

Coherent motion in the interaction model of cold glasses

Abdollah Langari

Institute for Advanced Studies in Basic Sciences, Zanjan 45195-159, Iran;
Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresden, Germany;
and Institute for Studies in Theoretical Physics and Mathematics, P. O. Box 19395-5531, Tehran, Iran
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We have studied the collective phenomena of multicomponent glasses at ultralow temperatures by taking into account the proper interaction between tunneling centers. We have considered both double- and triple- well potentials with different types of interactions. We show that a phase with coherent motion appears for a range of parameters when the path of tunneling is coursed by an interaction of the XY type, while the usual Ising-like interaction does not lead to the expected collective phenomena. In the phase of coherent motion, the dipole moment and the low-energy levels oscillate with a frequency proportional to the number of tunneling centers in the system. Simultaneous level crossing occurs between the ground and first excited states. The effects of long-range interactions and also of random couplings have been also studied for a one- and two-dimensional array of tunneling centers. We find that long-range interactions do not affect the coherent motion, while a wide distribution of random couplings destroys the collective effects.

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I. INTRODUCTION

At low temperatures glasses exhibit surprising phenomena, which are interesting both from a theoretical as well as from an experimental point of view. These properties have been attributed to the low-lying excitations which appear in almost all amorphous and disordered solids.¹ The most simple and successful model to explain many properties of glasses is the tunneling model (TM).^{2,3} In this model the excitations are described phenomenologically as a tunneling system. One may consider a double-well potential to be a tunneling system where an entity (an atom, group of atoms, . . .) tunnels between the wells. At low temperatures only the lowest-lying state of each well is relevant, so the model is effectively described by a two-dimensional Hilbert space where the basis kets represent the ground states of each of the well. Using the Pauli matrices, the Hamiltonian of an isolated two-level system (TLS) is given by

$$H_0 = \frac{1}{2}(\Delta\sigma^z + \Delta_0\sigma^x). \quad (1)$$

The eigenstates $|+\rangle$ and $|-\rangle$ of σ^z refer to the particle being in the right (R) and left (L) well, respectively (see Fig. 1). Δ is the asymmetry energy and Δ_0 is the tunneling matrix element. The analogy of H_0 with a spin-1/2 particle in a magnetic field can be used to explain the dynamics of TLS's in glasses. The interactions with acoustic and electric fields are usually treated as weak perturbations which enables the TLS model to explain successfully many of the anomalous thermal, acoustic, and dielectric properties of glasses.

Although the isolated TLS model works very well in many cases, there are some phenomena which can not be described only by isolated TLS's.⁴ In these cases it is expected that the interactions between the TLS's will resolve the problem.^{5,6} As an example, one may consider the effects of interactions in the two-level tunneling defect crystals, KCL:Li.⁷ In this system the density of defect ions (Li^+) is a tunable parameter. At low density, the distance of tunneling

centers is fairly large, so the interaction does not affect the behavior of the isolated TLS's. Upon increasing the density, dipole-dipole interactions between the TLS's become important and drive the system into a glassy state.⁸

Recently experiments on multicomponent glasses show novel phenomena at ultralow temperatures.⁹ By decreasing the temperature down to 5 mK the dielectric constant ϵ responds linearly to a small magnetic field of the order of 10 μT . In general, glasses are properly assumed to be linear dielectrics, so that ϵ depends quadratically on the electromagnetic field.¹⁰ Although the dependence on the magnetic field may come from nonlinear effects, the observed magnetic field dependence of ϵ in multicomponent glasses at very low temperatures is completely different in nature from the magneto effect in nonlinear dielectrics⁹ and can not be derived from thermodynamics by assuming glasses as simple magnetizable dielectrics.

The first theoretical approach addressing this behavior

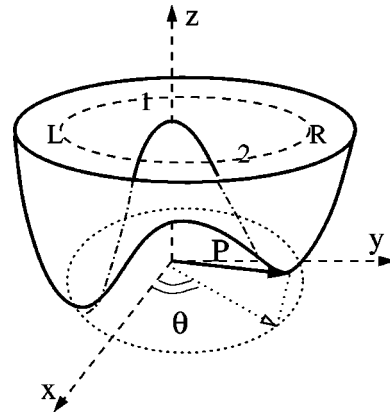


FIG. 1. A double-well potential in three-dimensional space. The wells are marked by L and R which are separated by a barrier. The tunneling may happen through this barrier via path 1 or 2. The position of a charged particle in the potential defines the dipole moment \mathbf{P} . The projection of \mathbf{P} onto the x - y plane is described by the angle θ measured from the x axis.

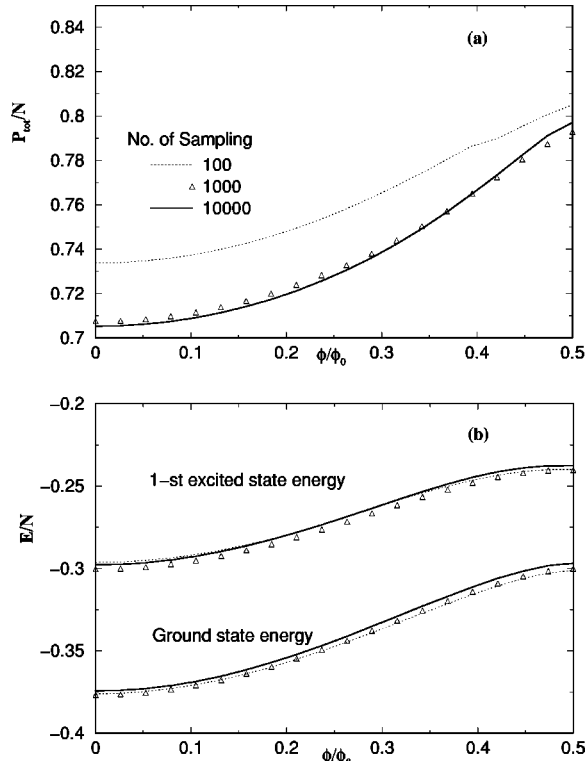


FIG. 2. (a) Dipole moment per site, (b) ground state and first excited state energy vs the magnetic flux ratio for $N=4$ interacting TLS's, Eq. (5). The tunneling centers are considered to be on a one-dimensional lattice. Data are shown for three different sampling numbers 100, 1000, and 10000. It is obvious that the data converge to the average value in the case of 10 000 samplings. Neither the dipole moment nor the energy levels show any oscillations signaling coherent motion.

