characteristic phase structures of the wave functions of a large class of systems [1]. These laws are at the origin of non-classical dynamical behaviour, which in particular occurs in systems with reduced spatial symmetry [1-3].

This breakdown of classical behaviour in the presence of phase singularities is consistent with a result of Bohm and Hiley [4], who introduced a quantum potential

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$$Q = (\hbar^2/2m) (\text{grad})^2 R(x)/R(x), \quad R(x) = |\psi(x)|,$$  
and showed, that non-classical behaviour results from the Schrödinger equation, if $Q$ is not negligible. According to this criterium classical behaviour cannot be expected in the presence of phase singularities, since they are located at nodes of the wave function, where $Q$ diverges.

Typical non-classical dynamical effects are Josephson type oscillations. They appear in small junctions and in superconducting and normal micro-circuits and have been the subject of intense research in recent years [5]. In this article we will discuss the ac-Josephson effect of a single electron in the light of the general laws [1] mentioned above. We will see that this effect is the limiting case of a very general behaviour, which is common to a large class of systems, which can be described by Schrödinger type equations.

We restrict our considerations to motion in one spatial direction. To be specific we consider a single particle with charge $q$ in the presence of a single potential barrier (Fig. 1) and subject to a homogeneous electric field $E_x$. This field can be expressed by a time-dependent vector potential

$$A_x(x) = \phi(t)/L, \quad \phi(t) = -cE_t Lt + \text{const.} \quad (1)$$

![Fig. 1. — One-dimensional system of length $L$ with a potential barrier of height $V$.](image)

We assume the boundary condition

$$|\psi(x)| = |\psi(x + L)|. \quad (3)$$

Condition (3) is fulfilled on a real loop of circumference $L$, but it is often also the correct physical condition on an open system. This is e.g. the case for a superconducting order parameter (which obeys the Ginzburg-Landau equation, which is of Schrödinger type), which finds bulk conditions on both sides of an insulating junction (corresponding to a high barrier in our one-particle problem), or for a single-particle solution with plane wave behaviour at a sufficient distance away from the barrier. Together with (3) the phase difference between $x$ and $x + L$, $\Delta_L = \eta(x) - \eta(x + L)$ (modulo 2 $\pi$), determines the self-adjoint representation of the Hamiltonian [6]. On a real loop, which is embedded in the real two- or three-dimensional physical space, this phase difference is zero (modulo 2 $\pi$) [2]. This corresponds to wave functions which are single-valued on the loop. On an open line all other values of $\Delta_L$ would also be acceptable from a physical point of view. In our following discussion these values would appear in the form of different choices of the origin of $\phi$ at $t = 0$ (see e.g. Refs. [1, 2]. Since this origin is irrelevant for the following, we set it equal to zero together with the constant in (2).

We consider the Hamiltonian

$$H = (1/2m)[(\hbar i)(d/dx) - q\phi(t)/(cL)] + V(x), \quad (4)$$

with $\psi(0) = \psi(0 + L)$, where $V(x) = V$ for $x_1 \leq x \leq x_2$ and zero otherwise ($x, x_1,$
We investigate the phase structure of the adiabatic solutions of the time-dependent Schrödinger equation for increasing barrier heights $V$. (Adiabatic solutions are eigenfunctions of $H(t)$ where $t$ is considered as a parameter. This is the limiting case for sufficiently small $E_r$.) In particular we are interested in the ground state. The time evolution of an adiabatic state is visible through its characteristic phase structure, which for the ground state of our system is particularly simple. The time evolution of the phase function illustrates the general laws discussed in reference [1], which lead to an odd periodic current with frequency $|qE_x L/h|$ if the symmetry is sufficiently low. In the system considered in this article an increase in the barrier height $V$ will let the periodic current tend towards an exactly monochromatic current. We will obtain this limit analytically. Further, the intermediate situations will be illustrated numerically.

