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Dimensional Interpolation for Random Walk

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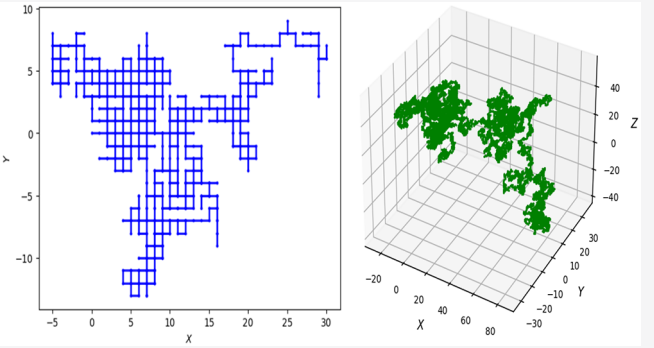
ABSTRACT: We employ a simple and accurate dimensional interpolation formula for the shapes of random walks at $D = 3$ and $D = 2$ based on the analytically known solutions at both limits $D = \infty$ and $D = 1$. The results obtained for the radius of gyration of an arbitrary shaped object have about 2% error compared with accurate numerical results at $D = 3$ and $D = 2$. We also calculated the asphericity for a three-dimensional random walk using the dimensional interpolation formula. The results agree very well with the numerically simulated results. The method is general and can be used to estimate other properties of random walks.



INTRODUCTION

A random walk is a random sequence of movements that begins at the same point. For example, consider an object that begins at zero on the integer number line, $\mathbb{Z}$, and at each step moves up or down the line, i.e., + 1 or −1, with equal probabilities. Random walk appears as a core phenomenon in various models, including the path traced by a molecule while traveling in a liquid or a gas, i.e., Brownian motion, the price of a fluctuating stock, and the financial status of a gambler. The random walk problem was introduced by Pearson in 1905,[1] and the developed theory has successfully been implemented in different branches of science and engineering, e.g., hydrodynamics,[2] astronomy,[3] chemistry,[4,5] polymer sciences,[6−8] mathematics,[9] biology,[10] and economics.[11] More specifically, condensed matter physics includes many applications for random walks, including percolation clusters,[12] lattice animals,[13,14] disordered magnetic systems and spin glasses,[15] anisotropy, and random fractals.[16] Dimensional scaling offers simple solutions at the limits $D = 1$ and $D \to \infty$, where D is the number of spacial dimensions. Using these limits, we interpolate between them to obtain accurate results for chemical physics at $D = 3$.[17−27] Recently, a dimensional interpolation formula was developed[28] to obtain the ground state energies for few electron atoms, simple diatomic molecules[29] and extended systems like metallic hydrogen.[30] Rudnick et al. studied the random walks in high spacial dimensions[21,31] and developed $1/D$ expansion to study the shape of a random walk in three dimensions. In this work, we employ a simple and accurate dimensional interpolation formula using dimensional limits $D = 1$ and $D \to \infty$ to analyze the random walk problem at $D = 3$ and $D = 2$, and obtain physical quantities like the radius of gyration and asphericity describing an arbitrarily shaped two- or three-dimensional objects.

BASIC DIMENSIONAL INTERPOLATION FORMULA

To recapitulate, we start with the dimensional interpolation formula for atomic, molecular, and extended systems.[29,30] For dimensional scaling of atoms and molecules, the energy erupts to infinity as $D \to 1$ and vanishes as $D \to \infty$. Hence, we adopt scaled units (with hartree atomic units) whereby $E_D = (Z/\beta)^2 \epsilon_D$ and $\beta = (1/2)(D - 1)$, so the reduced energy ϵ_D remains finite in both limits. The interpolation for atoms, developed in ref 28, is described by a simple analytic formula

$$\epsilon_D = \frac{1}{D}\epsilon_1 + \left(1 - \frac{1}{D}\right)\epsilon_\infty + \left[\epsilon_D^{(1)} - \frac{1}{D}\epsilon_1^{(1)} - \left(1 - \frac{1}{D}\right)\epsilon_\infty^{(1)}\right]\lambda \quad (1)$$

