Configuration-tree Theoretical Calculation of the Mean-Squared Displacement of Particles in Glass Formers

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Abstract. We report an analytical evaluation of the mean-squared displacement (MSD) of the particles in glasses based on their coarse grained trajectories. The calculation is conducted by means of a local random configuration-tree theory that was recently proposed by one of us [C.-H. Lam, J. Stat. Mech. \textbf{2018}, 023301 (2018)]. Results are compared with the numerical simulations of a lattice glass model, and good quantitative agreement has been obtained over a wide range of temperatures in the entire region of time with virtually no free parameters. To the best of our knowledge, the calculation is the first in its kind.

1. Introduction

Upon rapid cooling, many liquids undergo a dramatic – often more than ten decades – increase in their viscosity and eventually become glasses at a temperature $T_g$. The question of how the constituent particles of a liquid lose their mobility in this process remains a source of dispute, having generated a library of theories of varying sophistication and complexity \cite{1,2,3}.

Glasses are notoriously complex systems \cite{4}. Analytical yet accurate evaluations of any of their properties are very rare and valuable. A central quantity of interest is the mean-squared displacement (MSD) of particles, defined as

$$\text{MSD}(t) = N^{-1} \sum_j d_j^2(t),$$  \hspace{1cm} (1)

where $d_j(t)$ is the displacement of the $j$-th particle during a time $t$ and $N$ is the total number of particles in the glass. As a ubiquitous signature of glass formation, upon approaching $T_g$, $\text{MSD}(t)$ develops a plateau, which is a precursor of the so-called $\alpha$ relaxation that is characteristic of any glasses \cite{5}.

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In this contribution, we present an analytical calculation of $\text{MSD}(t)$ on the basis of a theory that was recently proposed by one of us [6], belonging to the class of dynamic facilitation descriptions [7, 8, 9, 2, 10, 11, 12]. Unlike related calculations in Refs. [13, 14], our calculation covers the full range of time scales, spanning both the time window before and that after the plateau and hence providing a complete picture of the caging dynamics. The theoretical result is then benchmarked against the ‘distinguishable particle lattice model’ (DPLM) [15], which is a lattice glass model realizing a dynamic facilitation mechanism motivated by glassy film simulation observations [16]. Good quantitative agreement has been achieved – including the position of the MSD plateau – over a wide range of temperatures with only two parameters, which can further be fixed by the diffusion coefficient $D$ of the particles resulting in no free parameter.

2. Theory

2.1. The concept of a random local configuration tree

Let us start with a brief recapitulation of the basic assumptions of the theory that has already been described in details in Ref. [6].

At temperatures close to $T_g$, a particle in a liquid mostly vibrates about a temporary equilibrium center, and occasionally makes a transient hop from one center to another. In the coarse-grained picture with the fast vibrations averaged out, only such hops are interesting and the phase space of the system reduces to a simple space of particle configurations. The system would then transit from one configuration to another via one or a sequence of particle hops – which are assisted by the vibrations acting as an effective heat bath – and relax its structure. Each hop is primarily initiated by a quasi-void [17], which propagates along a string of particles that displace one after another during the propagation. The strings generally come with different lengths. As an approximation, however, we assume that they are of the same length and each possess $\tilde{l}$ particles. In general, a void can propagate along one of $z$ strings lying in different directions. However, these strings each sense their own local energy landscape and they are not equally favorable.

At any instant, more than one void propagation may be occurring in a liquid. To simplify the analysis, let us divide the liquid into a number of local regions, each of volume $V$. We assume that $V$ is big enough so that a void propagation in one region does not affect the structural relaxation of neighboring regions, yet small enough so that one void propagation energetically affects the propagation of other voids in the same region (i.e. the fully interacting approximation [6]). Under this approximation, it suffices to consider the dynamics of one local region. Let us represent the configurations of this region by the nodes of a graph and possible transitions by the edges. Any pair of nodes connected by one edge signify the presence of a string. In a region containing $m$ voids, a node has $mz$ edges linked to it. It is reasonable to neglect the possibility of the region revisiting a previous node by a loop of edges, so that the graph becomes a tree with its
Figure 1. Sketch of the local configuration tree energy landscape. The energy for a node is represented by the height of the cylinder at the node. Left panel: Red (Grey) cylinders indicate the configurations with lower (higher) energies, which are considered to be more (less) energetically favorable. Blue (Cyan) edges are connecting the more (less) energetically favorable nodes with higher(lower) transition probabilities. Right panel: Red cylinders are assumed to have the same heights, approximating the fact that these configurations have almost the same low energy. Grey cylinders are now infinitely tall. Blue edges connect the nodes with red cylinders and represent the only possible transitions. Cyan edges are always connected to nodes with grey cylinders, for which transitions are impossible.

