Momentum deficit in quantum glasses

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Abstract

Using the concept of tunneling two level systems we explain the reduction of rotational inertia of disordered solid ⁴He observed in the torsional oscillator experiments. The key point is a peculiar quantum phenomenon of momentum deficit for two level systems in moving solids. We show that an unusual state which is essentially different from both normal and superfluid solid states can be realized in quantum glasses. This state is characterized by reduced rotational inertia in oscillator experiments, by absence of a superflow, and by normal behavior in steady rotation.

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1 Introduction

Owing to the large probability of quantum tunneling of the atoms (quantum solid), solid helium may be superfluid [1]. The general macroscopic motion of a superfluid solid is characterized by two mutually independent velocities: that of the solid bulk and the superfluid one. Since the superflow is irrotational, the moment of inertia of the superfluid solid is determined by the normal fraction density. On the contrary, the solid bulk velocity in a capillary is zero and the mass transfer is exclusively determined by the superflow.

Kim and Chan [2] observed the reduction of the solid 4 He moment of inertia below 0.2K in the torsional oscillator experiments and interpreted it as superfluidity of the solid. However, all attempts to observe a superflow (see [3] and [4]) were unsuccessful. Experiment [4] gives the upper limit of the critical velocity which is seven orders of magnitude smaller than the value obtained by Kim and Chan. The experimental data therefore disagree with the picture of a superfluid solid.

Further experiments [5] showed that the reduction of rotational inertia observed in highly disordered (glassy) samples of ⁴He is remarkably large, exceeding 20%. The reduction seems to be absent in ideal helium crystals (see [6] for a review).

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Anderson et al. and Philips [7] showed that the quantum tunneling of the atoms is responsible for anomalies in some low temperature properties (thermal, electromagnetic, and acoustic) of usual glasses. The key point is the presence of the so-called tunneling two level systems (TLS) in the solids. A TLS can be understood as an atom, or a group of atoms, which can tunnel between two localized states characterized by a small energy difference.

In this paper (also see earlier Letter [8]) we show that anomalous properties of disordered solid 4 He (the reduction of the rotational inertia, the absence of a superflow, and the absence of anomalies in perfect crystals) can be naturally explained on the basis of the concept of TLS. We show that a peculiar quantum phenomenon takes place. In the solid moving with a velocity \mathbf{v} , the contribution \mathbf{P} of a TLS to the total momentum of the solid under certain conditions (see below) can be different from $m\mathbf{v}$ where m is a contribution of the TLS to the total mass. The difference $\mathbf{p} = \mathbf{P} - m\mathbf{v}$ is determined by the velocity \mathbf{v} itself. The momentum deficit $-\mathbf{p}$ is proportional to the squared TLS tunneling amplitude.

As a result, an unusual state of quantum glasses can be realized. This state is essentially different from both normal and superfluid solid states. As a normal solid, this state is characterized by single velocity of macroscopic motion: the solid bulk velocity \mathbf{v} . But under certain conditions the momentum density is $(\rho - \rho_d)\mathbf{v}$ where ρ is the mass density, $\rho_d\mathbf{v}$ is the momentum density deficit, and ρ_d is a mass density deficit. In the present paper we calculate ρ_d in terms of TLS parameters. Being proportional to the squared TLS tunneling amplitude the density deficit can be considerable for highly disordered solid ⁴He and other quantum solids (hydrogen).

Our results are supported by the experiment by Grigorev et al. [9] who measured the temperature dependence of pressure in solid ⁴He, grown by the blocked capillary technique. At temperatures below 0.3 K where the reduction of the rotational inertia was observed, they found the glassy contribution to the pressure ($\propto T^2$). This corresponds exactly to the TLS contribution. On the other hand, the measurements of the melting pressure in perfect ⁴He samples showed no deviations from T^4 law [10].