The following general result is true [1]: if $V(x)$ has only the trivial periodicity $V(x + L) = V(x)$, as is the case in our system, the eigenfunctions of $H$,

$$\psi(x; \phi) = |\psi(x; \phi)| \exp[i \eta(x; \phi)], \quad (5)$$

show the following characteristic $\phi$-dependence:

$$\psi(x; \phi + \hbar c/q) = |\psi(x; \phi)| \exp[-i F(x)/\hbar], \quad (6)$$

where

$$F(x) = - \hbar x/L. \quad (7)$$

This means that the phase winding number

$$W(\phi) = (1/2 \pi) \int_0^L (\partial/\partial x) \eta(x; \phi) \quad (8)$$

obeys the general relation

$$W(\phi + \hbar c/q) = W(\phi) + \hbar c/q. \quad (9)$$

While the wave function itself is continuous as a function of $\phi$, the winding number $W$ changes discontinuously in jumps of integer values [1, 2]. This process is associated with the appearance of phase singularities, situated at cores of phase gradient vortices. In the general case of a three-dimensional system (threaded by a flux $\phi$) these singularities are located on nodal lines of $\psi$. If the configuration space is two-dimensional, they reduce to nodal points. When $\phi$ increases, these lines (points) periodically move across the physical domain into the hole threaded by the flux $\phi$. In our case, where the domain mathematically corresponds to a one-dimensional loop, this process can be visualized by extrapolating the phase $\eta(x)$ from the loop into the plane where the loop can be imbedded. This extrapolation is not unique, but the topology of the phase structure, i.e. the position of the vortex cores (the phase singularities) with respect to the loop is uniquely represented [2].

The current of an electron.

The current $j(\phi)$ along the loop reflects this phase structure, since $j$ has the general form

$$j(\phi) = [-q^2/(mc)] |\psi(x; \phi)|^2 \left[ A_x(x; \phi) - (\hbar c/q)(\partial/\partial x) \eta(x; \phi) \right]. \quad (10)$$

The eigenfunctions of the Hamiltonian (4) can be obtained in the usual way by a superposition of two plane waves in each part of the loop with constant $V(x)$ and then
connecting the piecewise solutions with the correct «branching» conditions. The solution has the general form \[2, 7\]

\[
\psi_a(s_a; \tau) = \exp \left[ -i \Gamma_a(s_a) \right] \{ \psi_1 \sinh (\theta_a - s_a \theta_a/L_a) + \psi_2 \exp \left[ i \gamma_a \right] \sinh (s_a \theta_a/L_a) \} / \sinh \theta_a
\]

(11)

\[
\psi_b(s_b; \tau) = \exp \left[ -i \Gamma_b(s_b) \right] \{ \psi_2 \sin (\theta_b - s_b \theta_b/L_b) + \psi_1 \exp \left[ i \gamma_b \right] \sin (s_b \theta_b/L_b) \} / \sin \theta_b,
\]

where \( s_a = x - x_1, \ s_b = x - x_2, \ L_a = x_2 - x_1, \ L_b = L - L_a. \) Here \( \psi_a(\psi_b) \) represents the solution in (outside) the barrier.

\[
\Gamma_{a,b}(x) = \int_{x_1, x_2}^x (q/\hbar c) A_x \, dx
\]

(12)

\[
\gamma_a = \Gamma_a(x_2), \quad \gamma_b = \Gamma_b(x_2 + L_b)
\]

(13)

\[
\theta_{a,b} = L_{a,b} (2m |E - V_{a,b}|)^{1/2}/\hbar
\]

(14)

with \( V_a = V, \ V_b = 0. \)

Here \( E \) is the corresponding energy eigenvalue at the given parameter value \( \phi(t) \) (only the case \( E < V \) is considered), and \( \psi_1, \ \psi_2 \) are the values of the solution at \( x_1, \ x_2 \) respectively (see e.g. Eq. (15) of Ref. \[7\]). With (11) the current (10) can be expressed as:

\[
\begin{align*}
\psi_a(t) &= \left| \psi_1 \right| \left| \psi_2 \right| (\theta_a/L_a \sinh \theta_a)(-q\hbar/m) \sin \left[ \eta(x_1) - \eta(x_2) - \gamma_a \right] \\
\psi_b(t) &= \left| \psi_1 \right| \left| \psi_2 \right| (\theta_b/L_b \sinh \theta_b)(-q\hbar/m) \sin \left[ \eta(x_2) - \eta(x_2 + L_b) - \gamma_b \right]
\end{align*}
\]

