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MOMENTUM DEFICIT IN QUANTUM GLASSES

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Using the concept of tunneling two-level systems, we explain the reduction of rotational inertia of disordered solid ^{4}He 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 that 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 the absence of a superflow, and by the 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]. General macroscopic motion of a superfluid solid is characterized by two mutually independent velocities, those of the solid bulk and of the superfluid one. Because the superflow is irrotational, the moment of inertia of a 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 0.2 K in the torsional oscillator experiments and interpreted it as superfluidity of the solid. However, all attempts to observe a superflow (see [3, 4]) were unsuccessful. The experiment in [4] gives the upper limit of the critical velocity which is seven orders of magnitude smaller than the value obtained in [2]. 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 ^{4}He is remarkably large, exceeding 20 %. The reduction seems to be absent in ideal helium crystals (see [6] for a review).

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It was shown in [7] 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 that 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 occurs. In a solid moving with a velocity $\mathbf{v}$, the contribution $\mathbf{P}$ of a TLS to the total momentum of the solid can under certain conditions (see below) be different from $m\mathbf{v}$, where m is the 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 a 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 the mass density deficit. In this paper, we calculate ρ_d in terms of TLS parameters. Being proportional to the squared TLS tunneling amplitude, the density deficit can be large for highly disordered solid ^{4}He and other quantum solids (hydrogen).

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

2. TLS IN MOVING SOLIDS

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

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

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

We 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 velocity operator 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 where $\mathbf{v} = 0$ 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 where $\mathbf{v}$ is finite. We obtain

$$H_0 + \mathbf{p}\cdot\mathbf{v} + mv^2/2; \quad \mathbf{p} + m\mathbf{v}. \tag{4}$$

The last terms in both expressions must be included into 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

$$H = H_0 + \mathbf{p}\cdot\mathbf{v}; \quad \mathbf{p}. \tag{5}$$

These two operators represent the energy and momentum of the tunneling TLS in the solid moving with the 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 $u = (m/\hbar)\mathbf{a}\cdot\mathbf{v}$. Using the standard formula (see [11, § 11]), we can express the momentum mean values $\langle\mathbf{p}\rangle_{1,2}$ in the stationary states 1 and 2 as

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

It follows that

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

In the case of a 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 the 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 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 regard the TLSs as almost closed systems, neglecting the interaction between different TLSs. The density matrix is

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

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

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

where $\boldsymbol{\omega}$ is the angular velocity and $\mathbf{M}$ is the TLS angular momentum. Because 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:

$$\mathbf{M} = \mathbf{R}\times\mathbf{p}, \quad \mathbf{v} = \boldsymbol{\omega}\times\mathbf{R}, \tag{10}$$

where $\mathbf{R}$ is the coordinate of the TLS center of gravity with respect to the origin located at the rotation axis. We obtain $H' = H_0$. This means that TLSs 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, $\mathbf{v} = \mathbf{v}(t)$. We note that the term $\mathbf{p} \cdot \mathbf{v}$ in Hamiltonian (5) describes the interaction between a TLS and the velocity field $\mathbf{v}(t)$. We assume that it is applied adiabatically. We consider two different physical situations.

4.1. TLS in thermodynamic equilibrium

At low temperatures in highly disordered solids, the TLS–TLS relaxation time τ is much shorter than the TLS–phonon relaxation time τ_p. We assume that during the adiabatic process, the TLSs remain in thermodynamic equilibrium. This means (see [12, § 11]) that the "transition duration" is much longer than τ but much shorter than τ_p. In oscillator experiments, the same conditions must be satisfied for the period of oscillations.

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

As is usual in statistical mechanics [12, § 11, § 15], we have

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

where

$$f = -T \ln \mathrm{Tr} \, \exp(-H/T) \tag{12}$$

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

The free energy in (12) can be written as

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

where $E_{1,2} = \mp E$ 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

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

or

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

where the mass deficit tensor is

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

4.2. Free TLS

We now consider the opposite limit case where 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 components $h_1 = -J$, $h_2 = Ju$, and $h_3 = \varepsilon$. The TLS density matrix w is generally determined by a real polarization vector s_α:

$$w = \frac{1 + s_\alpha \sigma_\alpha}{2}. \tag{19}$$

We have

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

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 obtain 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, Chapt. II, § 5c]) holds as a consequence of (23). In addition to the absolute value $s = |s_\alpha|$ of the polarization, the angle between the field h_α and s_α is an integral of motion. The process is adiabatic for a 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 set into motion, the polarization is directed along the field $(-J, 0, \varepsilon)$, and the absolute value of the equilibrium polarization is

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

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 then have

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

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

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

5. MOMENTUM DEFICIT

To calculate the momentum density, we have to integrate expression (16) with (17) and (26) over the TLS ensemble. Let $N d\varepsilon$ ($N = \text{const}$) be the number of TLSs per unit volume of the solid and per interval of the energy half-difference $d\varepsilon$ near some ε that 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 density deficit tensor is the same with the logarithmic accuracy in both cases (17) and (26):

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

Here, $\langle \ldots \rangle$ denotes 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

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

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 $u_c \sim 1$. 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 the parameters N, m, J, and a. For efficient tunneling of a TLS, the presence of a region with a lower local particle number density is necessary near the TLS. The ^{3}He impurity, due to the smaller mass of ^{3}He atoms, must bind to such regions (see [6]), thus destroying the TLS. This is a simple explanation of the depletion of the momentum deficit by ^{3}He impurities observed in the experiments in [2].

6. CONCLUSIONS

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

We have generalized the results in our work [8] to the wider region of rotation frequencies. Dynamic equations (23) for TLS are derived. In the general case, these equations should be solved together with elasticity theory equations using proper boundary conditions. The present theory is therefore nonlocal and is not excluded by the blocked annulus experiment as suggested in [14].

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