considered the Aharonov-Bohm effect upon a charged particle in a three-dimensional (3D) double-well potential.¹¹ In this approach, as explained briefly in the next section, the effect of magnetic field enters in the form of a flux-dependent hopping parameter in the standard TLS. Then the isolated TLS of Eq. (1) is studied with $\Delta_0 \equiv \Delta_0(\phi)$. To fit the experimental electric permittivity data (Fig. 3 in Ref. 11) the charge entity in the TLS should be $Q \approx 10^5 |e|$, where $|e|$ is the magnitude of the electron charge. The large value of Q is explained by assuming *coherent motion* of the charged particles in all of the TLS's on a mesoscopic scale. The coherent motion takes place when the interactions between the TLS's become important at ultralow temperatures. In this phase one may treat the motion of all of the TLS's in terms of a single TLS with a charge Q which is equal to the sum of all of the charges. Although this model effectively describes the magnetic field dependence of the electric permittivity, the type of interaction which may lead to coherent motion over the mesoscopic size of TLS remained open.

Our goal in this paper is to explain in a more quantitative way the collective effect of TLS's in the presence of a magnetic field by taking into account the interactions of the TLS's. In this approach we introduce the magnetic field in the flux-dependent hopping elements, while the interaction term traces the path of the tunneling process. The coherent

motion of the particles is simulated by probing the relative motion of each coupled TLS. We suppose that our model is the original interacting model of the effective TLS containing the renormalized parameters introduced in Ref. 11. We will study the effects of long-range (LR) interactions and also of random couplings using our model in order to justify our contention that it represents the collective phenomenon of cold glasses properly.

The outline of this paper is as follows: In the next section we will briefly explain the effective model of TLS's in which the magnetic field is included as a flux-dependent tunneling matrix element. In Sec. III the double- and triple-well models are studied in the presence of an Ising-like interaction. We introduce the XY-like interaction in Sec. IV. In this model, it is possible to trace the tunneling path in each TLS and hence to simulate the coherent motion. We will study the effect of long-range interactions and random couplings on the behavior of our model in different subsections. In these studies we have used an exact diagonalization method to obtain the physical quantities from our model restricted to one- or two-dimensional lattices. We finally present our conclusions in Sec. V.

II. EFFECTIVE MODEL OF TLS

We start first by explaining the effective model of an isolated TLS.¹¹ The basic idea in this approach is to consider the Aharonov-Bohm effect upon a charged particle in a two-dimensional double-well potential. The real-space representation of the potential might look similar to a Mexican hat, as shown in Fig. 1. In this figure the solid lines defines a potential with two minima separated by a finite barrier. The two minima are labeled L and R. A particle with charge Q bounded in this potential may tunnel from one well (L) to the other one (R) along the different paths labeled 1 and 2, corresponding to clockwise and anticlockwise rotations, respectively. Without loss of generality we assume that each path covers half a circle (π radians). Now we introduce a magnetic field B parallel to the z axis to our model. Within the two-level approximation, Eq. (1), the magnetic field affects the parameters of our model. If tunneling occurs through path 1 (L to R), the wave function of the particle is influenced by the factor $e^{i\pi\phi/\phi_0}$, where ϕ is the total flux passing through a closed tunneling path, ϕ_0 is the flux quantum defined by $\phi_0 = h/|Q|$, and h is Planck's constant. On the other hand, tunneling through path number 2 (L to R) adds the factor $e^{-i\pi\phi/\phi_0}$ to the wave function. Since the tunneling through both paths occurs with equal probability, the tunneling matrix element t between L and R is equal to the sum of the hopping through path 1 and 2 which is

$$t(\phi) = \Delta_0 (e^{i\pi\phi/\phi_0} + e^{-i\pi\phi/\phi_0})/2 = \Delta_0 \cos(\pi\phi/\phi_0). \quad (2)$$

The factor 1/2 arises from the equal probability of the paths in which the total path probability is conserved to be unity. Then, replacing the tunneling matrix element Δ_0 in Eq. (1) by $t(\phi)$, the Hamiltonian of an isolated TLS in the presence of a magnetic field becomes

$$H_0(\phi) = \frac{1}{2} \begin{pmatrix} \Delta & t(\phi) \\ t(\phi) & -\Delta \end{pmatrix}. \quad (3)$$

The next steps to calculate the physical quantities are similar to those for the standard isolated TLS's.^{2,3} To do so, one simply replace Δ_0 by $t(\phi)$ in all of the equations.

According to Ref. 11, the electric permittivity ϵ depends on temperature as well as magnetic flux through the minimal tunneling splitting $t_{min}(\phi)$. The maximum value of the resonant part of ϵ , ϵ_{res} , is obtained when the lower cutoff of the excitation $t_{min}(\phi)$ vanishes. This is important when the temperature is lowered since the relaxational part of ϵ becomes negligible. Thus the maximum value of ϵ occurs at $t_{min}(\phi) = 0$ or, equivalently, at $\phi = \phi_0/2$. By introducing the experimental values of $B = 0.1$ T (see Fig. 3 in Ref. 11) and the typical radius $r \approx 2 \times 10^{-10}$ m of a tunneling center one can obtain agreement with the experimental data, if one further assumes $\phi_0 \approx 10^{-5} h/|e|$. In other words, using the definition $\phi_0 = h/Q$, we arrive at $Q \approx 10^5 |e|$. The charge Q is suggested to be the effective charge of $N \approx 10^5$ electrons in TLS's which tunnel coherently. The coherent tunneling could arise from the interactions between the TLS's which are important in the low-temperature regime.

If we consider coherent motion with the above-mentioned characteristics, we expect to observe an oscillation with a frequency proportional to N in the ground-state energy and in some other physical quantity of the interacting model. This is simply understood by considering $\phi_0 = h/(N|e|)$ and substituting it in the energy eigenvalues of Eq. (3), leading to $\pm \frac{1}{2} \sqrt{\Delta^2 + \Delta_0^2 \cos^2(N\pi\phi/\phi_0)}$, where $\phi_0 = h/|e|$. We will show in the next sections that a special form of the interactions can produce such evidence for coherent motion with the specified property.

