

INTERSITE VORTEX TUNNELLING IN 2D LATTICE SYSTEMS

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The motion of a vortex is considered for a number of 2D quantum lattice models. For the case of small quantum fluctuations this motion can be described as successive tunnelling of the vortex core from cell to cell. We have found the temperature dependence of the tunnelling probability for a rather typical regime of incoherent tunnelling (strictly exponential relaxation). For the different systems under consideration (2D planar ferromagnet, Josephson junction arrays, quantum crystal free surface) this dependence is either exponential or algebraic. The diffusion coefficient is proportional to the tunnelling probability.

1. Introduction

Fifteen years ago it was discovered that the thermodynamics of two-dimensional (2D) systems with planar symmetry is determined by vortices [1]. The low-temperature (quasi-ordered) phase differs from the high-temperature (disordered) one by the fact that it does not contain free vortices which are thermodynamically unstable. The influence of vortices on the dynamic properties of both phases has been investigated in a series of papers by Ambegaokar and co-workers [2] on the assumption that the motion of the isolated vortex is strictly diffusive and can be entirely described by the diffusion coefficient.

Recently, rather active experimental investigations of such 2D systems with planar symmetry as regular arrays of Josephson junctions and superconducting networks have been pursued, as a number of other papers of this volume testify. It is evident that it is correct to compare the results of these experiments with theory [2] only if there exists a range of parameters for which the motion of a vortex on a lattice is diffusive (another possibility to be thought over is the formation of a band).

In this paper the existence of such domains for a number of simple quantum models is shown (for some of them it extends down to zero

temperature) and the temperature dependence of the diffusion coefficient is found. The results obtained are applicable for describing vortex tunnelling in such 2D systems as planar ferromagnets, Josephson-junction arrays (with or without dissipation) and quantum crystal free surfaces.

An attempt to study intersite vortex tunnelling has been previously endeavoured by Lobb, Abraham and Tinkham for the case of a resistivity shunted Josephson-junction array [3]. These authors considered only the classical limit and also conjectured that the only difference between this process and phase tunnelling in a single junction is the different barrier height. The latter simplification is qualitatively incorrect for the small dissipation limit and quantitatively incorrect for the large dissipation limit. In this paper we are primarily interested in temperatures low enough for tunnelling to proceed quantum mechanically.

When speaking of the motion of the vortex in the low-temperature (quasi-ordered) phase one should bear in mind that it should be either one of two constituents of a neutral pair or a thermodynamically unstable single vortex, created due to the decay of a neutral pair under the action of the external current or in some other special way.

A preliminary account of the principal results of this paper has been published previously [4].

2. Quantum XY model

In the simplest approximation the regular Josephson-junction array can be described by the Hamiltonian:

$$\hat{H} = \sum_j \frac{J}{2} \hat{n}_j^2 - \sum_{(jj')} V \cos(\varphi_j - \varphi_{j'});$$

$$\hat{n}_j \equiv -i \frac{\partial}{\partial \varphi_j}, \quad (1)$$

where φ_j is the phase of the j th superconducting island, $J = 4e^2/C$ (C is the self-capacitance of each island), and $V = \hbar I_c/2e$ (I_c is the critical current of each single junction). The mutual capacitance of different islands is not incorporated into eq. (1). This very model also describes the planar ferromagnet in the continuous spin approximation. For such interpretation, φ is the angle of rotation of the j th spin with respect to a certain fixed direction. We shall consider only the case of $V \gg J$ when quantum fluctuations are small and at zero temperature there exists a rigorous long-range order.

The configuration of the field φ , associated with a vortex (this configuration being a true local minimum of total potential energy) is centred on this or that lattice cell. When the vortex core transfers to the neighbouring cell (fig. 1) the phase difference for the sites denoted by 1 and 2 changes continuously from $\pi/2$ to $3\pi/2$, so the

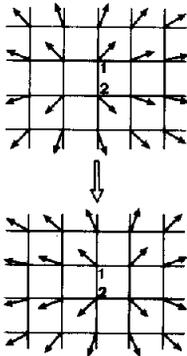


Fig. 1. Change of spin configuration for vortex core tunnelling between neighbouring cells. Here, as elsewhere throughout the paper, we consider for simplicity only the case of the square lattice.

energy $-V \cos(\Delta\varphi_{12})$ rolls over its maximum. The barrier height for the total potential energy is approximately equal to $0.40V$ [3]. At low temperatures this barrier is to be overcome by quantum-mechanical tunnelling.