root corresponding to the initial configuration [6]. This configuration tree is random in the sense that, in general its energetically favorable edges are randomly distributed. In this paper, we assume that the transition probabilities for the energetically favorable edges are finite but negligible for the unfavorable edges. In Figure 1, an illustration of the energy landscape is shown for the local configuration tree with one void and \( z = 4 \).

In the rest of this section, we derive and solve a set of rate equations governing the motions of a local region on the tree.

2.2. Level dynamics on the tree: rate equations

Let us consider a local region with \( m \) voids and suppose the region is at equilibrium initially sitting at the root of its configuration tree defined to be level \( n = 0 \). In time \( t \), the region will descend down the tree to some level \( n \) with a probability denoted by \( p_n(t; m) \). Our purpose here is to derive the rate equations satisfied by this probability. Our formulation is analogous to previous calculations for random walks on regular trees [18, 19].

To ease the discussion, let us look at an ensemble of \( N \) identical regions all initially at the root. At instant \( t \), the number of members in this ensemble at the root \( (n = 0) \) is \( Np_0(t; m) \). After a short interval \( dt \), this number becomes \( Np_0(t + dt; m) \), the difference due to a loss of those members transiting to level \( n = 1 \) and a gain of members at level \( n = 1 \) transiting to the root. The transition from the root to level \( n = 1 \) can take place through \( mz \) edges [6], which we label by \( \nu = 1, 2, ..., mz \). Let us denote by \( dt \times \tilde{w}_{0\rightarrow 1}^{\nu} \) the
probability of such a transition via edge \( \nu \). The total transition rate is then \( \sum_\nu \tilde{w}_0^{\nu} \) which averages to \( mz\tilde{w}_0 \), with \( \tilde{w}_0 \) being the rate per edge. As the transitions are assisted by an effective heat bath of vibrations, \( \tilde{w}_0^{\nu} \) in general depends on the energy difference \( \Delta E \) between the configurations connected by the \( \nu \)-th edge. Denoting by \( P(\Delta E) \) the probability for the occurrence of \( \Delta E \) assuming an initial equilibrium configuration, a formally exact expression for the average transition rate \( \tilde{w}_0 \) along any of the edges from the root is

\[
\tilde{w}_0 = \int_{-\infty}^{\infty} d(\Delta E)w(\Delta E)P(\Delta E),
\]

where the rate \( w(\Delta E) \) depends on the detailed microscopic dynamics. Now the number of members lost to level \( n = 1 \) is \( Np_0(t; m)dt mz\tilde{w}_0 \).

On the other hand, the transition for any member from level \( n = 1 \) to the root can take place only through the edge linking the root and the node where the member is currently located. The probability of this transition for a member sitting on the node of the \( \nu \)-th edge is then \( dt \times \tilde{w}_1^{\nu} \). Denote by \( N^\nu_1 \) the number of such members, which satisfies \( \sum_\nu N^\nu_1 = Np_1(t; m) \). The number of members gained to the root is then \( \sum_\nu N^\nu_1 dt \tilde{w}_1^{\nu} \). At low temperatures, very few edges are energetically favorable and \( N^\nu_1 \) are significant only for the nodes linked to these edges. The rest can then be ignored. As \( \Delta E \) for energetically favorable edges linking only low energy configurations are expected to be small, we can neglect the difference in their transition rates. As such, we shall replace \( \tilde{w}^{\nu}_1 \) with an average rate \( \tilde{w} \) for them. To actually compute \( \tilde{w} \), let us define the energetically favorable edges as those for which \( \Delta E \leq Ck_BT \), where \( C \) is a constant of order unity [6]. Now, the rate \( \tilde{w} \) for a favorable edge is approximated as follows

\[
\tilde{w}^{-1} = \frac{\int_{-\infty}^{Ck_BT} d(\Delta E)w(\Delta E)^{-1}P(\Delta E)}{\int_{-\infty}^{Ck_BT} d(\Delta E)P(\Delta E)},
\]

which will be further explained below. As such, the number of members gained amounts to \( Np_1(t; m)dt \tilde{w} \).