III. INTERACTION MODELS

In this section we consider an ensemble of TLS's. Each tunneling center is placed onto a lattice site. The on-site Hamiltonian is the same as Eq. (3), where 2Δ is the energy difference between the well bottoms. The tunneling centers (sites) interact through H_{int} . The Hamiltonian of the lattice is then of the following form:

$$H = \sum_{i=1}^N H_0^i(\phi) + H_{int}. \quad (4)$$

The coupling between sites (H_{int}) arises from electric dipole-dipole interactions. The magnetic dipole-dipole interactions, which are set up by the persistent currents of the tunneling centers, are negligible. Typically the magnetic interaction is of order 10^{-12} smaller than the electric dipole-dipole interaction for a tunneling system, assuming the average distance between tunneling centers is 10^{-8} m.

We first consider the following form for the electric dipole-dipole interaction:

$$H_{int} = \sum_{i,j} J_{i,j} \sigma_i^z \sigma_j^z, \quad (5)$$

where $J_{i,j} \sim 1/|r_i - r_j|^3$ is the coupling of dipole moments. A distribution for $J_{i,j}$ simulates different orientations of dipole moments. We have considered a one-dimensional array of sites and diagonalized the Hamiltonian exactly to find its low-energy spectrum. First we considered a model in which all couplings are fixed to a specified value. We did not observe any level crossing between the ground and first excited states.

In the next step, the coupling constants were chosen random from a distribution function. The distribution function f for Δ and Δ_0 is the same as in the standard model of TLS's, where $f(\Delta) = f_0$ and $f(\Delta_0) \sim 1/\Delta_0$. Since we consider a one-dimensional array with equal spacing, $f(r) = 1/N$, the coupling of dipole moments will have the following distribution:

$$f(J) = J_0 J^{-4/3}, \quad J_1 < J < J_2$$

$$f(\Delta, \Delta_0) = \frac{f_0}{\Delta_0}, \quad \begin{cases} 0 < \Delta < \Delta_{max}, \\ \Delta_{0min} < \Delta_0 < \Delta_{0max}, \end{cases} \quad (6)$$

where f_0 and J_0 are normalization factors. J_1 is the minimum strength of coupling where two dipoles are very far from each other at the order of system size (L), $J_1 \sim 1/L^3$, and J_2 is the maximum coupling arises from two nearest-neighbor dipoles separated by a lattice spacing (a), $J_2 \sim 1/a^3$. A system of $N=4$ sites is studied with random couplings which are chosen from Eq. (6). Typical values for the parameters are $\Delta_{max} = 0.5$ K, 0.001 K $< \Delta_0 < 1$ K, and 0.01 K $< J < 1$ K. We have computed the energy levels and the dipole moment of the model for 10 000 samples. Data are plotted in Fig. 2. We have only computed the data for $0 < \phi/\phi_0 < 0.5$, since the data are symmetric around $\phi/\phi_0 = 0.5$, similar to an even function.¹²

We consider an external electric field E in the z direction. Then the electric field interacts with the dipole moment of the TLS's via $H_E = -\vec{P}_{tot} \cdot \vec{E} = -EP^z$, which is added to the Hamiltonian. The dipole moment of the system can be obtained from $P_{tot} = -\langle 0 | \partial H / \partial E | 0 \rangle = \langle 0 | \sum_i \sigma_i^z | 0 \rangle$, where $|0\rangle$ is the ground state. The dipole moments vary by a few percent upon changing the flux ratio (magnetic field), Fig. 2(a), and do not show any oscillations. In Fig. 2(b), the ground- and first-excited-state energies do not cross each other when the flux ratio is changed; moreover, they do not show any oscillations. We have also considered another domain of the parameters, long-range interactions resembling a three-dimensional system, and a distribution of dipole couplings which allows both positive and negative values. In all cases, similar results were obtained, which are not presented here. We conclude that the TLS's with Ising-like interactions of form of Eq. (5) do not show any coherent motion.

It has been argued that it is not possible to observe coherent motion in a double-well potential, since a particle tunneling through either path 1 or 2 from one well arises at a unique point which is the other well.^{13,14} The tunneling entity may tunnel either coherently or randomly to reach the final configuration in a system of interacting TLS's. One way to overcome this problem is to introduce a three-well potential (3WP).¹⁵ We have performed similar computations using an interacting 3WP model.¹⁶ We have studied both fixed and

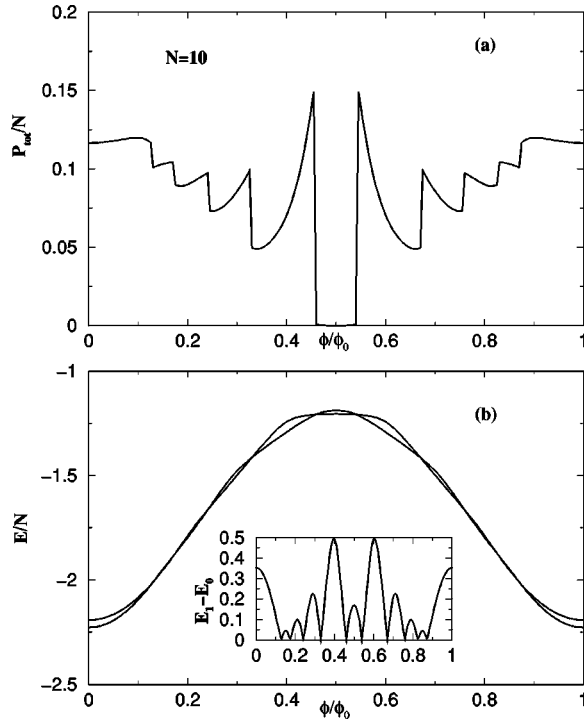


FIG. 3. (a) Dipole moment per site. (b) Ground- and first-excited-state energies vs the magnetic flux ratio with $N=10$ interacting TLS's from Eq. (9). The inset in (b) is the difference ($E_1 - E_0$) of the first-excited- and ground-state energies, which illustrate more clearly the level crossings. There are ten points of level crossings, and exactly at these points a sharp change in the dipole moment appears. We have treated a one-dimensional array of tunneling centers with the parameters $\Delta=0.2$, $\Delta_0=3$, and $J_{i,j}=J=1$.

random values of the parameters. We did not observe any oscillations in the dipole moment to indicate collective phenomena. The same conclusion is then obtained that the 3WP model with the z -component dipole-dipole interactions does not show evidence for coherent motion.

