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Quantum dynamics of a single dislocation

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Abstract

We discuss the zero temperature motions of an edge dislocation in a quantum solid (e.g., He_4). If the dislocation has one *kink* (equal in length to its Burgers vector b) the kink has a creation energy U and can move along the line with a certain transfer integral t. When t and U are of comparable magnitude, two opposite kinks can form an extended bound state, with a size l. The overall shape of the dislocation in the ground state is then associated with a random walk of persistence length l (along the line) and hop sizes b. We also discuss the motions of kinks under an applied shear stress σ: the glide velocity is proportional to $\exp(-\sigma^*/\sigma)$, where σ^* is a characteristic stress, controlled by tunneling processes. ***To cite this article: P.-G. de Gennes, C. R. Physique 7 (2006).***

Résumé

Mouvements quantiques d'une dislocation. On analyse le mouvement à température nulle d'une dislocation coin dans un solide quantique (He_4). La dislocation peut avoir un *cran* (d'énergie U) dans son plan de glissement. Le cran peut avancer ou reculer le long de la dislocation par effet tunnel, avec une certaine intégrale de transfert t. Deux crans de signe opposé peuvent former un état lié. En présence d'une contrainte extérieure σ, la ligne doit avancer avec une vitesse $\sim\exp(-\sigma^*/\sigma)$ où σ^* est une contrainte seuil, contrôlée par l'effet tunnel. ***Pour citer cet article : P.-G. de Gennes, C. R. Physique 7 (2006).***

Version française abrégée

Des expériences récentes [1,2] suggèrent que He_4 solide, en rotation, exhibe des moments d'inertie anormalement bas. L'idée théorique classique sur ce sujet est basée sur des *lacunes*, qui seraient mobiles par effet tunnel et auraient une condensation de Bose [3]. Mais, à basse température, ces lacunes tendent à s'évaporer à la surface [4,5]. Récemment, P.W. Anderson et ses collaborateurs ont proposé un mécanisme qui maintient des lacunes même à température nulle [6].

Nous discutons ici un autre aspect, fondé sur des dislocations. Les expériences sont faites avec un solide polycristallin, qui comporte des *joints de grain* : chaque joint est associé à une échelle de dislocations. Si, par effet tunnel, ces lignes gardent une certaine mobilité, un écoulement à température nulle est possible.

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Nous étudions ici surtout *une* dislocation unique. Elle doit se déformer et se déplacer par des crans (Fig. 1). L'idée du mouvement quantique de crans a déjà été émise pour un problème différent : le déplacement de marches atomiques à l'interface He_4 solide/He_4 superfluide [8,9]. La Section 2 discute la mécanique quantique d'une paire de crans, qui, le plus souvent, doivent former un état lié. La Section 3 discute l'effet d'une contrainte externe σ, qui entraîne les dislocations.

Dans la Section 4 on discute brièvement la forme statistique d'une ligne portant des crans, à température $T = 0$.

Des relations éventuelles entre ces mouvements de dislocations et les expériences mécaniques [1,2] sont présentées dans la Section 5. Mais, au stade actuel, si on part de dislocations indépendantes, notre modèle représente plutôt une sorte de déformation plastique à $T = 0$ qu'une vraie superfluidité : il n'implique aucune cohérence de phase à grande échelle.

1. General aims

The mechanics of quantum solids is not yet fully understood. Recent experiments at Penn State [1,2] suggest that He_4 (at pressures ∼60 atm) is a solid with anomalously low moments of inertia. An early approach to this was based on vacancies [3] with a certain transfer integral t between adjacent sites. The assumption is that the idea of vacancies

