Determination of pairwise interactions via the radial distribution function in equilibrium systems interacting with the Mie potential

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\textbf{Abstract}

Particle interactions play a fundamental role in condensed matter physics because they determine both the dynamical behavior and the equilibrium physical properties of a given system at temperature \( T \) and density \( \rho \). However, these interactions are not always precisely known in experiments, or in simulations of coarse-grained systems. A direct determination of the pair interaction potential in a given system could help understand observed behaviors and make further predictions. Given a number of equilibrium configurations of a system, it would be desirable to find a method to directly determine the pair potential by only using these snapshots. We propose two simple methods towards this goal for the specific case of the systems in 3 dimensional space with the Mie potential, which includes two exponents as \( m \) and \( s \). Well-equilibrated system configurations are produced by molecular dynamical simulations using the Mie potential with different exponent combinations \((m, s)\). In the first method, we construct a correspondence between the value and location of the first peak of the radial distribution function and the couple \((m, s)\), which allows us to determine the potential with an accuracy of 100\% when given a set of equilibrium configurations for an unknown potential. In the second method, we train an artificial neural network to learn this correspondence. We find that all \((m, s)\) combinations are correctly predicted. Both methods support the idea that the pairwise interaction can often easily be inferred by using equilibrium snapshots.

\textbf{Introduction}

Our world is colorful due to the existence of interactions among particles. Particle–particle interactions are of paramount importance in many-body systems as they determine the collective behavior and coupling strength [1]. For instance, in the simple case of the hard sphere interaction model, systems made of hard spheres display gas [2–4], fluid [3–8], crystals [9–14], disordered glasses [12,15] as well as hyperuniform structures [16]. For any model system, one can obtain all of its physical properties, including its phase diagram and microstructure, when the interactions among particles are fixed. In other words, interactions play a fundamental role in physics.

Often, particle–particle interactions are too complex to be obtained accurately in real physical systems. Very complicated expressions describing such interactions can be found in material science and chemical physics, obtained by different types of experimental and numerical methods [17–20]. In experiments, the particle–particle interactions can be completely unknown, while a determination of effective pairwise interactions can be useful to describe complex systems at a more coarse-grained level in computer simulations [21], and can also be useful for determining experimental parameters such as particle charge or screening length in colloidal systems, assuming the interaction is the Yukawa potential. Another potential application is the determination of the optimal pair potential to be used in order to produce a desired targeted structure, as in self-assembly [22].

In practice, one has instead access to some dynamical behavior or to some physical structural properties at equilibrium at the corresponding experimental conditions. Only when the particle–particle interactions in a system are well-characterized can one understand better its observed behaviors and even make predictions about unknown behaviors in different conditions. Thus, it is of great importance to find ways to determine particle–particle interactions directly from observations [23, 24].

Conceptually, the pairwise interaction for a specific physical system can be determined by analyzing the statistics of a system comprised of

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only two particles [25]. Although direct and simple, this method is not always accessible (for instance in experimental work or when a coarse-grained potential is sought) and it is desirable to devise methods that extract the pair interaction directly from the many-body interacting system at the desired thermodynamic conditions. In this context, this amounts to solving the inverse problem of extracting the pair potential from a given set of produced data. It is well known that, given the pair correlation function $g(r)$ there exists a one-to-one correspondence to the pair interaction potential $u(r)$ in virtue of the theorem derived by Henserson [26]. In practice however, there exists no analytic solution to this problem which must be tackled numerically. The most common method is perhaps the iterative Boltzmann inversion [27] where a candidate pair potential is proposed, and a computer simulation is used to measure its corresponding $g(r)$. The distance to the target pair correlation is used to improve the candidate potential in an iterative manner, in a way which can be refined [28]. Because an entire simulation is needed at each step the method is rather costly, and simpler methods would be welcome. Recently, an iterative method which does not require multiple simulations has been devised based in the particle insertion method [29]. This is an interesting step, but it only works for system that are dilute enough that particles can be inserted, which limits its applicability to dense liquids or solid phases.

In this paper, we focus on the systems interacting with the Mie potential in 3 dimensional space and devise a very simple idea to determine the two exponents of the Mie potential by only using an ensemble of equilibrium configurations obtained at thermal equilibrium. Although this problem is simpler than a full inversion problem to determine a completely unknown potential, it remains non-trivial and impossible to tackle analytically. Proposing a simple solution to the inverse problem in that narrower case is therefore a valuable contribution.