2 TLS in moving solids

The Hamiltonian H_0 of a given TLS in the frame of reference in which the solid bulk velocity \mathbf{v} is zero, can be written as

$$H_0 = -\varepsilon \sigma_3 + J\sigma_1. \tag{1}$$

Here $\mp \varepsilon$ ($\varepsilon > 0$) are energies of two localized states, J is the tunneling amplitude, and σ_i (i = 1, 2, 3) are the Pauli matrices.

Let us suppose that the tunneling of the TLS be accompanied by displacement of a mass m by a vector \mathbf{a} . The coordinates $\mathbf{r}_{1,2}$ of the center of gravity of the TLS before and after the tunneling can be written as $\mathbf{r}_{1,2} = \mp \mathbf{a}/2$. The operator form of the last equality is $\mathbf{r} = -\sigma_3 \mathbf{a}/2$. The operator of velocity is

determined by the commutator:

$$\dot{\mathbf{r}} = \frac{i}{\hbar} [H_0, \mathbf{r}] = -\frac{J\mathbf{a}}{\hbar} \sigma_2. \tag{2}$$

The TLS momentum in the frame in which $\mathbf{v} = 0$, is

$$\mathbf{p} = m\dot{\mathbf{r}} = -\frac{mJ\mathbf{a}}{\hbar}\sigma_2. \tag{3}$$

In an arbitrary frame of reference a description of the TLS by means of a discrete coordinate is impossible. But we can use Galilean transformations to find the TLS Hamiltonian and momentum in the frame in which \mathbf{v} is finite. We obtain

$$H_0 + \mathbf{p}\mathbf{v} + mv^2/2; \qquad \mathbf{p} + m\mathbf{v}, \tag{4}$$

respectively. The last terms of both expressions must be included to the total kinetic energy and momentum of the solid bulk. Therefore, the contributions of the TLS tunneling to the energy and momentum of the total system are

$$H = H_0 + \mathbf{pv}; \qquad \mathbf{p}. \tag{5}$$

These two operators represent the energy and momentum of the tunneling TLS in the solid moving with velocity \mathbf{v} . We note that the operators \mathbf{p} and H do not commute with each other.

The eigenvalues of the Hamiltonian H are $E_{1,2} = \mp E$, where $E = (\varepsilon^2 + \Delta^2)^{1/2}$, $\Delta = J(1+u^2)^{1/2}$, and $u = (m/\hbar)\mathbf{av}$. Using conventional formula ([11], §11) the mean values of momentum $\langle \mathbf{p} \rangle_{1,2}$ in the stationary states 1 and 2 are

$$\langle \mathbf{p} \rangle_{12} = \left\langle \frac{\partial H}{\partial \mathbf{v}} \right\rangle_{1,2} = \frac{\partial E_{1,2}}{\partial \mathbf{v}}.$$
 (6)

We have

$$\langle \mathbf{p} \rangle_{12} = \mp \frac{J^2 m^2}{\hbar^2 E} \mathbf{a}(\mathbf{a}\mathbf{v}).$$
 (7)

In case of nonzero \mathbf{v} , the TLS has nonzero mean values of momenta in both of its stationary states. We note that in the TLS ground state, the projection of the momentum $\langle \mathbf{p} \rangle_1$ on the direction of velocity \mathbf{v} is negative. This is the mechanism of the momentum deficit. The Hamiltonian H is the same as for spin 1/2 in an external magnetic field. The sign of $\langle \mathbf{p} \rangle_1$ corresponds to the spin paramagnetism.

3 Steady rotation

Equilibrium properties of a TLS in a steadily rotating solid are determined by the equilibrium density matrix w of the TLS in the steadily rotating frame.

We consider TLS as almost closed systems neglecting the interaction between different TLS. The density matrix is

$$w = \exp\frac{f' - H'}{T},\tag{8}$$

where f' and H' are the free energy and Hamiltonian in the rotating frame. We have

$$H' = H - \omega \mathbf{M} = H_0 + \mathbf{p}\mathbf{v} - \omega \mathbf{M},\tag{9}$$

where ω is the angular velocity, \mathbf{M} is the TLS angular momentum. Since the size of the TLS is supposed to be much smaller than the length scale of the rotating container, we can use the following expressions for the velocity and the angular momentum

$$\mathbf{M} = \mathbf{R} \times \mathbf{p}; \qquad \mathbf{v} = \omega \times \mathbf{R} \tag{10}$$

where **R** is the coordinate of the TLS center of gravity with respect to an origin situated at the rotation axis. We obtain $H' = H_0$. This means that TLS cause no anomalies. Steadily rotating quantum glasses behave like normal solids.