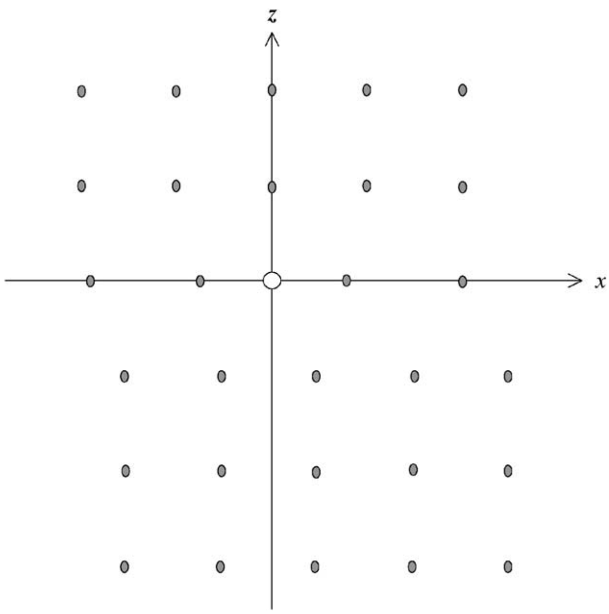

Fig. 1. An edge dislocation in a simple cubic lattice. Here, for tutorial reasons, we have put a vacancy at the core.

Fig. 1. Une dislocation coin dans un réseau cubique simple. Ici, pour des raisons pédagogiques, on a supposé qu'une lacune était fixée sur le coeur : alors les mouvements du coeur ressemblent à ceux d'une lacune.

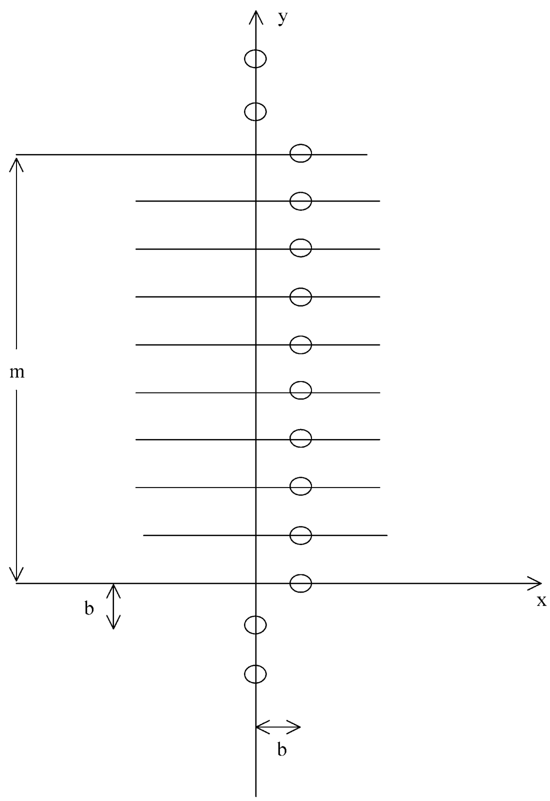

Fig. 2. Quantum motions of an edge dislocation (along y) moving in its glide plane (xy). We show two opposite kinks on the dislocation. Each kink can move up or down the y axis by one lattice distance b. The corresponding transfer integral is t. The creation energy for one kink is U.

Fig. 2. Mouvements quantiques d'une dislocation coin (parallèle à y en moyenne) se déplaçant dans son plan de glisse (xy). On voit deux crans sur la dislocation. Chaque cran peut sauter par effet tunnel d'une distance interatomique b dans la direction y. L'intégrale de transfert est t. L'énergie de création du cran est désignée par U.

form a gas (with short range repulsions) and display a Bose condensation. This, however, is not easy to justify, since the vacancies tend to drop out at the free surface of the crystal [4,5].

A different argument for the existence of vacancies has been proposed by P.W. Anderson and coworkers [6]. Their idea is that the optimal wave vector of the density modulations in the liquid differs slightly from the corresponding optimal reciprocal lattice vector in the ordered state: the difference may be achieved by a set of vacancies: this appears to be consistent with specific heat and X ray data.

In the present Note, we consider another type of defects: dislocation lines (Fig. 1): these lines can, in fact, be decorated by vacancies. Here we shall refer to vacancies as one simple picture of the line core. In the experiments of [1,2] we do expect that the solid He_4 is polycrystalline, with a number of *grain boundaries*. To each such boundary is associated a ladder of dislocation lines [7]. If, because of quantum effects, these lines retain a certain mobility, flow could possibly be allowed.

We concentrate here on a *single dislocation.* Clearly, this will not move as a whole, but through kinks as shown on Fig. 2. The idea of quantum kinks on a line was introduced long ago for a different problem: atomic steps at the surface of a He_4 crystal, bathing in superfluid Helium [8,9]. In Section 2, we discuss the quantum mechanics of kinks at a primitive level. In Section 3 we study the dislocation under an external shear stress.