It is well known that in the quasi-classical approximation the dynamics of a quantum system with a degenerate potential is determined by instantons, i.e. extremal trajectories in imaginary time, connecting different potential minima. For the considered model, both the equilibrium configuration of the field φ in a vortex and the time dependence of $\varphi_j(\tau)$ for the instanton trajectory, associated with vortex core tunnelling to a neighbouring cell, can be found exactly only if one replaces the cosine potential $-V \cos(\Delta\varphi)$ by a periodically continued parabolic potential:

$$V(\Delta\varphi) = -V + (V/2) \min_{p \in \mathbb{Z}_n} \{(\Delta\varphi - 2\pi p)^2\}. \quad (2)$$

The excess action for the instanton trajectory then is:

$$S_1 = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\pi}^{\pi} \frac{d^2\mathbf{k}}{(2\pi)^2} \pi^2 \hbar^2 \frac{V}{J} G_0(\mathbf{k}, \omega)$$

$$\propto \hbar \left(\frac{V}{J}\right)^{1/2},$$

where

$$G_0(\mathbf{k}, \omega) = \frac{1}{(\hbar^2/J)\omega^2 + V(4 - 2\cos k_x - 2\cos k_y)}. \quad (3)$$

The value of S_1 determines the bare zero-temperature tunnelling frequency $\Delta_0 \propto \exp(-S_1/\hbar)$, which in the case of non-interacting instantons would coincide with the band half-width. In the present problem Δ_0 has no direct physical meaning since instanton interaction cannot be omitted. It has not been evident, a priori, that S_1 is finite: in the next two sections we consider the models for which S_1 logarithmically diverges. Both the dependence $S_1 \propto (V/J)^{1/2}$ and the law of long-range instanton interaction (see eq. (4))

remain the same if one keeps the original potential instead of the one given by eq. (2).

In contrast to the standard problem of phase tunnelling in a single junction with the Hamiltonian: $\hat{H}_0 = (J/2)\hat{n}^2 - V \cos \varphi$, in the considered problem instantons have a long-range interaction in imaginary time. For a large distance τ in imaginary time:

$$\begin{aligned} \Delta S(\tau) &\approx \pm \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \iint_{-\pi}^{\pi} \frac{d^2\mathbf{k}}{(2\pi)^2} 2\pi^2 \hbar^2 \frac{V}{J} G_0(\mathbf{k}, \omega) \\ &\quad \times e^{-i\omega\tau} \\ &\propto \frac{\hbar^2}{J\tau}. \end{aligned} \quad (4)$$

A similar law of instanton interaction has been already encountered when the problem of quantum crystal growth was analysed [5, 6]. Reformulating the results of ref. [6] one can immediately conclude that for $k_B T \geq J$, intersite vortex tunnelling will proceed incoherently (exponential relaxation) and thus can be described by the tunnelling probability w . For the temperature range $J \ll k_B T \ll (JV)^{1/2}$:

$$w \propto \frac{\Delta_0^2 J^{1/2}}{\hbar(k_B T)^{3/2}} \exp\left[2\pi(\ln 2) \frac{k_B T}{J}\right], \quad (5)$$

and at $T = T_0 \sim (JV)^{1/2}/k_B$ a transition to the regime of thermally activated overbarrier tunnelling should take place. At $T > T_0$ the Arrhenius law will hold for $w(T)$.

For clarity we would like to recall that the form of the instanton interaction in imaginary time given by eq. (4) corresponds to logarithmic interaction at finite temperatures of the instantons introduced by Chakravarty and Leggett [7] (see also ref. [6]) for describing the density matrix evolution in real time (fig. 2). For $k_B T \geq J$ real-time instantons are bound into small-size pairs, each pair corresponding to an individual tunnelling event. The incoherence of tunnelling (the independence of different tunnelling events) is ensured by a large distance between these pairs, so the tunnelling probability is determined