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However, for molecular and extended systems in $D = 3$,[32−35] the interpolation formula becomes

$$\epsilon_3(R') = \frac{1}{3}\epsilon_1\left(\frac{1}{3}R'\right) + \frac{2}{3}\epsilon_\infty\left(\frac{2}{3}R'\right) \tag{2}$$

with

$$R \to R'/D \text{ for } D \to 1; \quad R \to \left(1 - \frac{1}{D}\right)R' \text{ for } D \to \infty \tag{3}$$

For the random walk problem an important quantity is the principal components of the radius of gyration R_i^2. These are one of the quantities for measuring the anisotropy of a D-dimensional random object. We propose the following interpolation formula for random walk problem

$$(R_i^2)_d = \frac{1}{D}(R_i^2)_1 + \left(1 - \frac{1}{D}\right)(R_i^2)_\infty \tag{4}$$

where D = dimension and $(R_i^2)_D$ is the ith principle component of the radius of gyration.

RANDOM WALK AT THE LARGE-D LIMIT

There are a number of ways to measure the anisotropy of a random object generated by a three-dimensional random walk. The shape of an arbitrary solid object in D-dimension is described by a quantity called the gyration tensor, which is described as

$$T_{ij} = \frac{1}{N+1}\sum_{l=1}^{N+1}(x_{li} - \langle x_i\rangle)(x_{lj} - \langle x_j\rangle) \tag{5}$$

with

$$\langle x_i\rangle = \frac{1}{N+1}\sum_{l=1}^{N+1} x_{li} \tag{6}$$

where x_{li} is the ith coordinate of the particle after l steps and N is the total number of steps.

Eigenvalues of $\overleftrightarrow{T}$ are the square of the components of the radius of gyration R_i^2. The gyration tensor was first introduced by Solc and Stockmeyer in their study of random flight chain.[36] These principal components determine the size and shape of a solid object and also inertial properties.[7] By convention ${R_1}^2 \geq {R_2}^2 \geq {R_3}^2$.... The combination of principal radii of gyration is known as the square of the radius of gyration

$$R^2 = {R_1}^2 + {R_2}^2 + {R_3}^2 + ... \tag{7}$$

The average value $\langle R^2\rangle$ for long, unrestricted open chain walks was calculated[37] to be $R^2 = N/6$, and for closed walks,[38,39] $R^2 = N/12$. From the principal radii of gyration, we can compute asphericity or the asymmetry parameter of a solid object which is a one parameter measure to describe how much it is deformed from the perfect sphere.[40−42]

For a N-step random walk problem at $D = \infty$, Rudnick et al.[21] showed that the gyration tensor becomes

$$\begin{aligned}(T_\infty)_{ij} &= \frac{i}{(N+1)^2}(N+1-j), \text{ for } i < j, \text{ and } 1 \\ &\leq i, j \leq (N+1), \\ &= \frac{j}{(N+1)^2}(N+1-i), \text{ for } i > j, \\ &= 0, \text{ otherwise.}\end{aligned} \tag{8}$$

The eigenvectors of T_{ij} can be written as[31]

$$\psi_n(i) = \left(\frac{2}{N+1}\right)^{1/2}\sin\left(\frac{n\pi i}{N+1}\right) \tag{9}$$

and the corresponding eigenvalues are

$$\lambda_n = \langle {R_n}^2\rangle_\infty = \frac{1}{4(N+1)}\left[\sin^2\left(\frac{n\pi}{2(N+1)}\right)\right]^{-1} \tag{10}$$

where N is the total number of steps. For large N, the principal components of the radius of gyration becomes

$$\langle {R_n}^2\rangle_\infty = \lambda_n = \frac{N+1}{\pi^2 n^2} \approx \frac{N}{\pi^2 n^2} \tag{11}$$

RANDOM WALK IN ONE DIMENSION

In one dimension, we have only two possible directions: forward and backward. For total number of steps = N, the probability of m forward steps and n backward steps can be written as

$$P(m, n) = \frac{1}{2^N}\frac{N!}{m!n!} \tag{12}$$

For large N, the probability function can be defined as

$$P(x) = \frac{2}{\sqrt{2\pi N}}e^{-x^2/2N} \tag{13}$$

where x is the distance from the origin.