Combining these considerations, we obtain the number balance equation

\[
Np_0(t + dt; m) - Np_0(t; m) = -Np_0(t; m)dt mz\tilde{w}_0 + Np_1(t; m)dt\tilde{w},
\]

or equivalently

\[
\partial_t p_0(t; m) = -mz\tilde{w}_0 p_0(t; m) + \tilde{w} p_1(t; m).
\]

By applying the same reasoning to other levels, we find

\[
\partial_t p_1(t; m) = -(1 + c_m)\tilde{w} p_1(t; m) + mz\tilde{w}_0 p_0(t; m) + \tilde{w} p_2(t; m),
\]

\[
\partial_t p_{n+1}(t; m) = -(1 + c_m)\tilde{w} p_n(t; m) + c_m \tilde{w} p_{n-1}(t; m) + \tilde{w} p_{n+1}(t; m).
\]

Here we have introduced the quantity \( c_m = (mz - 1)q \), with \( q = \int_{-\infty}^{Ck_BT} d(\Delta E)P(\Delta E) \) giving the likelihood of an edge being energetically favorable. \( c_m \) gives the number of children of a node at level 1 or beyond. One can readily show that \( \partial_t \sum_n p_n(t; m) = 0 \), i.e. the total probability (\( = 1 \)) is conserved.
Equation (3) provides $\tilde{w}$ by averaging the transition time $w(\Delta E)^{-1}$. At low temperatures, the long-time dynamics is dominated by a series of transitions along the levels on a thin tree branch with a degree $c_m$ close to unity for some dominant value of $m$. The average of the transition time, as opposed to that of the transition rate, thus gives a more accurate description for long-time dynamics. Furthermore, Eq. (3) is accurate even at higher temperatures. This is because $w(\Delta E)$ then admits small fluctuations and averaging over time or rate indeed give similar values.

From Eqs. (4) - (6), it follows that the average level
\[ \bar{n}(t; m) = \sum_n n p_n(t; m), \] (7)
the local region could have reached must satisfy the following equation,
\[ \partial_t \bar{n}(t; m) = (c_m - 1)\tilde{w} [1 - p_0(t; m)] + mz\tilde{w}_0 p_0(t; m), \] (8)
subjected to initial conditions $\bar{n}(0; m) = 0$ and $p_0(0; m) = 1$. An integration gives
\[ \bar{n}(t; m) = \int_0^t dt' \{(c_m - 1)\tilde{w} [1 - p_0(t'; m)] + mz\tilde{w}_0 p_0(t'; m)\}. \] (9)
It is interesting to see that $\bar{n}(t; m)$ is completely determined if $p_0(t; m)$ is known. For small $t$, we may take $p_0(t; m) \rightarrow 1$, and then $\bar{n}(t; m) \rightarrow mz\tilde{w}_0 t$, i.e. the initial growth of $\bar{n}(t; m)$ which is formally exact.

Inspecting Eq. (8) or (9), we note that there are two types of solutions depending on whether $c_m$ is greater or less than 1. For $c_m > 1$, $\bar{n}(t; m)$ increases without bound, implying that the local region will be descending down the tree and access all of its configurations in time. In the meantime, $p_0(t; m)$ must decay to zero, yielding
\[ \bar{n}(t; m) \approx (c_m - 1)\tilde{w} t \] (10)
for large $t$. We may call such regions mobile regions.

For $c_m < 1$, however, $\bar{n}$ cannot increase arbitrarily. Instead, it will initially increase as the second term on the right-hand side of Eq. (8) is larger than the first term, but finally saturate when the two terms balance each other. In this regime, the local region is trapped in a few configurations, in the number of
\[ 1 + \frac{mz\tilde{w}_0}{(1 - c_m)\tilde{w}}, \] and cannot escape. These regions may be called immobile regions.