The manuscript is organized as follows. In Section “Theoretical basis”, we explain the theoretical basis for the idea. In Section “Numerical dynamics simulations and numerical computations by Method 1”, we provide details of our molecular dynamical simulations and the method of fitting correlations to check whether the idea well stands or not. In Section “Numerical computations by Method 2: artificial neural network (ANN)”, we provide the second method of the artifical neural network model underneath the Machine Learning to check whether the idea well stands or not. In Section “Results and discussion”, we demonstrate the validity of the predicted potentials under these two methods. In Section “Conclusion”, we make a short conclusion.

Theoretical basis

As is well-known, a pairwise additive interaction potential is defined as a mathematical function of the distance between the two particles considered. Many different kinds of pairwise potential functions are being used in the literature, such as the hard sphere potential [23], the Lennard-Jones potential [30] which is a special case of the more general Mie potential [31], or the Yukawa potential with or without hard core [29]. The Mie potential reads [31]

$$u(r_{ij}) = \frac{A}{r_{ij}^{m}} - \frac{B}{r_{ij}^{n}}.$$

When $m = 12$ and $s = 6$, Eq. (1) reduces to the Lennard-Jones potential [31]. In this paper, we consider equilibrated systems characterized by the Mie potential with 51 different $(m, s)$ combinations in 3 dimensional space.

The radial distribution function (RDF) (also called pair correlation function) reads [32]

$$g_2(r_1, r_2) = \frac{V^2 N^!}{N^2 (N - 2)!} \frac{1}{Z_N} \int \cdots \int e^{-\beta U_N} dr_1 \cdots dr_N.$$

Here $r_i$ are the particle coordinates, $U_N(r_1, \ldots, r_N)$ is the potential energy of the system due to the interactions between particles, $Z_N = \int \cdots \int e^{-\beta U_N} dr_1 \cdots dr_N$ is the configurational integral taken over all possible combinations of particle positions in the canonical ensemble. It is related to the canonical partition function $Z$ as

$$Z_N = Z \cdot N! \lambda^3 N,$$

where $\lambda = (\frac{\hbar}{2 \pi m})^{1/2}$ is the de Broglie thermal wavelength.

If the fluid system consists of spherically symmetric particles and the potential is fixed, $g_2(r_1, r_2)$ depends only on the relative distance between particles 1 and 2, $r_1 = |r_2 - r_1|$, so that

$$g_2(r_1, r_2) = g_2(r_{12}).$$

The canonical partition function for the fluid system composed of spherically symmetric particles with the Mie potential can be obtained using mean-field methods [33]

$$Z = \frac{V^N}{N! \lambda^3 N} \exp \left(-A \rho \frac{1}{2} - W \rho \frac{3}{2} \right),$$

with $A = 4 \pi \int_0^\infty r^4 \rho(r) g(r) dr$ and $W = 4 \pi \int_0^\infty r^4 \rho(r) g(r) dr$. As a result, we have that,

$$Z = Z(\rho, \beta, m, s).$$

Combining Eqs. (2), (4), (6), the radial distribution function can be written as

$$g_2 = g_2 \left(r_{12}, \rho, \beta, m, s \right).$$

Eq. (7) is reasonable as when the Mie potential is fixed (and so $(m, s)$ are fixed) and the system is equilibrated at constant density $\rho$ and temperature $T = 1/\beta$, we get that $g_2$ is a unique function of $r_{12}$. For a system with fixed density and temperature,

$$g_2 = g_2 \left(r_{12}, m, s \right) = g_2(r, m, s).$$

As is also well-known, for a fluid system at equilibrium, the radial distribution function exhibits several peaks. We characterize the first peak by its location and amplitude $(r_{1st}, g_{1st})$. By solving

$$\frac{d g_2}{d r} \bigg|_{r=r_{1st}} = 0$$

one can then obtain $m$ and $s$ because $r_{1st}$ and $g_{1st}$ are unique functions of $(m, s)$.