(15)

where \( \psi_a, \ \psi_b \) denote the expression for the current on the intervals \( L_a, \ L_b \) respectively. Here \( \psi \) and \( j \) are fully determined by \( E(\phi), \ \psi_1(\phi), \ \psi_2(\phi) \), which are obtained by solving the corresponding linear system \[2\] for the unknown values \( \psi_1 \) and \( \psi_2 \) at a given \( \phi = \phi(t) \).

Let us calculate the adiabatic current as a function of \( t \) for different barrier heights \( V \). Equation (15) suggests, that a monochromatic behaviour is obtained if \( \eta(x_1) = \eta(x_2) \) changes linearly with time (\( \gamma_a \) is already linear in \( t \) according to (1), (2), (12) and (13)). We will now show, that such a monochromatic behaviour is indeed obtained mathematically as a limiting case.

From the Schroedinger equation it follows, that the current is divergence free, hence the expression (15) for the current in the barrier interval of length \( L_a = x_2 - x_1 \) equals the expression for the current on the complementary interval of length \( L_b \) (which due to the periodic boundary conditions is also bounded by \( x_1 \) and \( x_2 \)). From the equality of these two current expressions one obtains

\[
\Delta \equiv \eta(x_1) - \eta(x_2) = \arctan \left( -X \sin \gamma + \sin \gamma_a \right)/(X \cos \gamma_b \cos \gamma_a),
\]

(16)

where

\[
X = \frac{\theta_b L_a \sinh \theta_a}{\theta_a L_b \sin \theta_b},
\]

(17)

If \( V \) is sufficiently high, \( \partial E(\phi)/\partial \phi \) can be set equal to zero (for the ground state a simple estimation yields the condition \( V \approx \hbar^2/(2\hbar \cdot mL_a L) \); similar limits could be given for the excited states). One obtains then (expressing \( \phi \) in units of \( \hbar c/q \))

\[
\partial \Delta/\partial \phi = - \frac{1}{L} \frac{X^2 L_b - L_a + X(L_b - L_a) \cos \phi}{1 + X^2 + 2 X \cos \phi}
\]

(18)

\[
\partial^2 \Delta/\partial \phi^2 = - \frac{X(X^2 - 1) \sin \phi}{(1 + X^2 + 2 X \cos \phi)^2},
\]

(19)
Further, from (17) we obtain:

$$|X| \geq \frac{\sinh [L_a(2m|E-V|)^{1/2}] \hbar}{L_b(2m|E-V|)^{1/2}}$$

(20)

Therefore, for very high $V$ the expression $|X|$ tends towards infinity, hence $\delta^2 \Delta \delta \phi^2$ tends towards zero and $\delta \Delta / \delta \phi$ tends towards $-L_b/L$. This means that in this case we have

$$\Delta = -L_b \phi / L,$$

(21)

or

$$\Delta - \gamma_a = -(L_a + L_b) \phi / L = -\phi.$$ (22)

Hence

$$j \sim \sin \phi$$

(23)

according to the first equation of (15).

Equation (23) leads to the predicted monochromaticity, since $\phi$ obeys (2) and the prefactor in front of $\sin \phi$ can be considered as $\phi$-independent (see appendix). One obtains (expressing $\phi$ again in ordinary units)

$$j(t) \sim \sin \omega t, \quad \omega = q \Delta V / \hbar.$$ (24)

Here $\Delta V = E_x L$ is the potential drop along $L$ (or the electromotive force around the loop) and $\omega$ is the Josephson frequency for a single particle with charge $q$.

Numerical results.