We have developed a python program to simulate a random walk in one-dimension. For $N = 1000$ steps, an example of a one-dimensional random walk is plotted above in Figure 1.

We calculate the moment of inertia tensor T from eq 5 which has one eigenvalue, ${R_1}^2$, the principle component of the

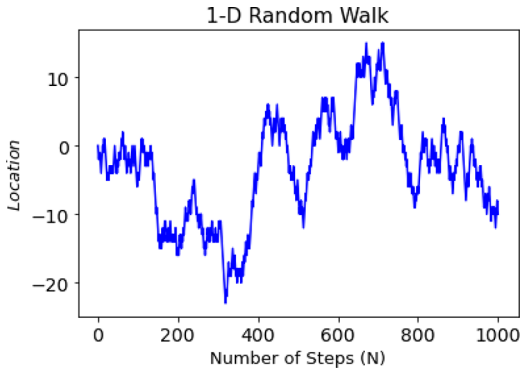

Figure 1. Random walk in one dimension with 1000 steps. The x-axis describes the number of steps, and the y-axis describes the position of the random walker after each step from the origin. The forward and backward directions are assumed to be positive and negative, respectively.

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radius of gyration. We repeat the simulation 100 000 times and take the average of all R^2's to obtain $\langle R_1^2 \rangle$ = 166.285179.

RANDOM WALK IN TWO DIMENSIONS

In two dimensions the particle can go in any of the two directions X and Y. We simulate a random walk in two spacial dimensions with N = 1000 steps starting from the origin $(0,0)$. The simulation result of a two-dimensional random walk is plotted in Figure 2.

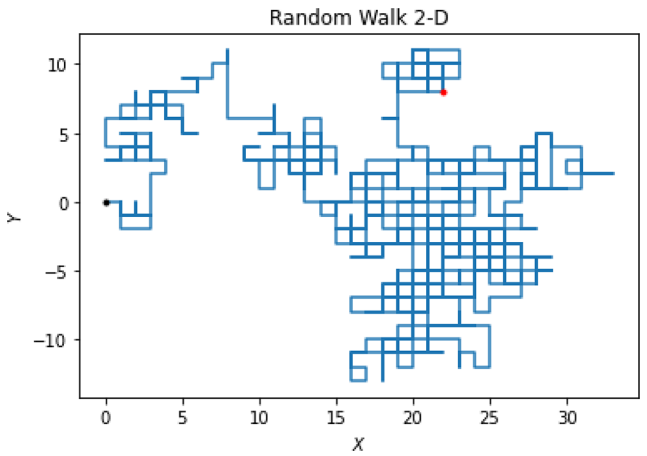

Figure 2. Random walk in two dimension with 1000 steps. The blue and red dots are beginning (origin) and ending points, respectively.

We calculate the moment of inertia tensor T_{ij} from eq 5, which has two eigenvalues, R_1^2, R_2^2, the principle components of the radius of gyration. By convention $R_1^2 \geq R_2^2$. We repeat the simulation 100 000 times. The averages of all R_i^2's are given by $\langle R_1^2 \rangle$ = 138.94300 and $\langle R_2^2 \rangle$ = 27.90438. The radius of gyration is given by $R^2 = (R_1^2 + R_2^2)$ = 166.84739. The distribution of all (R_1^2, R_2^2) obtained from different simulations is calculated and the frequency and probability distribution of the R_1^2 is plotted in Figure 3.

RANDOM WALK IN THREE DIMENSION

In three dimensions the particle can go in any of the three X, Y, and Z directions.