The above reasoning proposes an explicit demonstration, within a mean-field approach, that the exponents $m$ and $s$ can be determined directly from the pair correlation function. Given its approximate nature, we cannot use these expressions to perform the inversion in Eq. (9) analytically and we must thus resort to computer simulations. If the values of $r_{1st}$ and $g_{1st}$ are measured accurately, one can obtain the values of $m$ and $s$ by inverting the expressions for $r_{1st}$ and $g_{1st}$. It is interesting to discuss the physical meaning of some special points of the RDF; for instance, the peaks. Peaks in the RDF reflect some important physical microscopic structures. As qualitatively deduced by Liu et al. [34], a structure with higher symmetry will produce a lower density of RDF peaks. One can capture at least three independent pieces of information in a peak of the RDF peak [35]; its position gives the average separation of the pair of atoms in question; its integrated width and shape of the peak gives the underlying atomic probability distribution.

In the following, we use the distance histogram (DH) method to measure the values of $r_{1st}$ and $g_{1st}$ from a given set of data. The DH method is the most widely used method to measure the radial distribution function as a function of the distance between the two particles [36, 37]. This is the basis for the numerical analysis proposed in the following sections.
Molecular dynamics simulations and numerical computations by Method 1

We define the reduced distances \( r^* = r/\sigma \), density \( \rho^* = \rho\sigma^3 \), and temperature \( T^* = k_BT/\epsilon \). In Section "Theoretical basis", we described the theoretical basis to obtain the two unknown exponents \((m, s)\) from the value and location of the first peak of the RDF of equilibrated system configurations obtained with the Mie potential.

To test this idea, we perform computer simulations. We simulate Mie potential systems composed of \( N = 2048\) particles at six different reduced densities of \( \rho^* = 0.8, 0.9, 1.0, 1.1, 1.2, \) and 1.3 and three reduced temperature of \( T^* = 1/1.30, 1/1.35, 1/1.40 \) using conventional molecular dynamics simulations in 3 dimensional space. Temperature is imposed using a Nose–Hoover thermostat. Periodic boundary conditions are used. Specially, the reduced time step reads \( \Delta t^* = 0.005(t^* = t\sqrt{\epsilon/\sigma m}) \), the reduced maximal time reads \( t^*_{\text{max}} = 500 \), and the inertia parameter reads 10. The analysis and discussion in the present work are based on the converged results after \( 10^5 \) time steps using a cutoff radius of \( r^*_\text{cut} = L/2 \) with \( L \) being the linear size of the simulated box to guarantee that all systems are equilibrated. The core Fortran codes are from Frenkel and Smith [24] and available on request. The exponents of the Mie potential chosen in the interval \( m \in [8, 13] \) and \( s \in [2, m - 1] \). All systems were found to be thermodynamically stable. Note that the global stability of the considered cases of \( s = 2 \) and \( s = 3 \) confirmed numerically is presumably an artifact resulting from the chosen \( r^*_\text{cut} \) value, and that these systems would be thermodynamically unstable when considering infinite-range interactions. In total, we have studied 51 \((m, s)\) combinations. For each equilibrated Mie system with \((m, s)\), \( 10^4 \) statistically independent configurations are stored to compute the radial distribution function using the DH method with a regular grid with discretization \( \Delta r = 0.01\sigma \). From these numerical results, we obtain \( g_s(r) \), and we can extract the value and location of its first peak \((r^*_1, g^*_1)\) for each \((m, s)\) combination. A detailed description of the DH method can be found elsewhere [33]. Numerically, we fit a short interval around the first peak using a third-order polynomial function to get a smooth curve and extract the value and location of its first peak from the corresponding polynomial function.

The measured values for the combinations \((m = 8, s = 2, 3, 4, 5, 6, 7)\), \((m = 10, s = 2, 3, 4, 5, 6, 7, 8, 9)\) \((m = 12, s = 2, 4, 6, 7, 8, 10)\) and \((m = 13, s = 2, 2, 6, 8, 10, 12)\) provide a total of 26 data points which are used to obtain empirical expressions for \((r^*_1, g^*_1)\). For instance, in the case of \( \rho^* = 0.8 \) and \( T^* = 1/1.35 \) the fittings form reads:

\[
\begin{align*}
 r^*_1(m, s) & = 0.7044 + 0.06615m + 0.1906s - 0.003014m^2 - 0.03709ms \\
 & - 0.03859s^2 + 0.001775m^2s + 0.007326ms^2 + 0.001251s^3 \\
 & - 0.0003539m^2s^2 - 0.0002707ms^3 - 1.944 \times 10^{-6}s^4 \\
 & + 1.45 \times 10^{-5}m^2s^3 + 9.892 \times 10^{-7}ms^4 - 1.103 \times 10^{-6}s^5. \\
g^*_1(m, s) & = 0.6661 + 0.2141m + 0.08667s - 0.00694m^2 - 0.04018ms \\
 & - 0.01882s^2 + 0.002458m^2s + 0.008879ms^2 - 0.003937s^3 \\
 & - 0.000522m^2s^2 - 4.325 \times 10^{-5}m^3s + 0.001732s^4 \\
 & + 7.691 \times 10^{-6}m^2s^3 + 1.102 \times 10^{-5}ms^4 - 1.2 \times 10^{-5}s^5.
\end{align*}
\] (10)

Equivalent expressions for the other five densities are enclosed for the case of \( T^* = 1/1.35 \) in the Supporting Material (SM). Other expressions for other two cases of \( T^* = 1/1.30, 1/1.40 \) have also been obtained, see SM. For each density, we simulate a total of 51 combinations of exponents. We checked that the quality of the predictions became less if we only use lower-order polynomial in Eqs. (10), (11).

To check the accuracy of a given prediction for \((r^*_1, g^*_1)\), we introduce an error function between the prediction and the measured values defined as

\[
\chi^2 = \left( \frac{g^*_1 - g^*_1_{\text{fit}}}{g^*_1} \right)^2 + \left( \frac{r^*_1 - r^*_1_{\text{fit}}}{r^*_1} \right)^2.
\] (12)

With these definitions, our procedure to determine the unknown exponents \((m, s)\) from a given set of equilibrium configurations is as follows:

(a) For a set of \( 10^4 \) configurations for which we wish to infer the exponents \((m, s)\) we measure numerically \( g_s(r) \) by the DH method;

(b) We fit the region of the first peak using a polynomial function and extract the value and the location of the first peak \((r^*_1, g^*_1)\);

(c) For all possible pair \((m, s)\) with integer values we use Eqs. (10), (11) to calculate \((r^*_1, g^*_1)\);

(d) For each pair \((m, s)\) we estimate the error \( \chi^2 \) in Eq. (12) between the fitted and measured values;

(e) The \((m, s)\) combination with the lowest \( \chi^2 \) is selected as the best candidate for the two exponents of the Mie potential corresponding to the numerical data.

Numerical computations by Method 2: artificial neural network (ANN)

The spirit of machine learning (ML) is to automatically learn a set of rules from a set of data using an appropriate algorithm, to be able to make predictions for a new set of data. Artificial neural network (ANN) models act as a nonlinear data modeling device in ML [38–41]. We propose to use a very simple ANN model to determine the two exponents \((m, s)\) of the Mie potential by using the value and location of the first peak of the RDF as inputs.

The structure of our ANN model is displayed in Fig. 1. The Matlab software is used to build the model. The ANN model is composed of the input layer, the hidden layer, and the output layer while the neurons exist in the layers. In the input layer, the input information is received, and each neuron represents an input variable and directly transmits the information to the neurons in the hidden layer without processing. In the hidden and output layers, each output receives a weighted sum of the inputs plus a bias, and then transmits the sum through an activation function to generate an output. We use a feed-forward neural network. The input variables are \((r^*_1, g^*_1)\) and the output variables are the two exponents \((m, s)\). Because the two exponents \((m, s)\) to be determined are integers, we need to transform the real numbers obtained in output back into integers. We consider the case of \( T^* = 1/1.35 \) as an example to illustrate the details. For each density, the 51 \((m, s)\) samples are divided into two disjoint sets of data. The numerical values of \((m = 8, s = 2, 3, 4, 5, 6, 7)\), \((m = 10, s = 2, 3, 4, 5, 6, 7, 8, 9)\) \((m = 12, s = 2, 4, 6, 7, 8, 10)\), \((m = 13, s = 2, 4, 6, 8, 10, 12)\) provide a total of 26 samples which form the part I (PI). The other 25 samples form the part II (PII). In PI, 80\% of the 26 samples (20 samples) are used for training, 10\% (3 samples) are used for validation, and 10\% (3 samples) are used to perform the testing. These three databases are randomly assembled. Both ‘tansig’
and ‘purelin’ functions in Matlab software are selected as the activation functions in the hidden layer and output layer, respectively. The training accuracy of the ANN model is measured by the mean-squared error (MSE) defined as