We thus conclude that other interaction forms must be present in the model in order to lead to coherent motion. Actually, Ising-like interactions do not depend upon the relative motion of the particles in different tunneling centers because there is no information regarding the tunneling path present in the Hamiltonian. These interactions only depend upon the final configuration of the system and are not able to trace the relative motion of different entities. To overcome this difficulty, we will introduce an interaction in the next section which depends upon $|\theta_i - \theta_j|$, where θ_i is the angle defined in Fig. 1. In this case, the interaction contains information regarding the paths of motion and, more precisely, regarding the relative motion of different tunneling entities. We will show that a phase with coherent motion appears for N coupled TLS's. Surprisingly, this occurs over a range of parameters, in agreement with the observed experimental data.

IV. MODIFIED INTERACTION HAMILTONIAN

A. One-dimensional model

In the last section we studied various forms of the interaction that might enable us to represent the coherent motion

as a collective phenomenon. The coherent motion in the context of a tunneling model is a phase in which all of the particles in each potential contribute to the overall tunneling process coherently. The classical picture of such a phase is the simultaneous motion of all of the particles in the same direction, i.e., clockwise or anticlockwise on a circular path. To identify such a motion for a particle in the potential of Fig. 1, we define an angle θ which is measured from the x axis by the projection of the dipole moment onto the xy plane. When a particle tunnels from one well to the other one, the projected vector traces a semicircular path. In this picture the important quantity is the relative angle $|\theta_i - \theta_j|$ between pairs of particles in different tunneling centers. Since the magnitude of this difference is meaningful modulo 2π , we may define $\cos(|\theta_i - \theta_j|)$ as being proportional to the interaction term. Then in the classical picture the interaction Hamiltonian would be

$$H_{int}^c = \sum_{i,j} J_{i,j} \cos(|\theta_i - \theta_j|), \quad (7)$$

where $J_{i,j}$ defines the strength of the interaction. To arrive at the quantum picture, which is important at low temperatures, we consider the dipole moment of the particle as an operator acting on the i th site. If we define the projection of the dipole moment onto the xy plane as $\vec{p}_{\perp,i} = \sigma_i^x \hat{x} + \sigma_i^y \hat{y}$, then the cosine term is proportional to the inner product of the projected vectors, $\cos(|\theta_i - \theta_j|) \propto \vec{p}_{\perp,i} \cdot \vec{p}_{\perp,j}$. By using the Pauli matrices, the quantum version of Eq. (7) is written in the following form:

$$H_{int}^q = \sum_{i,j} J_{i,j} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y). \quad (8)$$

Then, the total Hamiltonian of interacting system is

$$H_t = \sum_{i=1}^N H_0^i(\phi) + \sum_{i,j} J_{i,j} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y). \quad (9)$$

Before starting to study the properties of H_t , we would like to mention the most important difference between Eqs. (5) and (8). The Hamiltonian of Eq. (5) has discrete Z_2 symmetry whereas Eq. (8) has continuous $U(1)$ symmetry. Moreover, we are now able to trace the tunneling path using the continuous symmetry and to define the phase of coherent motion.

We will first study the properties of H_t using constant parameters, and then we shall consider the effects of random couplings subject to a parameter distribution function.

Let us consider a one-dimensional array of tunneling centers with the total Hamiltonian defined by H_t . We shall examine two quantities, the dipole moment, the induced dipole moment, as we have defined it earlier, and the two lowest-lying energy levels. In Fig. 3 we have plotted the dipole moment per site and the first two energy levels of $N=10$ interacting TLS's. The following couplings have been used to observe the present behavior: $\Delta=0.2$, $\Delta_0=3$, and $J_{i,j}=J=1$. The dipole moment is induced by the external electric field when this effect is allowed due to the asymmetry in

the height of the wells, $\Delta \neq 0$. Thus the amplitude of the dipole moment is proportional to Δ , which is small. Moreover, we observed N oscillations in the dipole moment, which is the signature of coherent motion. Exactly at the position of a sharp change in the dipole moment, a level crossing between the first two low-lying states occurs, as has been plotted in Fig. 3(b).

To show the level crossings more clearly, we have shown the difference between the first-excited-state energy E_1 and the ground-state energy E_0 in the inset of Fig. 3(b). These observations confirm that the model introduced in Ref. 11 can be the effective model for the interacting system defined in Eq. (9). In this sense, the oscillations in the dipole moment or the number of level crossings between the first two low-lying states represent the number of tunneling entities which move coherently. Therefore, the Hamiltonian of Eq. (9) describes a system of N interacting TLS's in the coherent motion phase. In the following, we will discuss the range of parameters over which this phase is observed. The specified couplings are in accordance with the low-temperature regime, where the collective phenomena of cold glasses has been observed. By changing the parameters, the phase may appear at higher or lower temperatures.

When N is increased, the difference between the energy levels and the distance between two level crossing points are both reduced. Then, the level crossing occurs for two states which are nearly degenerate. In this case, the states are similar to each other, and their dipole moments differ only slightly, so we do not observe a pronounced discontinuity. In the thermodynamic limit, these two states become degenerate. Thus we would like to stress that the phenomena we have predicted are mesoscopic effects which occurs for finite N and not in the thermodynamic limit $N \rightarrow \infty$. This is surprisingly in agreement with the effective theory of TLS's,¹¹ in which the number of interacting TLS's is assumed to be $\sim 10^5$.

The other feature which supports the notion that the observed phenomena are mesoscopic is the even and odd dependence of the dipole moments.¹⁴ The result for an odd value of N ($=11$) is plotted in Fig. 4. The main difference between even and odd N appears in the form of the oscillations in the dipole moment. For the even- N case, at the locations of each level crossing, the ground state changes from one state to another, leading to a discontinuity in the dipole moment. The case of odd- N values is different. Hence the oscillations arise from a smooth change in P_{tot}/N . In particular, the oscillations arise from the beat frequencies of the nearly degenerate ground and first excited states, without any level crossing. By changing the magnetic flux ratio the ground and first excited states switch positions, due to the alternation in their relative energy differences. Each time the ground state comes close to first excited state, a peak in the dipole moment occurs.