The preceding analytical results are illustrated by the following numerical calculations. Figure 2 shows the phase $\eta(x)$ of the ground state wave function for different values of $\phi$ and three different barrier heights $V$. One sees, that $\eta(x)$ becomes linear outside the barrier for high barrier height. It is linear in the whole spatial domain for $\phi = 2\pi$ times an integer, but it jumps in the middle of the barrier at $\phi = \pi$ times an odd integer. These jumps correspond to the fact, that if the system is considered as a loop, at these $\phi$-values the centre of a phase gradient vortex (i.e. a phase singularity) with individual winding number one is situated on the perimeter of the loop, exactly in the middle of the barrier. Hence the phase $\eta(x)$ jumps by an amount of $\pi$ if this point is crossed in $x$-direction. (For the motion of the vortex pattern in the extrapolation plane of the loop see Ref. [2].)

Figure 3 shows the phase difference $\Delta$ across the barrier as a function of $\phi = -t_c \Delta V$ for different barrier heights $V$. It illustrates the linearity of $\Delta$ with $t$ for high barriers («weak links »).

Discussion.

It has been shown previously [1, 2], that for systems described by Schroedinger type equations (with the boundary conditions mentioned above), which describe charged particles in the presence of an electric field, the periodic passage of quantized vortices (whose centres are phase singularities, which also are called phase slip centres) is a consequence of the mathematical structure of the equation. If the spatial translational symmetry is only the trivial one, i.e., $V(x + L) = V(x)$, the frequency of passage of the vortices is equal to $q \Delta V / \hbar$ [1]. This is just the time periodicity of the adiabatic current in the system.

In the present paper a limiting case of this general behaviour has been investigated. We considered an electron in the ground state driven by an electric field across a single potential barrier. We showed, that for sufficiently high barriers the periodic current tends to a
Fig. 2. — Numerical values of the phase \( \eta(x) \) of the ground state wavefunction as a function of \( \phi = - eE_x L \tau \) for different barrier heights \( V \). Full lines: \( V = 3.75 \) eV; pointed lines: \( V = 0.375 \) eV; dashed lines: \( V = 0.0375 \) eV. \( L = 100 \) Å, \( L_2 = x_2 - x_1 = 10 \) Å.

Fig. 3. — Phase difference \( \Delta \) across the barrier as a function of \( \phi \) for the same values of \( V \) as in figure 2.

*monochromatic* current with the frequency \( \nu = \omega / (2 \pi) = q \Delta V / h \) (Eq. (24)). Equations (15) and (22), (2) together constitute the same type of equations as the Josephson equations in the superconducting case (apart from a constant prefactor depending on the parameters of the superconductor and apart from the factor two in the charge), see equations (42) and (38), (28) of reference [8].
In the present case of a single electron the differential equation (the Schroedinger equation) is known in the entire spatial range of the system, i.e., including the barrier region and its edges. The behaviour of the particle can therefore be derived from this equation without any additional assumptions on the structure of the wave function outside the barrier (once the boundary conditions of the Hamiltonian are given). Our results show in particular, that the crucial linear relation of the phase difference $\Delta \phi$ with respect to time and to the potential difference $\Delta V$ (Eq. (21), where $\phi$ is expressed by (2)) holds only in the limit of a very high barrier (corresponding to a weak link in the superconducting and superfluid cases). In the derivation of this limit the nature of the barrier appears explicitely through (18). On the other hand, in the superconducting and superfluid cases the corresponding linearity (Eqs. (1) and (38) of Ref. [8] and Eq. (19) of Ref. [9], where the chemical potential enters instead of the electrostatic potential) is derived independently of the nature of the barrier, by a separate argument for the phase of the order parameter in the bulk outside the weak link. This is because in general no macroscopic wave equation exists inside the weak link, whose width is of the order of the coherence length or smaller. (An exception may be the case of thick junctions in dirty superconductors close to the transition temperature. Here similar methods as in the present Schroedinger case could be applied, with the order parameter fitted together with corresponding boundary conditions [11].)