2.3. Solutions to the rate equations

While Eqs. (4) - (6) may be numerically integrated in a straightforward manner, here we solve them by the method of Laplace transform. So we define
\[ P_n(s; m) = \int_0^\infty dt \ e^{-st} p_n(t; m), \] (11)
where $s$ resides in the upper half complex plane. In terms of $P_n(s;m)$, Eqs. (4) and (5) can be written as

$$\begin{align*}
sp_0(s;m) - 1 &= -mzw_0p_0(s;m) + \tilde{w}p_1(s;m), \\
sp_1(s;m) &= -(1 + c_m)\tilde{w}p_1(s;m) + mzw_0p_0(s;m) + \tilde{w}p_2(s;m).
\end{align*}$$

(12) (13)

Here we have used the initial condition that $p_n(0;m) = \delta_{n,0}$. Expressing $P_{n=1,0}$ in terms of $P_2$, we find

$$P_n(s;m) = \alpha_n(s;m) + \beta_n(s;m)P_2(s;m),$$

(14)

where $\alpha_{n=0,1}$ and $\beta_{n=0,1}$ are some coefficients given as follows

$$\begin{bmatrix}
\alpha_0(s;m) & \beta_0(s;m) \\
\alpha_1(s;m) & \beta_1(s;m)
\end{bmatrix}
= \frac{1}{(s + mzw_0)[s + (1 + c_m)\tilde{w}] - mzw_0\tilde{w}}
\times
\begin{bmatrix}
s + (1 + c_m)\tilde{w} & \tilde{w}^2 \\
mzw_0 & \tilde{w}(s + mzw_0)
\end{bmatrix}.$$  

(15)

Analogously, Eq. (6) is transformed as

$$sp_n(s;m) = c_m\tilde{w}[P_{n-1}(s;m) - P_n(s;m)] + \tilde{w}[P_{n+1}(s;m) - P_n(s;m)].$$

(16)

This equation is invariant under a translation of $n$ and thus the general solution is of the form

$$P_n(s;m) = P_2(s;m)c^{n-2}, \quad n > 1.$$  

(17)

The quantity $c$ is obtained by substituting this expression into (16). We find

$$c^2 - (1 + c_m + s\tilde{w}^{-1})c + c_m = 0.$$  

(18)

This has two solutions. One solution leads to $P_n$ that diverges for large $n$ and must be excluded. The other solution is given by

$$c(s;m) = \frac{1}{2} \left(1 + c_m + s\tilde{w}^{-1} - \sqrt{(1 + c_m + s\tilde{w}^{-1})^2 - 4c_m}\right).$$

(19)

Finally, the normalization condition of the probabilities implies that

$$\sum_{n=0}^{\infty} P_n(s;m) = \int_{0}^{\infty} dte^{-st} = s^{-1}.$$  

(20)

Combining this with Eqs. (14) and (17), we obtain

$$P_2(s;m) = \frac{s^{-1} - \alpha_0(s;m) - \alpha_1(s;m)}{[1 - c(s;m)]^{-1} + \beta_0(s;m) + \beta_1(s;m)},$$

(21)

which can be used to generate all $P_n(s;m)$. Going back to $p_n(t;m)$, we need to invert the Laplace transform

$$p_n(t;m) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} dse^{st}P_n(s;m),$$

(22)

which can be numerically evaluated using standard algorithms.
3. Calculating MSD(t)

The migration of a region on the configuration tree can be mapped unto the real-space motions of the particles in this region, thereby allowing us to calculate the MSD, $\text{MSD}(t)$ of these particles.

To this end, let us observe that, as the region moves down the tree by one level, what happens in real space is that a void propagates along a string and each particle in this string hops by an average distance $a$ comparable to the atomic separation. Suppose the region has descended to level $n$ in a period $t$. During this period, in total $n\tilde{l}$ particle hops have occurred in string of length $\tilde{l}$, excluding the hops due to back-and-forth repetitions between any pair of nodes, which are highly correlated and do not contribute to the MSD. Some particles may have hopped more than once. As long as the hops are uncorrelated, as is statistically reasonable for non-repetitive hops, the squared displacement of a particle over ensemble average is simply $a^2$ times the number $n_{\text{hop},j}$ of non-repetitive hops particle $j$ has executed, i.e. $\langle d_j^2 \rangle = n_{\text{hop},j}a^2$ with $\sum_j n_{\text{hop},j} = n\tilde{l}$.