The origin of this different behavior for even and odd N is related to the different types of degeneracies of the ground state at the magnetic flux ratio where the levels cross for even N and beat for odd N . The degeneracy is twofold and can be labeled by the eigenvalues of a parity. Suppose in H_t we set $\Delta = 0$, the symmetric TLS or in the absence of exter-

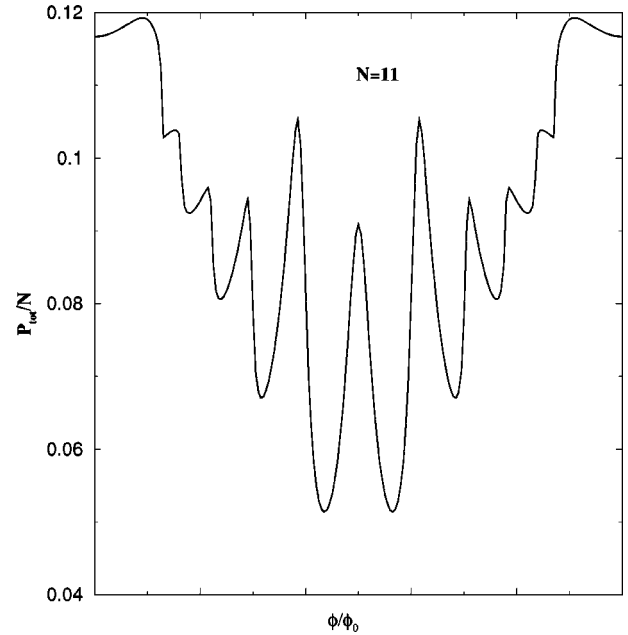


FIG. 4. Dipole moment per site vs the magnetic flux ratio for odd-size ($N=11$) interacting TLS's. The coupling constants of the one-dimensional Hamiltonian are $\Delta=0.2$, $\Delta_0=3$, and $J_{i,j}=J=1$.

nal electric field. Then the Hamiltonian $H_t(\Delta=0)$ is invariant under the parity operation $\Pi(\hat{z}) = -\hat{z}$, which defines the $Z2$ symmetry. Then each eigenstate of the Hamiltonian will be an eigenstate of Π . Since $\Pi^2 = \mathcal{I}$, the identity operation, the eigenvalues of Π are $+1$ or -1 . When the electric field is turned on, $\Delta \neq 0$, the $Z2$ symmetry is broken and we expect it to remove the degeneracy at the level crossing points. Actually, this is true for odd N , for which the degeneracy is removed by an electric field as, in the linear stark effect, there is no level crossing and the dipole moment changes continuously. This means the first two low-lying eigenstates of the Hamiltonian with odd N have different $Z2$ parity, whereas they have the same parity for even N . The degeneracy still remains at a level crossing for even N and leads to discontinuous changes in the dipole moment. Thus we should search for another symmetry which might be responsible for the degeneracy present for even N . We define the mirror image of a one-dimensional array about its center by $\Omega(i) = N - i + 1$ where i is the site label and N is the length of array. Again $\Omega^2 = \mathcal{I}$, which defines the eigenvalues $\omega_{1(2)} = +1(-1)$, respectively. Since Ω commutes with H_t , all eigenstates of the Hamiltonian are also eigenstates of Ω . Thus, we conclude that the first two low-lying eigenstates of the even- N Hamiltonian have different Ω parity.

Now we discuss the range of parameters which gives the phase with coherent motion. The main coupling constants in our model are Δ_0 and J . Since the value of Δ corresponds to the asymmetry of the wells, it is considered to be much smaller than the other parameters. At large Δ value, the energy difference of the two wells is too high to allow tunneling, so some of the particles will be frozen in the lowest well of their own tunneling center and do not contribute to the coherent motion. Then the probability of having all particles moving coherently will be reduced. This can be shown by

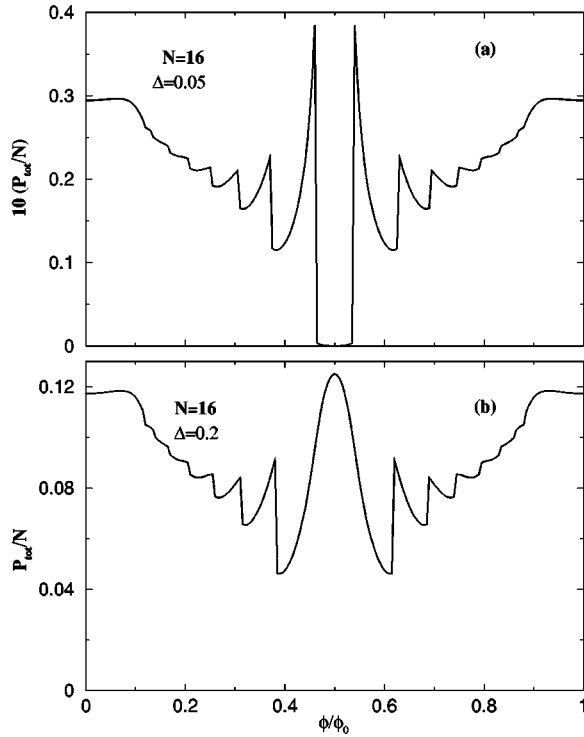


FIG. 5. The dependence of dipole moment per site on the asymmetry parameter vs magnetic flux ratio of $N=16$ interacting TLS's. (a) All TLS's contribute to the coherent motion, where $\Delta=0.05$. (b) The effective number of TLS's in coherent motion is reduced to 15 when $\Delta=0.2$. The other coupling constants are $\Delta_0=3$ and $J_{i,j}=J=1$.

computing the dipole moment for different values of Δ . In Fig. 5, we plotted the dipole moment of a one-dimensional array of $N=16$ TLS's with different asymmetries, $\Delta=0.05$ in part (a) and $\Delta=0.2$ in part (b). We observe 16 peaks in Fig. 5(a), but this number is reduced to 15 in Fig. 5(b), which shows that only 15 of the tunneling centers are effectively moving coherently. With increasing Δ , this number decreases.