4 Adiabatic process

The result is different if the solid bulk velocity depends on time $\mathbf{v} = \mathbf{v}(t)$. Suppose it is applied adiabatically. We consider two different physical situations.

4.1 Thermodynamic equilibrium

Assume that during the adiabatic process, the solid itself remains in thermodynamic equilibrium. This means (see [12], §11) that the "transition duration" is much longer than the relaxation time in the solid but much shorter than the period during which the solid can be regarded as thermally insulated. The second of these two time scales is very long due to the Kapitza thermal resistance. In oscillator experiments the same conditions have to be satisfied for the period of oscillations.

Suppose the velocity is applied as a result of an axisymmetric container rotation. Otherwise, additional terms should be included to the Hamiltonian to take the macroscopic displacement of the container walls into account (see [12], §11).

As usual in statistical mechanics ([12], §11 and §15) we have

$$\langle \mathbf{p} \rangle = \left\langle \frac{\partial H}{\partial \mathbf{v}} \right\rangle = \left(\frac{\partial f}{\partial \mathbf{v}} \right)_T,$$
 (11)

where

$$f = -T\log \operatorname{Tr} \exp(-H/T) \tag{12}$$

is the TLS free energy and H is determined by the first expression in (5) with $\mathbf{v} = \mathbf{v}(t)$.

The free energy (12) can be written as

$$f = -T\log\left(\exp\frac{-E_1}{T} + \exp\frac{-E_2}{T}\right). \tag{13}$$

Here $E_{1,2} = \mp E$ are the eigenvalues of the Hamiltonian H. The mean value of the TLS momentum is

$$\langle \mathbf{p} \rangle = \frac{m\mathbf{a}}{\hbar} \left(\frac{\partial f}{\partial u} \right)_{T}. \tag{14}$$

Simple calculation gives

$$\left(\frac{\partial f}{\partial u}\right)_T = -\frac{J^2 u}{E} \tanh \frac{E}{T} \tag{15}$$

or

$$\langle p_i \rangle = -m_{ik}^{(d)} v_k, \tag{16}$$

where the mass deficit tensor is

$$m_{ik}^{(d)} = \left(\frac{Jm}{\hbar}\right)^2 a_i a_k \frac{\tanh(E/T)}{E}.$$
 (17)

4.2 Free TLS

Consider the opposite limiting case when the time scale of velocity variations (the period of oscillations) is much shorter than the TLS relaxation time. The TLS can be regarded as free. The Hamiltonian H of a TLS (see (5)) can be written as

$$H = -h_{\alpha}\sigma_{\alpha},\tag{18}$$

where $\alpha = 1, 2, 3$ and h_{α} is the "field" having the following components $h_1 = -J, h_2 = Ju, h_3 = \varepsilon$. Generally the TLS density matrix w is determined by a real polarization vector s_{α} :

$$w = (1 + s_{\alpha}\sigma_{\alpha})/2. \tag{19}$$

We have

$$\langle \sigma_{\alpha} \rangle = \text{Tr}(w\sigma_{\alpha}) = s_{\alpha}.$$
 (20)

The mean value of the TLS momentum is

$$\langle \mathbf{p} \rangle = -\frac{mJ\mathbf{a}}{\hbar} s_2. \tag{21}$$

From the equation for the density matrix

$$\dot{w} = \frac{i}{\hbar}[w, H] \tag{22}$$

we get the equation for s_{α} :

$$\hbar \dot{s_{\alpha}} = e_{\alpha\beta\gamma} h_{\beta} s \gamma, \tag{23}$$

where $e_{\alpha\beta\gamma}$ is the Levi-Civita tensor.