We simulate a random walk in three spacial dimensions with N = 1000 steps starting from the origin $(0,0,0)$. The simulation result of a three-dimensional random walk is plotted in Figure 4. We calculate the moment of inertia tensor T_{ij} from eq 5, which has three eigenvalues, R_1^2, R_2^2, R_3^2, the principle components of the radius of gyration. By convention $R_1^2 \geq R_2^2 \geq R_3^2$. We repeat the simulation 100 000 times. The distribution of all (R_1^2, R_2^2, R_3^2) obtained from different simulations is calculated and the frequency and probability distribution of the R_1^2 is plotted in Figure 5.

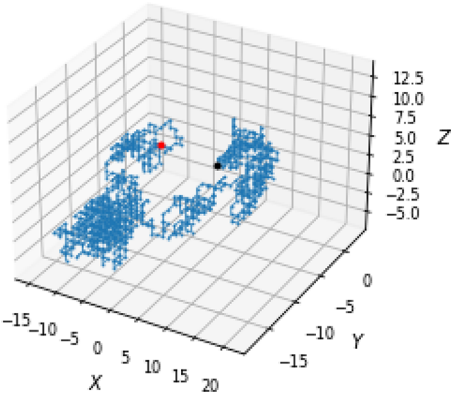

Figure 4. Random walk in three dimension with 1000 steps. The blue and red dots are beginning (origin) and ending points, respectively.

The averages of all R_i^2's are given by $\langle R_1^2 \rangle$ = 126.82723, $\langle R_2^2 \rangle$ = 28.68618, and $\langle R_3^2 \rangle$ = 10.57850. The radius of gyration is given by $R^2 = (R_1^2 + R_2^2 + R_3^2)$ = 166.0919.

INTERPOLATION AT D = 3

We employ the interpolation formula in eq 4 developed by Herschbach[28] for R_i^2 in three dimensions as follows:

$$(R_i^2)_3 = \frac{1}{3}(R_i^2)_1 + \frac{2}{3}(R_i^2)_\infty \tag{14}$$

where $(R_i^2)_D$ is the ith component of the radius of gyration in the D-dimension.

From eq 10, we see that

$$(R_n)^2 = \frac{1}{4(N+1)}\left[\sin^2\left(\frac{n\pi}{2(N+1)}\right)\right]^{-1}, \text{ for } n = 1, 2, 3 \text{ , and } N = 1000 \tag{15}$$

Therefore, from eq 15 $(R_1^2)_\infty$ = 101.422588. On the other hand $(R_1^2)_1$ = 166.2851794.

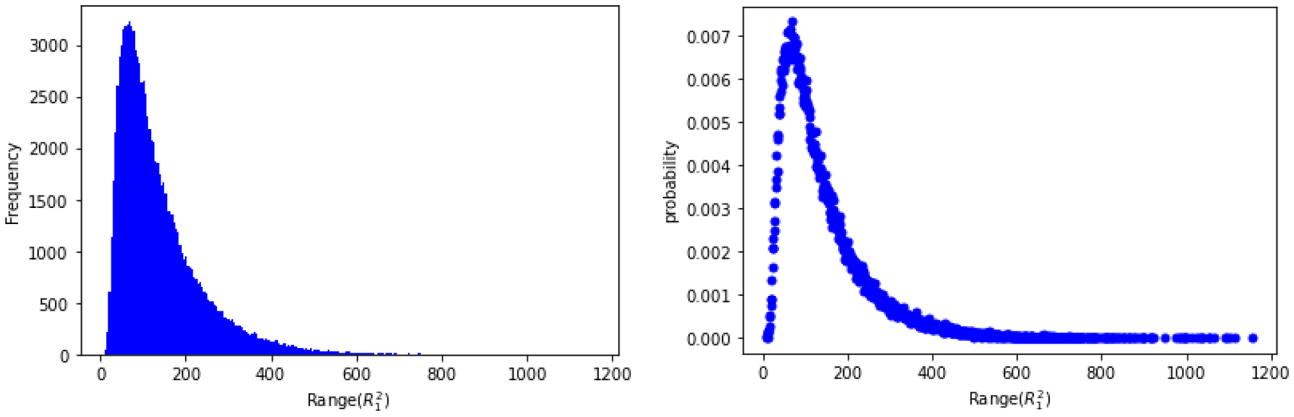

Figure 3. Plots of frequency and probability of R_1^2, as a function of its values occurring during different simulation.