In Section 4 we give a more formal presentation of one dislocation viewed as a sequence of spin $1/2$ fermions, with the $\uparrow$ spin describing kinks to the right and $\downarrow$ spin kinks to the left. We do not construct the detailed ground state of this model, but we do present a plausible argument for the overall shape of the fluctuating line (in zero stress).

Our central assumption is that the transfer integral t for kinks need not be very small when compared with the classical He_4–He_4 interactions. When the kink moves from one site to the next, an elastic deformation of the surrounding crystals lowers the barrier energy: this is very similar to the Peierls–Nabarro effect for the motion of dislocations invented more than 60 years ago [10].

2. Quantum mechanics of a pair of kinks

Consider the dislocation shape shown in Fig. 2, with two kinks of opposite sign, distant by a length mb ($m > 0$). We call ψ_0 the wave function of the unperturbed line (no kinks), and ψ_m the wave function of state m.

For simplicity, in this section, we fix the bottom kink at one position ($m = 0$) and let the top kink wander. This simplifies the notation, and preserves the physics (except for numerical coefficients).

The Hamiltonian $\mathcal{H}$ of the line has the following matrix elements:

$$(\psi_0|\mathcal{H}|\psi_0) = 0, \qquad (\psi_m|\mathcal{H}|\psi_m) = 2U, \qquad (\psi_m|\mathcal{H}|\psi_{m\pm1}) = -t \tag{1}$$

U is the creation energy for one kink; t is the transfer integral. The eigenvalue equations for the energy E are:

$$E\psi_m = 2U\psi_m - t(\psi_{m+1} + \psi_{m-1}) \tag{2}$$

$$E\psi_0 = -t\psi_1 \tag{3}$$

We shall find two cases:

(a) If $2U < t$ there is no bound state for the pair of kinks: kinks can be created freely, and the line wanders enormously. (This might correspond to melting ... ?)

(b) If $(2U - t)/t = \varepsilon$ is positive, the ground state describes two bound kinks, with a wave function:

$$\psi_m = \bar{\psi} \exp(-\,pm) \quad (m > 0) \tag{4}$$

where p is related to the energy E by Eq. (2)

$$E = 2U - 2t\cosh p \tag{5}$$

Eq. (2) written for $m = 1$ gives $\bar{\psi} = \psi_0$. Eq. (3) then leads to

$$E = -t\mathrm{e}^{-p} = -\frac{t^2}{2U} \tag{6}$$

Thus p is defined by

$$\mathrm{e}^{p} = \frac{2U}{t} \equiv 1 + \varepsilon \tag{7}$$

We concentrate here on the limit of small ε and, thus, of small p ($p \cong \varepsilon$). This corresponds to a bound state of large size l. The probability distribution for the bound state is proportional to $|\psi^2|$, and the size is $l = b/2p$.

3. Motions under a shear stress

Returning to Fig. 2, we now apply a shear stress $\sigma_{xz} = \sigma$ on the line, creating a Peach–Koehler [7] force σb (per unit length of line) along x. When we increase the interkink distance bm by one unit, we gain an energy $-\sigma b^3$. Eq. (2) is replaced by

$$E\psi_m = \left[2(U-t) - \sigma b^3 m\right]\psi_m - t\frac{\partial^2\psi}{\partial m^2} \tag{8}$$

(where we have gone to the continuum limit, valid for large l). The bound state is connected to free states by a tunneling barrier, extending from $m = 0$ to $m = m_0$, with a local decay constant $K(m)$

$$K^2 = \frac{2(U-t)}{t} - \frac{E}{t} - \frac{\sigma b^3 m}{t} \cong \varepsilon^2 - \frac{\sigma b^3 m}{t} \tag{9}$$