The adiabatic theorem (see [13], chap II, §5c) takes place as a consequence of (23). Besides the absolute value $s = |s_{\alpha}|$ of the polarization, the angle between the field h_{α} and s_{α} is the integral of motion. The process is adiabatic for free TLS if the time scale of velocity variation is much longer than $\hbar/|h_{\alpha}|$. The last condition is very liberal for quantum solids.

Until the solid is put in motion, the polarization is directed along the field $(-J, 0, \varepsilon)$, and the absolute value of equilibrium polarization is

$$s = \tanh \frac{\left(\varepsilon^2 + J^2\right)^{1/2}}{T}.$$
 (24)

With the same absolute value, the polarization is directed along the field $(-J, Ju, \varepsilon)$ when the velocity $\mathbf{v} = \mathbf{v}(t)$ is applied. We have

$$s_2(t) = \frac{Ju(t)}{E(t)} \tanh \frac{\left(\varepsilon^2 + J^2\right)^{1/2}}{T}.$$
 (25)

Again, the TLS momentum is determined by (16), but now the mass deficit tensor is

$$m_{ik}^{(d)} = \frac{J^2 m^2}{\hbar^2 E} a_i a_k \tanh \frac{\left(\varepsilon^2 + J^2\right)^{1/2}}{T}.$$
 (26)

5 Momentum deficit

To calculate the momentum density we have to integrate the expression (16) with (17) and (26) over the TLS ensemble. Let $Nd\varepsilon$ (N= const) be the number of TLS per unit volume of the solid and per interval of the energy half-difference $d\varepsilon$ near some ε which is much smaller than the characteristic height U of the energy barriers in the solid. The total momentum density \mathbf{j} is

$$j_i = \rho v_i - \rho_{ik}^{(d)} v_k, \tag{27}$$

where the tensor of the density deficit is the same with the logarithmic accuracy for both cases (17) and (26):

$$\rho_{ik}^{(d)} = \left\langle m^2 J^2 a_i a_k \right\rangle \frac{N}{\hbar^2} \int_{\max(\Delta, T)}^{U} \frac{d\varepsilon}{\varepsilon}.$$
 (28)

Here $\langle ... \rangle$ means the averaging over the TLS ensemble at $\varepsilon = 0$, and $\max(\Delta, T)$ is of the order of Δ if $T \ll \Delta$ and of the order of T if $T \gg \Delta$. Both T and Δ are much smaller than U.

For an isotropic system (glass) we have $\rho_{ik}^{(d)} = \rho_d \delta_{ik}$, where

$$\rho_d = \frac{N}{3\hbar^2} \left\langle m^2 J^2 a^2 \right\rangle \log \frac{U}{\max(\Delta, T)}.$$
 (29)

We see that the characteristic temperature of the phenomenon is of the order of Δ . The critical velocity v_c is determined by the condition that $u_c \sim 1$. We have $v_c \sim \hbar/(ma)$. The critical velocities observed experimentally (see [2]) are very small. This suggests the macroscopic character of the most effective TLS. In principle, this is possible. The pressure dependence of ρ_d is determined by the competition of all parameters N, m, J, and a. For efficient tunneling of a TLS the presence of a region which has lower local particle number density is necessary near the TLS. The ³He impurity, due to the smaller mass of ³He atoms, must bind to such regions (see [6]) destroying TLS. This is a simple explanation of the depletion of the momentum deficit by ³He impurities observed in the experiments [2].

6 Conclusions

We have shown that a new quantum phenomenon of momentum deficit takes place for TLS in moving solids. As a result, an unusual state of quantum glasses (solid helium, solid hydrogen) can be realized. Like normal solid, this state is characterized by a single velocity of macroscopic motion: the solid bulk velocity. This explains the negative results of experiments [3] and [4]. The reduction of rotational inertia observed by Kim and Chan [2] is a direct consequence of momentum deficit.

Our prediction is that steadily rotating quantum glasses behave like normal solids. TLS cause no reduction of moment of inertia in this case.

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