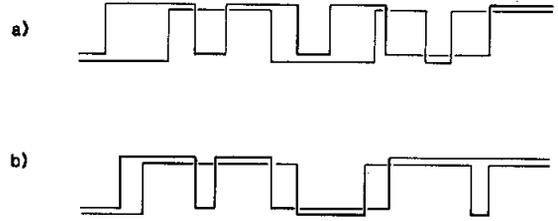


Fig. 2. The real-time evolution of the density matrix of a degenerate system can be schematically described by two trajectories, corresponding to the two arguments of the density matrix. The figure illustrates the case of a two-fold degenerate system. (a) A quantum two-level system. In this case different hoppings of trajectories from well to well (real-time instantons) do not interact with each other and are distributed in time uncorrelatively. (b) A system with an infinite number of degrees of freedom (a particle interacting with environment or, as in the case of the present paper, a vortex, moving from cell to cell). Instantons are interacting. For the case of a strong interaction they form small-size pairs (blips [7]) separating the long time intervals for which the density matrix is diagonal (sojourns [7]).

by the statistical weight of an isolated instanton pair.

Eq. (5) was derived just in that very approximation of non-interacting instanton pairs. The result obtained coincides with the one derived via traditional methods of evaluating $w(T)$ by the imaginary part of the free energy. The diffusion coefficient D is trivially related to w as $D = a^2 w$ (a is a lattice constant).

In the considered regime of incoherent tunnelling the interaction of the vortex with another vortex (in the case of a neutral pair), or with the array boundaries, or with inhomogeneities, can be taken into account by multiplying eq. (5) by a Boltzmann factor associated with the diffusive motion in the external potential: $\exp(\pm \varepsilon / 2k_B T)$, where ε is the relative shift of the levels for neighbouring positions of the vortex core, $|\varepsilon| \ll (k_B T)^2 / J$. For lower temperatures ($k_B T \ll J$) one should simultaneously take into account both the partial restoration of tunnelling coherence (due to the interaction between different tunnelling events) and its destruction (due to level shifts of different origin). This is a more complicated problem. In general, inhomogeneities lead to an extension of the domain of incoherent tunnelling to lower temperatures.

The interaction of charges on distant super-

conducting islands can be safely ignored only if, for example, the Josephson-junction array is fabricated on a superconducting substrate, which, being isolated from superconducting islands, nonetheless can supply the image charge for every island that is charged. In the absence of such a substrate one should replace the first term of eq. (1) by $\sum_{jl} \frac{1}{2} J_{jl} \hat{n}_j \hat{n}_l$, where

$$J_{jl} \begin{cases} = J & \text{for } j = l, \\ \approx J_{\infty}/|j-l| & \text{for } |j-l| \gg 1. \end{cases}$$

In the case when the distance between the nearest islands is comparable to all three linear dimensions ($J_{\infty} \sim J$) the temperature dependence of the incoherent tunnelling probability changes from (5) to $w(T) \propto T^{-5/2} \exp[c(k_B T)^3/J_{\infty}^2 V]$, $c = \text{const}$, which holds for the more narrow temperature range: $(J_{\infty}^2 V)^{1/3} \ll k_B T \ll (JV)^{1/2}$.

3. Array of dissipative Josephson junctions

If the influence of a normal shunt resistance R on the properties of a single junction can be described by adding to its Euclidian action the Caldeira–Leggett non-local term [8]:

$$S_D(\Delta\varphi) = \iint_{-\beta/2}^{\beta/2} d\tau d\tau' \frac{\eta}{4\pi} \left[\frac{\Delta\varphi(\tau) - \Delta\varphi(\tau')}{\frac{\beta}{\pi} \sin \frac{\pi}{\beta} (\tau - \tau')} \right]^2 \quad (6)$$

(where $\eta = \hbar^2/4e^2 R$, $\beta = \hbar/k_B T$), then the array as a whole should be described by the action:

$$S = \int_{-\beta/2}^{\beta/2} d\tau \left[\sum_j \frac{\hbar^2}{2J} \left(\frac{\partial \varphi_j}{\partial \tau} \right)^2 - \sum_{(jj')} V \cos(\varphi_j - \varphi_{j'}) \right] + \sum_{(jj')} S_D(\varphi_j - \varphi_{j'}). \quad (7)$$

The phase diagram of the model (7) has been studied by Chakravarty et al. [9].