Thus

$$K = \varepsilon\left(1 - \frac{m}{m_0}\right)^{1/2} \tag{10}$$

with

$$m_0 = \frac{\varepsilon^2 t}{\sigma b^3} \tag{11}$$

The overall tunneling amplitude is

$$\exp\left[-\int_0^{m_0} \bar{K}(m)\,\mathrm{d}m\right] \equiv \exp(-I) \tag{12}$$

where

$$I = \varepsilon\int_0^{m_0} \mathrm{d}m\left(1 - \frac{m}{m_0}\right)^{1/2} = \frac{2}{3}\varepsilon m_0 \tag{13}$$

and the glide velocity V is expected to be of the form

$$V = V_0\exp(-2I) = V_0\exp\left(\frac{-\sigma^*}{\sigma}\right) \tag{14}$$

where σ^* is a characteristic stress

$$\sigma^* = \frac{4}{3}\varepsilon^3\frac{t}{b^3} \tag{15}$$

The prefactor V_0 is dimensionally expected to be of order $tb/\hbar$. Thus we obtain from Eq. (14) a very nonlinear relation between velocity and stress.

4. Statistical shape of the line in zero stress

(1) *Formal approach*: we may picture the dislocation (following Fig. 3) by a sequence of positive or negative kinks, with an attractive interaction $2U$ between two adjacent kinks of opposite sign. We also forbid the presence of two kinks of the same sign on one same site (this corresponding to a high energy). We may then describe the kinks as spin $1/2$ fermions (plus/minus spin corresponding to plus/minus kinks) with creation operators $\psi^+_{m\uparrow}$, $\psi^+_{m\downarrow}$. The corresponding Hamiltonian is

$$\mathcal{H} = -t\sum_m(\psi^+_{m\uparrow}\psi_{m+1\uparrow} + \psi^+_{m\downarrow}\psi_{m-1\downarrow}) - 2U\sum_m \psi^+_{m\uparrow}\psi_{m\uparrow}\psi^+_{m\downarrow}\psi_{m\downarrow} \tag{16}$$

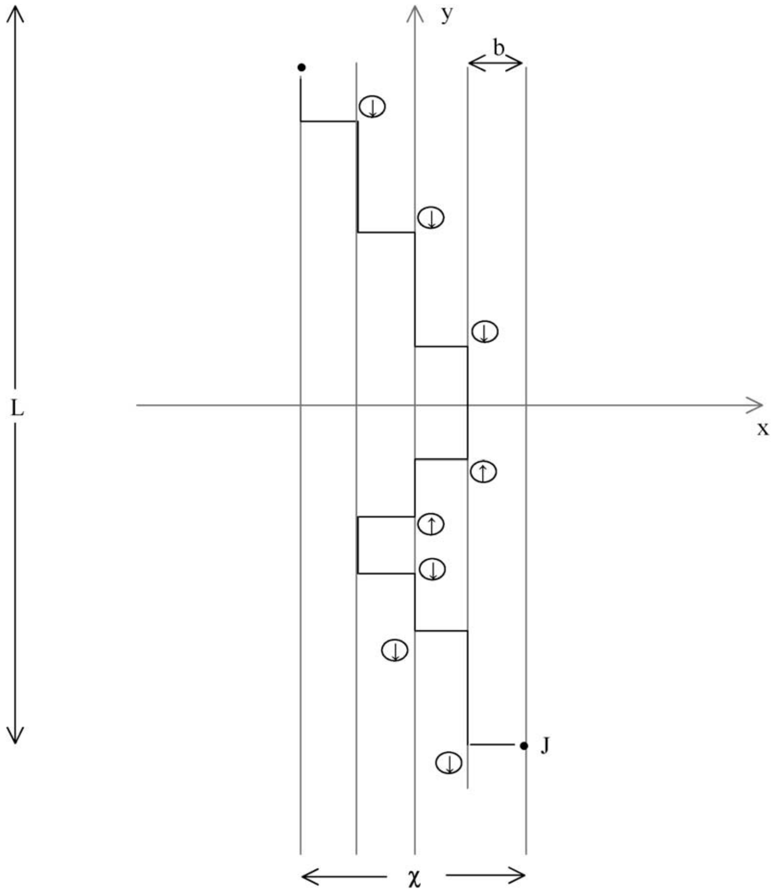

Fig. 3. Representation of a fluctuating line as a fluid of spin 1/2 fermions with a contact attraction between neighboring fermions of opposite spin.