Our analysis shows, that the single-particle ac-Josephson effect is a quantum effect due to quantized vortex motion. This is analogous to the ac-Josephson effect in superfluids [9, 10] and superconductors [12]. We emphasize, that the periodic passage (with time period $\tau = h/(q \Delta V)$) of the phase gradient vortex centres (phase singularities, phase slip centres) perpendicular to the direction of the potential drop, which leads to the phase jumps across the middle of the barrier with time period $\tau$, is crucial for the frequency equation (24) (which corresponds to Eq. (42) of Ref. [8] in the superconducting case). This fact is not obvious from the usual [8] macroscopic derivation of the Josephson equations. It means that (21) (and (38) of Ref. [8]) is actually only true within disconnected time intervals slightly shorter than $\tau$, since periodically (with period $\tau$) the phase $\eta(x)$ on one side of the barrier globally increases by $2\pi$, see figures 2 and 3. But this jump occurs just at values, where the argument of $\sin(\phi)$ in (23) is itself equal to an (odd)integer multiple of $\pi$. Hence this jump has no mathematical consequences for the equation (23) of the current and may pass unnoticed.

The derivation in the present paper has been a missing link in the analogy between macroscopic systems described by quantum wave functions of Ginzburg-Landau type and the behaviour of a single particle in Schroedinger quantum mechanics. Here the influence of the barrier on the phase function and its consequences for ac-Josephson behaviour could be analyzed in detail. We hope that our analysis will contribute to the understanding of this effect.

An experimental verification of the predicted behaviour of the electron current appears to be rather difficult. Presently one can hope to measure a current of roughly $2\text{nA}$ in a mesoscopic ring (without a barrier) of $2 \mu\text{m}$ in diameter (by detecting the created magnetic flux with a squid). This current corresponds to the sum of about thousand single-electron currents, and its amplitude turns out to be of the order of the current of a single electron at the Fermi level in such a ring. However, in the presence of a barrier the amplitudes of the individual and hence of the total current are reduced. Therefore the monochromatic limit of the current seems not yet to be detectable with present experimental methods.

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We should like to thank A. Benoît for information on the present experimental possibilities.
Appendix.

We study the prefactor of \( \sin \phi \) in (23), which depends on the wavefunction \( \psi(x) \) given by (11). Here \( |\psi_1| = |\psi_2| \), which is arbitrarily set equal to one. This determines the normalization factor \( N^2 = \int_0^L |\psi(x)|^2 \, dx \) of the normalized function \( \psi(x)/N \). After some algebra we find from (11)

\[
N^2 = A + B \cos \phi
\]

where

\[
A = L_a \left[ 1/(\theta_a \tanh \theta_a) - 1/\sinh^2 \theta_a \right] + 1/(\alpha \sin^2 \theta_a)[\theta_a/\sin \theta_a - 1] + \\
L_b \left[ 1/\sin^2 \theta_b - 1/(\theta_b \tanh \theta_b) \right] + 1/(\alpha \sin^2 \theta_b)[1 - \theta_b/\tanh \theta_b]
\]

\[
B = [L_a \theta_b/(\alpha L_b \sin \theta_b)][\theta_a/\sin \theta_a - 1] + [L_b \theta_a/(\alpha L_a \sin \theta_b)][1 - \theta_a/\tanh \theta_b]
\]

\[
\alpha = 1/(L_a \theta_a \tanh \theta_a) + 1/(L_b \theta_b \tanh \theta_b)
\]

If \( V \) is very high, \( \partial E/\partial \phi \) tends to zero, hence \( \theta_b \) and \( \theta_a \) are constant with respect to \( \phi \). In addition \( \theta_a \) tends towards infinity (at least in the case \( L_a \ll L \) considered here), and one can see that \( B \) is negligible compared to \( A \) for all values of \( \theta_b \). Therefore, after normalization of the wavefunction, the product \( |\psi_1| |\psi_2| = 1/N^2 \) (which represents the relevant prefactor in (23)) is constant with respect to \( \phi \).

References

[5] For a review see e.g. LIKHAREV K. K., Dynamics of Josephson Junctions and Circuits (Gordon and Breach Science Publishers, New York) 1986;