The interaction of the instantons associated with vortex core tunnelling to a neighbouring cell for the model (7) at $T = 0$ is logarithmic, just as

in the case of phase tunnelling in a single junction with linear Ohmic dissipation [10]. The pre-logarithmic factor κ is proportional to the effective viscosity η and is determined entirely by the equilibrium configuration of the field φ in a vortex:

$$\kappa = \frac{\eta}{\pi} \sum_{(jj')} [\Delta\varphi_{jj'}(\tau = +\infty) - \Delta\varphi_{jj'}(\tau = -\infty)]^2;$$

$$\Delta\varphi_{jj'} = \varphi_j - \varphi_{j'},$$

where κ contains contributions from all junctions forming the array. For the case of a periodically continued parabolic potential (2) the value of κ can be calculated exactly; $\kappa = 2\pi\eta$. For the cosine potential it is also close to $2\pi\eta$.

The properties of periodic systems with linear Ohmic dissipation being known [11], one can immediately conclude that for $\kappa > \kappa_c = 2\hbar$ vortex tunnelling remains incoherent at arbitrary small temperatures, the tunnelling probability w depending on the temperature algebraically:

$$w \propto T^{\kappa/\hbar-1} \quad (8)$$

For $T = 0$ and $\kappa > \kappa_c$ the vortex is localized.

The consideration of the other kind of dissipation (originating from quasi particle tunnelling through a normal metal layer) which should be described by the non-Gaussian non-local action [12]:

$$S_D(\Delta\varphi) = \iint_{-\beta/2}^{\beta/2} d\tau d\tau' \frac{4\eta}{\pi} \times \left[\frac{\sin \frac{\Delta\varphi(\tau) - \Delta\varphi(\tau')}{4}}{\frac{\beta}{\pi} \sin \frac{\pi}{\beta} (\tau - \tau')} \right]^2,$$

leads not to qualitative changes, but only to a small ($\sim 10\%$) decrease of the parameter κ :

$$\kappa = \frac{\eta}{\pi} \sum_{(jj')} \left[4 \sin \frac{\Delta\varphi_{jj'}(+\infty) - \Delta\varphi_{jj'}(-\infty)}{4} \right]^2$$

entering eq. (8).

4. Quantum crystal free surface

We consider one more model, which has the Hamiltonian:

$$\hat{H} = \sum_{\langle ij \rangle} \left[\frac{J}{2} (\hat{n}_j - \hat{n}_{j'})^2 - V \cos(\varphi_j - \varphi_{j'}) \right], \quad (9)$$

and in the terms of the Josephson-junction array corresponds to a non-physical case of an inverse capacitance matrix containing negative elements.

Nonetheless this very model can be applied for describing such a realistic physical system as quantum crystal free surface [13, 14]. For such interpretation the first term in eq. (9) describes the energy of steps on the crystal surface (n is the height of the surface, in lattice units, with respect to a certain level) and the second term describes the hopping of atoms along the surface. The latter becomes more clear if one notes that the operators $a_j^\pm = \exp(\mp i\varphi_j)$ possess only such non-zero matrix elements as $\langle n_j \pm 1 | a_j^\pm | n_j \rangle = 1$ so the two terms of $-V \cos \Delta\varphi_{jj'} = -(V/2)(a_j^+ a_{j'}^- + a_j^- a_{j'}^+)$ correspond to an increase (decrease) of n_j by 1 simultaneously with a decrease (increase) of $n_{j'}$ by the same value.

The phase diagram of the model (9) has been investigated in ref. [14]. In the present paper we are interested only in the case $J, k_B T \ll V$, when the surface is in an atomically rough superfluid phase, quite analogous in its properties to the low-temperature phase of the quantum XY model (1).

The calculation of instanton interaction for the model (9) can be carried out with the help of the same formula (4) where one should replace $G_0(k, \omega)$ by

$$G_0(k, \omega) = \left[\frac{\hbar^2 \omega^2}{J(4 - 2 \cos k_x - 2 \cos k_y)} + V(4 - 2 \cos k_x - 2 \cos k_y) \right]^{-1}.$$

Just as in the case of the model (7) this interaction is logarithmic (the action of an isolated instanton logarithmically diverges). Thus, we again find ourselves in a position to conclude that the probability of intersite vortex tunnelling w decays with temperature algebraically:

$$w \propto T^{(\pi/8)\sqrt{V/J}-1}; \quad T \ll (VJ)^{1/2}/k_B, \quad (10)$$

the tunnelling being incoherent for arbitrary small temperatures. The exponent entering eq. (10) has the same value both for the original cosine potential $-V \cos(\Delta\varphi)$ and for its parabolic replacement (2). The same holds for the numerical coefficient in the exponent of eq. (5).

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