The contribution of each non-repetitive hop to the MSD is just $a^2/V\phi$, where $\phi$ is the particle density and $V\phi$ is the number of particles in the region. As such, for a region reaching level $n$, the MSD is $n\tilde{l}a^2/V\phi$. Ensemble averaging this by $p_n(t;m)$, we obtain the MSD for this region as

$$\text{MSD}(t;m) = \frac{\tilde{l}a^2}{V\phi}\bar{n}(t;m). \quad (23)$$

Here $\bar{n}(t;m)$ can be directly obtained from Eq. (9) with $p_0(t;m)$ provided in Sec. 2.3.

To obtain the MSD for the entire liquid, we have to take an average of $\text{MSD}(t;m)$ over all local regions. The number of voids in one region may differ from that in another. Suppose the average number of voids per region is $\bar{m} = V\phi_v$, where $\phi_v$ is the density of voids. With small correlations between voids the steady-state distribution of them over the regions then approximately follows Poisson’s law, i.e. the probability of a region with $m$ voids is

$$f(m;\bar{m}) = \frac{\bar{m}^m e^{-\bar{m}}}{m!}. \quad (24)$$

Now averaging $\text{MSD}(t;m)$ by this distribution, we finally arrive at

$$\text{MSD}(t) = \sum_m f(m;\bar{m})\text{MSD}(t;m) = \frac{\tilde{l}a^2}{V(\Omega^{-1} - \phi_v)} \sum_m f(m;\bar{m})\bar{n}(t;m). \quad (25)$$

Here $\Omega$ is the volume of a particle or of a void, i.e. $\Omega^{-1} = \phi + \phi_v$. Note that Eq. (25) is closed with Eq. (9), which gives $\bar{n}(t;m)$.

From Eq. (25), we can obtain the diffusion coefficient $D$ for the liquid. By definition,

$$D = \lim_{t \to \infty} \frac{\text{MSD}(t)}{2dt}, \quad (26)$$

where $d$ is the dimension of the system. As discussed in Sec. 2.2 for mobile regions with $c_m = (mz - 1)q > 1$, $\bar{n}(t;m) = (c_m - 1)\bar{w}t$ for $t \to \infty$. For immobile regions, however,
\( \bar{n}(t; m) \) approaches a constant for \( t \to \infty \). Thus, only mobile regions contribute to \( D \). We find

\[
D = \frac{\tilde{w}a^2\Omega}{2d\mathcal{V}(1 - \phi_v\Omega)} \sum'_{m} f(m; \tilde{m})(c_m - 1),
\]

(27)

where the prime restricts the summation to mobile regions. This result on \( D \) was first obtained in Ref. [6], where the behavior of \( D \) has been thoroughly investigated.

4. Comparison with simulations

While the theory is expected to be valid for a variety of glassy systems exhibiting string-like motions, here we check it with the DPLM, for which most of the required parameters are known precisely and adjustable parameters are minimum.

As this model has already been studied thoroughly in Ref. [15], here a short description is provided for the convenience of readers. The DPLM assumes a number of distinguishable hard-core particles living on a square lattice with lattice constant \( a = 1 \). Interactions occur between neighboring particles in the form \( V_{ij} \), each of which is sampled from a distribution \( g(V) \) before a simulation begins. Here \( i \) and \( j \) denote a pair of neighboring sites while \( s_i \) and \( s_j \) denote the types of the particles sitting at the sites, respectively. Each particle is of its own type. A void is simply the absence of a particle. We have chosen \( g(V) \) to be a uniform distribution in the range of \( V \in [-0.5, 0.5] \). The string length is chosen to be \( \tilde{l} = 1 \). The kinetic Monte Carlo rules of activated hopping is employed for the dynamics of the particles. Each particle can hop to an empty neighboring site at a rate

\[
w(\Delta E) = w_0 e^{-\left(E_0 + \Delta E / 2\right)/k_B T},
\]

(28)

where \( w_0 \) and \( E_0 \) are constants and \( \Delta E \) is the change in the system energy due to the hop. Though the equilibrium properties of this model are exactly solvable, it displays many characteristic behaviors of a glass former [15].