So by considering a small value for $\Delta \sim 1/N$ for a mesoscopic size (N) system, the ratio of the other two parameters ($\lambda = \Delta_0/J$) controls the behavior of the system. If we fix $J=1$, then Δ_0 is the tunable parameter. We have found two different phases in our model. When $\lambda < \lambda_1$ the number of level crossings is less than N . In this phase, just some of the tunneling centers contribute to the coherent motion, and for very small values of λ the tunneling probability is negligible and, consequently, there is no coherent motion. This occurs when the interaction coupling (J) is very strong and causes the system to be frozen into a ground state which is only defined by the interaction term. In the other phase, when $\lambda > \lambda_1$, the model shows N level crossings between the first two low-lying levels and consequently the dipole moment oscillates with a frequency proportional to N . This phase corresponds to coherent motion. By increasing λ , the model behaves similar to that for independent TLS's, since Δ_0 is the strongest parameter in the Hamiltonian, and hence the interaction term becomes negligible. Practically the coherent motion phase becomes observable in the range of parameters

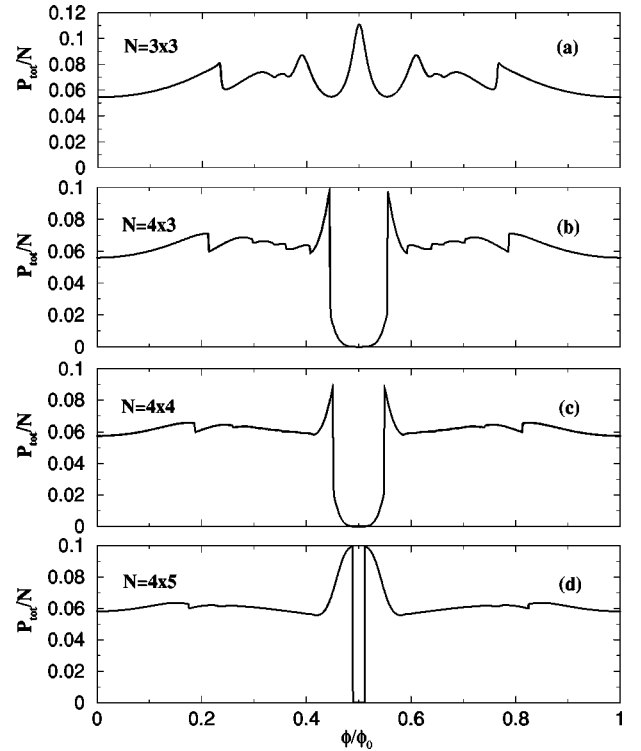


FIG. 6. Dipole moment per site for the two-dimensional model vs the magnetic flux ratio. The lattice sizes are (a) $N=9$, (b) $N=12$, (c) $N=16$, and (d) $N=20$. The coupling constants are $\Delta=0.2$, $\Delta_0=6$, and $J_{i,j}=J=1$, where the interaction is only between nearest neighbors.

$\lambda_1 < \lambda < \lambda_2$. We have found that for the one-dimensional model, $\lambda_1(1D)=3$, and for a two-dimensional lattice, it is $\lambda_1(2D) \approx 6$. So we assume $\lambda_1(3D) \sim 10$ for a three-dimensional model. If we choose a typical value of $\Delta_0=1$ K, then the strength of the dipole-dipole interaction (J) would have to be $J=100$ mK in order to observe a collective phenomenon. This estimated value of J obtained from our model is surprisingly in agreement with the expected value of the dipole-dipole interaction, assuming the average distance between two tunneling centers is $R=10^{-8}$ m and the average dipole moment of each TLS is $P=2|e|\hbar \times 10^{-10}$ m.

B. Two-dimensional model

In this subsection we present the results of our calculations for the dipole moment of the Hamiltonian defined in Eq. (9) on a two-dimensional square lattice. We only considered the nearest-neighbor (NN) interaction. The coupling constants are fixed to the values $\Delta=0.2$, $\Delta_0=6$, and $J_{i,j}=J=1$. The dipole moment per site on the finite 2D model is plotted in Fig. 6 for lattice sizes of $N=3 \times 3$, 4×3 , 4×4 , and 4×5 . The expected oscillations in the dipole moment are observed in all cases. The oscillations are more apparent for the smaller N ($=9, 12$) cases. As we discussed previously, by increasing N the difference between the energy levels is decreased, and consequently the magnitude of the oscillations in the dipole moment is reduced. Moreover, we still

distinguish the different types of oscillations for odd and even system sizes, which is clear by comparing Figs. 6(a) and 6(b) for $N=9$ and 12, respectively. In the case of odd N , the oscillations do not lead to a discontinuity in the dipole moment, whereas it is discontinuous for even N . Our data for the two-dimensional system confirm that the proposed model is able to obtain a coherent motion in higher dimensions. This will be justified by considering long-range interactions in the next subsection.

C. Long-range interactions

We now consider the effect of including LR interactions in our model. Since we are attempting to describe a glassy system, the positions of the TLS's are not limited to the sites on a regular lattice. Hence, each tunneling center may have many neighbors. In this respect, we have studied long-range interactions in both one- and two-dimensional models. We have calculated the dipole moment and the low-energy spectrum in order to compare them with the results for NN interactions studied in the last two subsections.

In a one-dimensional array of long-range interacting TLS's, the indices i and j run over all lattice points. Since the interactions originate from dipole-dipole couplings, the strength of the interaction between sites i and j should be equal to $J_{i,j}=J/(r_{i,j}^3)$. We have plotted the resulting dipole moment per site for an array of size $N=11$ in Fig. 7(a). In this plot, we have presented data for both NN and LR interactions. The nearest-neighbor coupling strength is taken to be $J=1$ in both cases. There is no qualitative change in the behavior of the dipole moment versus the magnetic flux ratio. This is due to the ordering in the coherent motion phase. Suppose that (i,j) and (j,k) are two NN sites. If the system is in the coherent motion phase, the relative angles between NN sites is constant, $|\theta_i - \theta_j| = c_{ij}$, $|\theta_j - \theta_k| = c_{jk}$. By turning on the LR interaction between (i,k) , the constraint $|\theta_i - \theta_k| = c_{ik}$ is imposed on the system, consistent with the previous system configuration, as seen by noting that $c_{ik} = c_{ij} + c_{jk}$. Thus, adding LR interactions does not destroy the coherent motion. Moreover, the oscillations are more pronounced in the case of LR interactions, and also the distance between two peaks becomes approximately equally spaced. Then we observe more clearly the oscillations in the dipole moment with a frequency proportional to the lattice size. When we consider LR interactions to all neighbors in the lattice, the system resembles a three-dimensional one, since each site has many neighbors. This adds for the support to the notion that this model may describe three-dimensional coherent motion.