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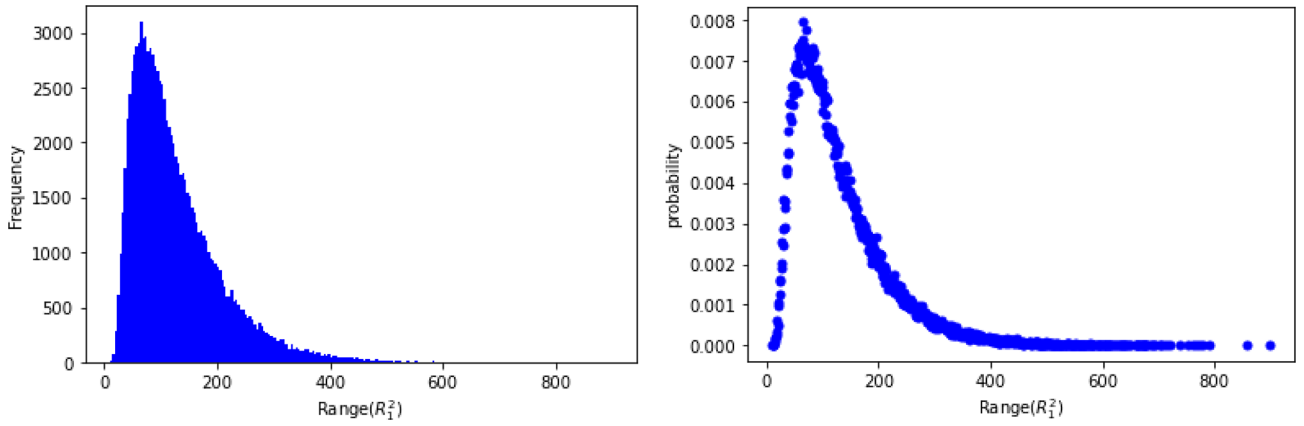

Figure 5. Frequency and probability distribution of R_1^2 obtained for the three-dimensional random objects generated by repeating a 1000 step random walk 100,000 times.

From the above eq 14 we can calculate

$$(R_1^2)_3 = \frac{1}{3}(R_1^2)_1 + \frac{2}{3}(R_1^2)_\infty = 123.04345 \tag{16}$$

The computer simulation of the three-dimensional random walk gives $(R_1^2)_{sim}$ = 126.82723, which is a very close estimation with 2% error.

In one dimension, there is only one component of the radius of gyration. Therefore, for interpolating the other component of the radius of gyration we extrapolate the values of R_n^2 at one dimension. For $D = \infty$, and large N, the principal components of the radii of gyration are as follows:

$$R_n^2 = \frac{1}{n^2}R_1^2 \tag{17}$$

so that

$$(R_1^2)_{\inf}:(R_2^2)_{\inf}:(R_3^2)_{\inf} = 9:4:1 \tag{18}$$

f

On the other hand, at $D = 3$, in the literature,[7] the authors showed that the following limiting ratios have been found to approach for the large N limit

$$\langle R_1^2\rangle:\langle R_2^2\rangle:\langle R_3^2\rangle = 11.80:2.69:1 \tag{19}$$

From eqs 18 and 19, we see that the ratios between the radius of gyration change with the change of dimension. We propose a model for the dimensional dependence of R_n^2 as follows:

$$R_n^2 = \left(\frac{1}{n^2\left(1 + \frac{a_n}{D}\right)}\right)R_1^2, \text{ for } n = 2, 3, \ldots \tag{20}$$

where a_2, a_3, ... are constants and D is the dimension. Now from the standard result at $D = 3$, from eq 19, we can get two sets of equations, which has a solution $a_2 = 0.28996$ and $a_3 = 0.9333$.