Note that \( \Delta E \) is also the energy change due to a void propagation. In the configuration-tree theory, we call an edge in the local tree energetically favorable if \( \Delta E \) for the corresponding void propagation is less than an upper cutoff \( Ck_B T \), where \( C \) is a parameter of the order of unity. Thus, the probability \( q \) that an edge is energetically favorable can be directly evaluated from \( g(V) \) and the equilibrium properties of the DPLM, see Ref. [15]. Since \( \Omega = 1 \) for the DPLM, this parameter \( C \) and the volume of a local region \( \mathcal{V} \) are the only parameters needed to evaluate \( \text{MSD}(t) \) by Eq. (25). These parameters can actually be further fixed by fitting the analytical expression of \( D \), Eq. (27) to the numerical simulations of the DPLM. This has been carried out in Ref. [6] using \( \tilde{w} = w_0 \), where it was found that \( C = 1.7 \) and \( \mathcal{V} = 12 \) give the best fit over a wide range of temperatures and void densities. This choice is appropriate for the activated hopping dynamics in (28) where \( \Delta E \) averages to 0. In the present paper, \( \tilde{w} \) is more accurately evaluated by Eq. (3). We thus adopt \( C = 1 \) and \( \mathcal{V} = 12 \), which provide a good fit of the data set. These values not only fit nicely the data for activated
hopping dynamics but also for the Metropolis dynamics and a wide choice of $g(V)$, as to be shown elsewhere. As such, virtually no free parameters are involved in the analytical calculation of $\text{MSD}(t)$.

Using the Laplace-transformation approach, by applying Eq. (21) together with the coefficients from Eqs. (15) and (19) as well as the rates defined by Eq. (2) and Eq. (3), one can calculate $P_2(s; m)$. Then, $P_0(s; m)$ follows from Eqs. (12) and (13) and can be inserted into Eq. (22) to obtain $p_0(t; m)$. Substituting $p_0(t; m)$ into Eq. (9), we find $\bar{n}(t; m)$, which is further inserted in Eq. (25) to obtain the MSD. Eq. (25) and these associated equations thus constitute our closed form solution for the MSD. Alternatively, identical results can be obtained using an ordinary differential equation (ODE) integration approach. In this case, the rate equations in Eqs. (4) - (6) are numerically integrated to obtain, in particular, $p_0(t; m)$. The MSD can then be obtained similarly using Eqs. (9) and (25).

The quantitative agreement of the theory with the simulations for a wide range of temperatures is shown in Figure 2. In the plot, we have chosen a void density $\phi_v = 0.01$ for the left panel while 0.05 for the right panel. As shown in the figure, the agreement is very good at high temperatures, while at low temperatures the theory slightly deviates from the simulations but the agreement is still impressive. More importantly, the theory captures the formation of the plateau very well for all temperatures. In particular, the plateau value of the MSD is accurately determined and this is highly non-trivial. The nearly exact agreement for $\text{MSD}(t) \leq 2 \times 10^{-3}$ for all curves also shows the validity of the rates $\tilde{w}_0$ used in our theory.

5. Conclusion and outlook

Based on the recently proposed local random configuration-tree theory, we have analytically calculated the MSD of particles in glass formers. The results have been
compared with numerical simulations of a lattice glass model – the DPLM, and an overall good agreement has been achieved at the quantitative level with virtually no free parameters. This kind of accuracy of a glass theory is rare, if not unprecedented.

In this paper we have only applied the theory to the DPLM, for the required parameters are precisely known here. In the near future, we shall apply it to other glass formers, including computational (e.g. polydisperse Lennard-Jones liquids) and experimental systems. For such systems, the MSD should be based on coarse-grained trajectories \[17\] with fast vibrations averaged out. There will be far more parameters involved. However, these parameters fall in groups and each group can be tightly constrained by computational or experimental observations. We shall also use the theory to shed light on the effects of particle swap on particle dynamics in these systems, which has recently attracted lots of attention \[20, 21, 22, 23, 24, 25, 26\].

Another interesting line of investigation would be to look at other physical quantities from the configuration-tree theory point of view, such as the self-intermediate scattering function and the particle displacement distribution function. The former is especially important for its widespread use in the experimental literature. We are currently working on generalizing our theory to calculate these functions.

Finally, we make a few remarks on the role of voids in our theory. There are two basic tenets in the theory. The first is the existence of a local random configuration tree, which in our opinion is quite general and robust. The second explicitly assumes the presence of voids and string-like particle motions. While string-like motions have ample evidences, the concept of voids is sometimes contested. Regarding this the following point is worthy of notice: A void capable of initiating string-like motions is not necessarily as well-defined spatially as in the DPLM. It could consist of free volumes fragmentarily and distributed.

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References