In Fig. 6(b) we present our results for a similar situation for a two-dimensional lattice. The lattice size is $N=4 \times 3 = 12$, where a TLS exists at each lattice point. For simplicity we have only considered the next nearest-neighbor (NNN) interactions, using it to represent a long-range interaction, since it does not change the generality. In this case, the NN coupling is $J_1=1$ and the NNN coupling is $J_2=0.125$, which are supposed to behave as $1/r^3$. As discussed for the 1D case, there are no qualitative changes in the results. In

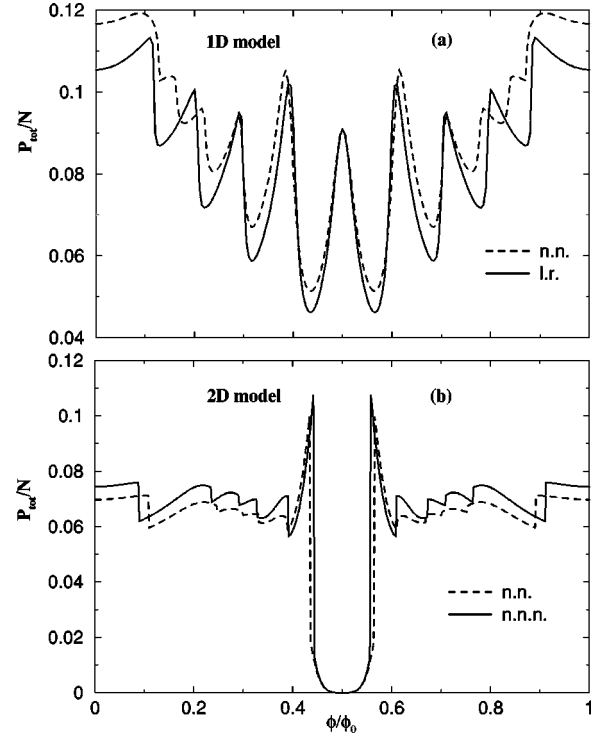


FIG. 7. The effect of long-range (LR) interactions on the dipole moment per site for one- and two-dimensional lattices vs the magnetic flux ratio. (a) The 1D lattice size is $N=11$ and the coupling constants are $\Delta=0.2$, $\Delta_0=6$, and $J_{i,j}=J=1$ for NN, and $J_{i,j}=1/(r_{i,j}^3)$ for LR interactions. (b) The 2D model is a $4 \times 3 = 12$ square lattice where $\Delta=0.2$, $\Delta_0=5$, and $J_1=1$ for NN and $J_2=0.125$ for next-NN interactions, the latter representing a long-range interaction.

comparison with the NN results, the oscillations in the dipole moment are observed to be clearer and more equally spaced.

D. Random couplings

So far, we have studied the Hamiltonian defined in Eq. (9) for one- and two-dimensional lattices with NN and LR interactions. In all of these cases we have considered a deterministic model, in which all of the couplings were constant and homogeneous for all lattice points. Since we are attempting to describe a phenomena in a glassy media, we expect to have a distribution of coupling constants.

The first model is to take the same distribution that has been used to treat noninteracting TLS's of Eq. (6). For a one-dimensional array of TLS's interacting via Eq. (8) we have calculated the dipole moment and the first two low-lying energy levels of a system with $N=4$ where the ranges of parameters are $0 < \Delta < 0.2$, $0.05 < \Delta_0 < 3$, and $0.05 < J < 1$. We have calculated the average values for 10 000 samples. The general behavior is the same as Fig. 2. The dipole moment does not demonstrate any oscillations, but instead shows monotonic behavior over the domain model. Moreover, the first two energy levels exhibit neither a level crossing nor a level frequency beating. This calculation verifies that the model with this type of distribution function does not describe coherent motion. We note that the type of

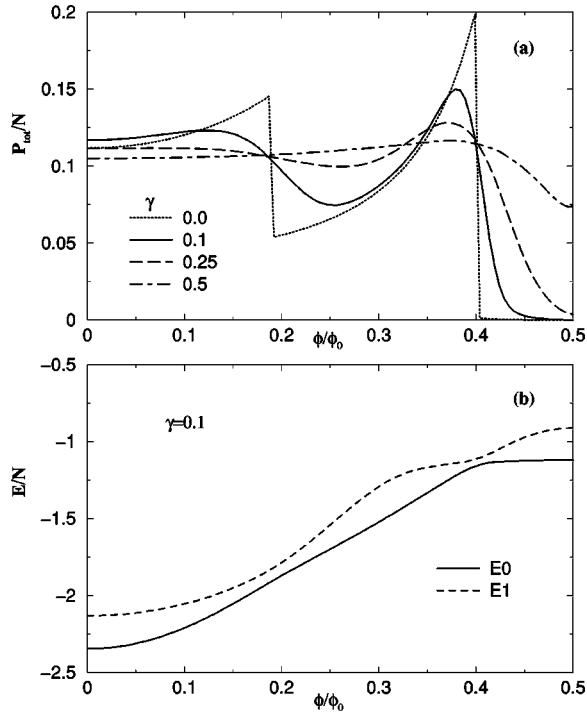


FIG. 8. (a) Dipole moment per site vs the magnetic flux ratio with Gaussian randomness for an $N=4$ one-dimensional array of interacting TLS's. The width \tilde{a} of the Gaussian distribution satisfies $\tilde{a} = \gamma\bar{x}$, where \bar{x} is the average value of the random variable. Data are presented for $\gamma=0, 0.1, 0.25, 0.5$. For small values of γ the oscillations in the dipole moment are strong and clearly evident, providing evidence for coherent motion. With increasing γ , the model loses its evidence for collective behavior. (b) Ground- and first-excited-state energies of the model for $\gamma=0.1$ which show the level frequency beating, a sign of coherent motion.

distribution function $f(\Delta, \Delta_0)$ defined in Eq. (6) follows from the assumption that the TLS's in glasses are considered to be isolated. Thus we argue that for interacting TLS's the distribution function should be modified.