With these ratios we can calculate the r_n^2 at $D = 1$ to be

$$(R_2^2)_1 = \frac{1}{5.15985}(R_1^2)_1 \text{ and } (R_3^2)_1 = \frac{1}{17.39997}(R_1^2)_1 \tag{21}$$

For $N = 1000$, from eq 21, at $D = 1$, we can calculate the quantities $(R_2^2)_1$ = 32.2267 and $(R_3^2)_1$ = 9.5566. And from eq 15 at $D = \infty$, we compute the quantities $(R_2^2)_\infty$ = 25.3557 and $(R_3^2)_\infty$ = 11.26925. With the values of R_i^2 at $D = 1$ and $D = \infty$, we calculate $(R_2^2)_3$ = 27.64604, and the computer simulation gives $(R_2^2)_{sim}$ = 28.68618. However, $(R_3^2)_3$ = 10.6983, and the computer simulation gives $(R_3^2)_{sim}$ = 10.5785.

The total radius of gyration from the interpolation is given by

$$(R^2)_3 = (R_1^2)_3 + (R_2^2)_3 + (R_3^2)_3 = 161.38 \tag{22}$$

which is a fairly good estimation for the $(R^2)_{sim}$ = 166.0919, obtained from random walk simulation at $D = 3$.

Now, we also calculate the ratios between the radii of gyrations obtained from the interpolation: $(R_1^2)_3:(R_2^2)_3:(R_3^2)_3$ = 11.5:2.58:1, where as ratios between the radii of gyrations obtained from simulation is given by $(R_1^2)_{sim}:(R_2^2)_{sim}:(R_3^2)_{sim}$ = 11.98:2.71:1.

The above estimates from dimensional interpolation are close estimates, because not one of the random number generators is a perfect random number generator. Therefore, the computer simulation of the random walk at $D = 3$ is only an approximation for a perfect random walk in three dimensions. We expand our calculation by considering different step sizes to establish the validity of our interpolation formula. The averages are taken over 1000 samples. We compute the radii of gyration for different step sizes N = 10, 50, and 100, respectively. For $D = 1$ we obtain $(R_1^2)_1$ = 1.8226 for $N = 10$, $(R_1^2)_1$ = 8.29468 for $N = 50$, and $(R_1^2)_1$ = 17.5066 for $N = 100$. On the other hand, for $D \to \infty$ limit, we obtain $(R_1^2)_\infty$ = 1.1221 for $N = 10$, 5.1690 for $N = 50$, and 10.2342 for $N = 100$. Using eqs 15 and 21 with the interpolation formula in eq 14 we calculate $(R_1^2)_3$, $(R_2^2)_3$, and $(R_3^2)_3$ respectively, and we compare with the results obtained from the computer simulation of random walk in three dimensions in Table 1.

INTERPOLATION AT $D = 2$

We employ the interpolation formula from eq 4 for R_i^2 in three-dimension as follows:

$$(R_i^2)_2 = \frac{1}{2}(R_i^2)_1 + \frac{1}{2}(R_i^2)_\infty \tag{23}$$

where $(R_i^2)_D$ is the ith component of the radius of gyration in the D-dimension.

Therefore from Eq 10, $(R_1^2)_\infty$ = 101.422588. On the other hand $(R_1^2)_1$ = 166.28518.

From the above equarion, eq 23, we can calculate

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Table 1. Dimensional Interpolation for Random Walk at $D = 3$ with Different Step Size N

step size (N)	$D = 3$ (simulation)	$D = 3$ (interpolation)
10	$\langle R_1^2\rangle = 1.3640$	$\langle R_1^2\rangle = 1.35563$
	$\langle R_2^2\rangle = 0.3242$	$\langle R_2^2\rangle = 0.3086$
	$\langle R_3^2\rangle = 0.1139$	$\langle R_3^2\rangle = 0.1142$
50	$\langle R_1^2\rangle = 6.3367$	$\langle R_1^2\rangle = 6.2109$
	$\langle R_2^2\rangle = 1.4336$	$\langle R_2^2\rangle = 1.3982$
	$\langle R_3^2\rangle = 0.54268$	$\langle R_3^2\rangle = 0.5428$
100	$\langle R_1^2\rangle = 12.7003$	$\langle R_1^2\rangle = 12.6584$
	$\langle R_2^2\rangle = 2.9590$	$\langle R_2^2\rangle = 2.8371$
	$\langle R_3^2\rangle = 1.0776$	$\langle R_3^2\rangle = 1.0939$

$$(R_1^2)_2 = \frac{1}{2}(R_1^2)_1 + \frac{1}{2}(R_1^2)_\infty = 133.8539 \tag{24}$$