Fig. 3. Représentation de la ligne avec ses fluctuations quantiques : il y a un gaz de crans le long de y. A chaque cran (positif/négatif) est associé un spin 1/2 (↑ / ↓). Il y a une attraction au contact pour deux crans de spin opposé.

The Fermi statistics ensures that we cannot have two kinks of the same sign on one site (m).

(2) It may be that the Hamiltonian $\mathcal{H}$ has a ground state wave function which can be constructed by an extension of the Bethe ansatz. Here we shall present only a simple conjecture, aiming at a description of the ground state fluctuations in the regime where we do have extended bound states of kinks.

The basic idea is based on the size l of the bound states (Eq. (8)). The average distance between kinks of the same spin is also expected to be $\sim l$. Thus we may roughly think of the dislocation line as a sequence of random steps, each having a length l (along x), each step being equal to $\pm b$. Then we expect a random walk behavior at large scales, with an overall fluctuation amplitude X (for a line length L along y) scaling like

$$X^2 = \frac{L}{l} b^2 \tag{17}$$

where L/l is the average number of lateral jumps ($\pm b$).

5. Concluding remarks

(A) Rheological behavior: we may extend the ideas of Section 3 to a population of parallel dislocations (with a line length per unit volume n). Under the stress σ these lines drift and generate a shear rate

$$\mathring{\gamma}_{xy} = \mathring{\gamma} = nbV \tag{18}$$

Eq. (18) can be checked by writing the dissipation $\sigma\mathring{\gamma} = T\mathring{S}$ (per unit volume) in terms of a Peach–Kochler force σb, working on each moving line of velocity V. Combining Eq. (18) with Eq. (14), we arrive at

$$\mathring{\gamma} = nbV_0 \exp(-\sigma^*/\sigma) \tag{19}$$

This looks like plastic flow rather than superfluid flow. See, however, point B(c) below:

(B) The whole construction presented in this Note is extremely fragile.

(a) It assumes that the transfer integrals t are large and comparable to the kink energies U: this would have to be examined using detailed simulations with realistic potentials for He_4 atoms (at various pressures). The optimal shape of a kink is probably not a sharp step, but a smooth curve extending over a few lattice distance along y. This will modify the transfer integral t.

(b) We assumed more specifically that the relative difference ε between $2U$ and t is small. This is an interesting limit because, in this case, the barrier length m_0 in Eq. (12) is large: even if two neighboring kinks have an interaction energy (say between next nearest neighbors), more complex than the contact term $2U$, the formula (14) should remain valid. However, this nice regime is probably not achieved in practice: we rather expect $t \ll U$, giving very tight bound states.

(c) Do these features lead to some anomalous behavior for a polycrystalline He_4 solid? We should explore not a single dislocation, but rather a ladder of such dislocations (with long range interactions between them). We should then find out whether these ladders can move under stress, and lead to an anomalous flow, before the ultimate moment where their motions allow the crystal to eliminate all its grain boundaries. These questions are, at present, totally obscure.

(C) A technical point: all our discussion of kink pairs assumed that one of them was fixed, while the other one made quantum jumps. In actual fact both kinks are mobile. This imposes a heavier notation, and modifies all numerical coefficients. We decided not to insist on these refinements, because in any case the model based on a simple cubic lattice is not really relevant. What we would need for the future is a sophisticated discussion of kink shapes and transfer integrals in an hcp lattice.

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References

[1] E. Kim, M. Chan, Nature 427 (2004) 225.
[2] E. Kim, M. Chan, Science 305 (2005) 1941.
[3] A. Andreev, I.M. Lifshitz, JETP 29 (1969) 1107.
[4] A.J. Leggett, Phys. Rev. Lett. 25 (1970) 1543.
[5] K. Liu, M.E. Fisher, J. Low Temp. Phys. 10 (1973) 655.
[6] P.W. Anderson, W. Brinkman, D. Huse, Science 310 (2005) 1164.
[7] J. Friedel, Dislocations, Pergamon Press, London, 1964.
[8] A.F. Andreev, A.Y. Parshin, Soviet Phys. JETP 48 (1978) 763.
[9] D.O. Edwards, S. Mukherjee, M. Pettersen, Phys. Rev. Lett. 64 (1990) 902.
[10] R. Peierls, Proc. Phys. Soc. 52 (1940) 34.