Hence, we choose a Gaussian distribution for the parameters in our model,

$$g(x) = \frac{1}{\tilde{a}\sqrt{2\pi}} e^{-(x-\bar{x})^2/2\tilde{a}^2}, \quad (10)$$

where $\bar{x} \equiv \langle x \rangle$ is the average value of the variable x and $\tilde{a} \equiv \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ its width. Now we consider a Gaussian distribution for all of the parameters in our model. In Fig. 8(a), the dipole moment of a one-dimensional array of TLS's with $N=4$ is plotted versus the magnetic flux ratio for four different values of the parameter γ . This parameter defines the variance of the distribution by $\tilde{a} = \gamma\bar{x}$. The average values of parameters are $\bar{\Delta} = 0.2$, $\bar{\Delta}_0 = 3$, and $\bar{J} = 1$. We have computed the average values of the physical quantities over 10 000 samples. In this notation, $\gamma=0$ is the deterministic case in which there is no random variable, leading to very sharp oscillations in the dipole moment. As discussed in the last sections, the dipole moment behaves discontinuously at the

level crossing points when N is even. The total number of oscillations is 4, with 2 in the region $\phi/\phi_0 \in [0, 0.5]$ [Fig. 8(a)] and 2 in the $\phi/\phi_0 \in [0.5, 1]$ region, which are not presented to save computation time. For $\gamma=0.1$, the variance is equal to 10% of the average value and still the oscillations in the dipole moment are clear, confirming coherent motion. For $\gamma=0.1$ we have also presented the two lowest-energy levels in Fig. 8(b), in which the effect of level frequency beating instead of level crossing can be seen. Since we included random variables in the model, we do not expect sharp level crossing. But the oscillations with frequency proportional to N in the energy levels show the dependence of the energy on the number of interacting TLS's, suggesting collective behavior. If variance is less than or equal to 10% of the average value, we still will observe evidence for coherent motion. By increasing γ , the amplitude of the oscillations is reduced, and for $\gamma=0.5$, there are almost no oscillations. In other words, a wide distribution of randomness destroys the collective behavior. Hence, we have shown that the proposed model exhibits coherent motion provided that the distribution of the coupling constants is sufficiently narrow.

V. CONCLUSION

We have attempted to find an appropriate interaction between TLS's in order to explain the experimental evidence for collective phenomenon in multicomponent glasses at ultralow temperatures. Our first attempt was to distinguish the features of double-well and triple-well potentials in the presence of Ising-like interactions. The Ising interactions are intended to simulate the z component of the dipole-dipole interactions between two wells when one uses a distribution of exchange couplings to simulate different dipole moment orientations. Our calculations confirm that none of the two- and three-well models with Ising-type interactions can provide evidence for a coherent motion phase. This is true for both fixed and random couplings. The crucial point arises from the symmetry of the interaction. The Ising interaction has a discrete symmetry, whereas a continuous symmetry is required in order to trace the path of the tunneling process for the simulation of coherent motion.

Second, we considered an XY interaction proportional to the $\cos(|\theta_i - \theta_j|)$, where θ_i is the angle of the dipole moment projected onto the xy plane (see Fig. 1). Thus the interaction is sensitive to the relative angle of the dipole moments in two coupled TLS's. In the coherent motion phase, the relative angle of each coupled TLS's is constant, so the ensemble of TLS's demonstrates a collective phenomenon in which all of the particles tunnel in the same direction (clockwise or anticlockwise). One may treat at this phenomenon effectively by a single TLS with a charge equal to the sum of the charges of all of the correlated TLS's. The XY interaction has a continuous $U(1)$ symmetry which properly traces out the path of tunneling and simulates the coherent motion. We have studied this model on one- and two-dimensional lattices in which the tunneling centers are restricted to the lattice points. We have predicted the coherent motion phase in a range of coupling constants by calculating the dipole moments and the

low-energy levels of the coupled TLS's. The range of parameters is $\lambda_1 < \Delta_0/J < \lambda_2$ where $\lambda_1 \approx 10$ is estimated for a 3D system. If we consider the typical value for $\Delta_0 \approx 1$ K and assume that $\lambda_2 = 1000$, we obtain $1 \text{ mK} < J < 100 \text{ mK}$. This is in agreement with the experimental observations at few millikelvin.⁹

The effects of long-range interactions were studied in a model exhibiting the expected clearly and equally spaced oscillations in the dipole moment. By definition, in the coherent motion phase the relative angle between coupled TLS's is constant. Adding LR interactions imposes constraints between non-nearest neighbors which are effectively satisfied by imposing a NN constraint. Thus LR interactions do not destroy the coherent motion phase. Moreover, results obtained with LR interactions resemble those obtained in higher spatial dimensions, which suggests that our model may be relevant for the 3D case as well. The glassy properties of our model were examined by introducing random couplings. We have found that the form of the random distribution depends upon the interacting or noninteracting model. If we assume the distribution of isolated TLS's [Eq. (6)], for the interacting model, we will not observe any evidence for the coherent motion phase. Thus we have considered a Gaussian distribution for all of the parameters in our model. When the width of the Gaussian distribution is narrow, we still observe the oscillations in the dipole moment represent-

ing collective behavior. For a wide distribution of parameters the coherent motion phase is destroyed.

Finally we conclude that the XY-like interactions between TLS's, combined with the Aharonov-Bohm effect of the single-particle Hamiltonian, allow us to construct a successful model exhibiting the important features suggestive of the collective phenomenon of coherent motion in low-temperature glasses. Since we have observed an oscillation versus flux ratio for many excited-state energies, we expect that finite-temperature calculations show also a similar behavior: namely, oscillations in the dipole moment proportional to N . There are still many aspects of the model such as the density of states as well as finite temperatures which should be investigated in future studies.

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