From the computer simulation of the two-dimensional random walk gives $(R_1^2)_{sim} = 138.94300$, which is a close agreement with the interpolation result in eq 24.

Using eq 21 we write the ratio between R_2^2 and R_1^2 at $D = 1$

$$(R_2^2)_1 = \frac{1}{5.15985}(R_1^2)_1 \tag{25}$$

For $N = 1000$ from eq 25, at $D = 1$, we calculate $(R_2^2)_1 = 32.2267$. From eq 15 at $D = \infty$, we calculate the following quantity, $(R_2^2)_\infty = 25.3557$. With the above data at $D = 1$ and $D = \infty$, we compute $(R_2^2)_2 = 28.7912$ and the computer simulation gives $(R_2^2)_{sim} = 27.9044$.

The total radius of gyration from the interpolation is given by

$$(R^2)_2 = (R_1^2)_2 + (R_2^2)_2 = 162.6451 \tag{26}$$

which is a fairly good estimation for the $(R^2)_{sim} = 166.84739$, obtained from random walk simulation in two dimensions with a 2.5% error.

Like the three-dimensional case, we also calculate the ratios between the radii of gyrations obtained from the interpolation: $(R_1^2)_2:(R_2^2)_3 = 133.8539:28.7912 = 4.65:1$, whereas ratios between the radii of gyrations obtained from simulation is given by $(R_1^2)_{sim}:(R_2^2)_{sim} = 138.9430:27.90438 = 4.97:1$. We expand our calculation by considering different step sizes to establish the validity of our interpolation formula at $D = 2$. The averages are taken over 1000 samples. We compute the radii of gyration for different step sizes $N = 50$, 100 respectively. For $D = 1$ we obtain $(R_1^2)_1 = 8.29468$ for $N = 50$ and $(R_1^2)_1 = 17.5066$ for $N = 100$. On the other hand, for $D \to \infty$ limit we obtain $(R_1^2)_\infty = 5.1690$ for $N = 50$ and 10.2342 for $N = 100$. Using eqs 15 and 21, with the interpolation formula in eq 14, we calculate $(R_1^2)_3$ and $(R_2^2)_3$ respectively, and compare with the results obtained from the computer simulation of random walk in two dimensions in Table 2.

Table 2. Dimensional Interpolation for Random Walk at $D = 2$ with Different Step Size N

step size (N)	$D = 3$ (simulation)	$D = 3$ (interpolation)
50	$\langle R_1^2\rangle = 7.2121$	$\langle R_1^2\rangle = 6.7318$
	$\langle R_2^2\rangle = 1.4513$	$\langle R_2^2\rangle = 1.4605$
100	$\langle R_1^2\rangle = 14.0010$	$\langle R_1^2\rangle = 13.8704$
	$\langle R_2^2\rangle = 2.8198$	$\langle R_2^2\rangle = 2.9760$

ASPHERICITY

The radius of gyration is a measure of the average extent of a random walk. However, to get a better idea of its shape we define a quantity called asphericity, which is denoted as $A_D \in [0,1]$.[31,40,42] This quantity determines how much a solid object deviates in shape from a perfect sphere. For example, for a perfectly spherical object its asphericity $A_D = 0$. On the other hand, this quantity has an upper bound of one, a limit that is reached when the walk is extended in one dimension only. Mathematically, the expression for A_D is defined as follows:

$$A_D = \frac{\sum_{i>j}^{D}\langle (R_i^2 - R_j^2)^2\rangle}{(D-1)\left\langle \left(\sum_{i=1}^{D} R_i^2\right)^2\right\rangle} \tag{27}$$

At the large D-dimension, Rudnick et al.[31,40] showed that the expression of asphericity can be written as

$$A_D = \frac{2}{5} + \frac{12}{25D} + O\left(\frac{1}{D^2}\right) \tag{28}$$

For $D \to \infty$, $A_\infty = (^2/_5)$. On the other hand, for $D = 1$, $A_1 = 1$.

In refs 43 and 44, the authors introduces a dimensional interpolation formula with $D = 0$ and $D = \infty$ and calculate asymmetry (similar to asphericity), which is defined as

$$\mathcal{A}_D = \frac{1}{D-1}\left\langle \frac{\sum_{i>j}^{D}(R_i^2 - R_j^2)^2}{\left(\sum_{i=1}^{D} R_i^2\right)^2}\right\rangle \tag{29}$$

Although both the above quantities measure the anisotropy, the asymmetry $\mathcal{A}_D$ is slightly different from the asphericity A_D, defined in eq 27. The asphericity of each walk in the ensemble is calculated first and then the result is averaged. Whereas, for calculating the asphericity A_D, we take the average over the numerator and denominator separately. See 21 and 41 for more details.

Equation 28 gives a dimensional dependence of A_D at the large-D limit as a power series of $1/D$. Although this power series expression for A_D does not produce the result at $D = 1$, which is $A_1 = 1$. For the interpolation at $D = 3$ we modify the above expression in eq 28 for A_D for the large-D limit and use the result for A_D at $D = 1$. We rewrite the expression for the asphericity in the D-dimension:

$$A_D = \frac{2}{5} + \frac{a}{D} + \frac{a^2}{D^2} + \frac{a^3}{D^3} + \ldots \tag{30}$$

Here a is a parameter to be fixed from a known value of A_D at a given dimension. For the purpose of calculations, we only consider the terms up to the cubic order in (a/D) . For $D = 1$, we know that $A_D = 1$. We put this $D = 1$ result in the above equation, eq 30, and get the following condition for a

$$5a^3 + 5a^2 + 5a = 3 \tag{31}$$

which has a solution $a = 0.3894$. Now, substituting the value of a and $D = 3$ in eq 30 we obtain

$$A_3 = 0.5488 \tag{32}$$

We performed numerical simulation of a random walk at $D = 3$ with $N = 1000$ steps. Then, we took an average over 100000 samples to calculate the asphericity using eq 27 $A_{sim} = 0.5240$, which is a close estimation of the above theoretical prediction.

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CONCLUSION

The simplicity of the $D \rightarrow \infty$ limit allows the removal of the derivative terms from the Hamiltonian for electronic structure calculations[35] to find the minimum energy of the system. For the random walk, at $D \rightarrow \infty$ limit, the walker can take a step that is orthogonal to all the previous ones along a D-dimensional axis. The simplicity of the $D = 1$ limit keeps derivatives in a Hamiltonian and is a true hyperquantum limit. Combining these extreme partner limits delivers the dimensional interpolation formula. We have used the interpolation formula successfully for two-electron atoms[28] and generalized it for few electron atoms, simple diatomic molecules,[29] and metallic hydrogen.[30] In this article, we implemented the dimensional interpolation formula for the random walks and calculated physical quantities like radii of gyration and asphericity in two and three dimensions to show its robustness in different topics in physics and chemistry.

The complexity of the N-step random walk problem at $D = 3$ is of the order 6^N, whereas in $D = 1$, it is of the order 2^N. Therefore, in $D = 3$, the complexity of the simulation grows exponentially ($6^N/2^N = 3^N$) with the number of steps and with the number of dimension. Whereas, for random walks at $D = \infty$ there is an analytical formula, which is described above. It is relatively easy to calculate the $D \rightarrow \infty$ and $D = 1$ limits, so the interpolation formula can predict results for the physical dimensions, $D = 2$ or 3. The interpolation formula is general and might be used to obtain accurate results for other complex systems such as spin systems on different latices used extensively for magnetic materials and quantum computing simulations.

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Notes

The authors declare no competing financial interest.

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