$$MSE = \frac{\sum (m_p - m_s)^2 + \sum (s_p - s_s)^2}{2N_p}$$

(13)

where \((m_p, s_p)\) and \((m_s, s_s)\) are respectively the predicted and exact values, and \(N_p\) is the number of samples. Using trial and error, we determined the optimal number of the neurons of the hidden layer with the mean square error (MSE), as is illustrated in Fig. 2(a). It is easy to see that the MSE is equal to 0.0004695 for PI, 0.002162 for PII, and 0.001316 for the mean MSE for 8 neurons.

The trained ANN model will be used for the prediction of the other 25 samples in part II (PII) which were not used in the model training stage. The other two temperature cases of \(T^* = 1/1.30\) and \(T^* = 1/1.40\) follow the same scheme but require different \((m, s)\) combinations for PI and are available on request.

Results and discussion

Stability of the first peak of the RDF from the DH method

For a homogeneous system, the radial distribution function can be defined as \([29]\) \(g(r) = \rho^2(r)/\rho\). It is given by the ratio of the local number density measured from a reference particle \(\rho^2(r)\) over the bulk number density \(\rho\). According to this definition, the RDF is typically measured using the distance histogram (DH) method \([42]\).

We have followed the behavior of the measured value and location of the first peak of the RDF of the Lennard-Jones fluids at \(\rho^* = 0.8\) and \(T^* = 1/1.35\). For a small number of configurations (a few hundreds), the measured values appear to fluctuate due to statistical uncertainties. Only when the number of configurations is large enough the measured values become stable. We find that \(r_{\text{peak}}\) and \(g_{\text{peak}}\) become statistically reliable when the number of configurations becomes larger than \(\approx 10^4\). We conclude that the measured \(g_{\text{peak}}\) will not take a constant value unless the number of configurations is quite large. In this work, the number of configurations (NC) is taken to be \(10^4\) for each \((m, s)\) combination, which provides a compromise between numerical precision and computational load. According to the above discussion, NC = \(10^4\) is large enough to obtain a reasonable stability of both the value and the location of the first peak of the RDF. It is observed that both the obtained \(r_{\text{peak}}\) and \(g_{\text{peak}}\) by the DH method are completely stable with NC = \(10^4\) for all the \((m, s)\) combinations we considered as follows. In the following, we show and analyze the results for the case of \(T^* = 1/1.35\). Similar results hold for the other two temperature cases, as shown in Supporting Materials.

Numerical results for Method 1: Empirical fits

Equilibrated Mie systems with 51 different \((m, s)\) combinations at \(\rho^* = 0.8, 0.9, 1.0, 1.1, 1.2, 1.3\) and \(T^* = 1/1.35\) are produced by MD simulations. The numerical results for the evolution of \(r_{\text{peak}}\) and \(g_{\text{peak}}\) with \((m, s)\) are displayed in Figs. 3, 4. The curved surface in Fig. 3 represents Eq. (10), and the curved surface in Fig. 4 represents Eq. (11) while the symbols correspond to the measurements.

From Fig. 3, we see that the location of the first peak of the RDF decreases with \(s\) when \(m\) is fixed. Recall that \(m\) is the exponent of the repulsive part of the Mie potential and \(s\) is the exponent of the
attractive part. Physically, increasing $s$ at fixed $m$ implies the increasing of attraction in large $r$ and the decreasing of repulsion in small $r$, which enhances the first peak of the RDF and shifts its position to smaller $r$ values.

We have a total of 51 different $(m, s)$ combinations at each thermodynamic condition $(\rho^*, T^*)$. We use 26 of them to obtain Eqs. (10), (11) and the other 25 are used to check the accuracy of the method proposed in Section “Molecular dynamics simulations and numerical computations by Method 1”.

We find that all of the 25 $(m, s)$ combinations that are not used to construct the fits at each thermodynamic condition $(\rho^*, T^*)$ can be correctly predicted with no exception. We check that the 26 $(m, s)$ combinations used for fitting can also be correctly predicted in the same manner.

In order to clearly show the difference between the 1st best candidate and the 2nd best candidate in each case, we have presented the results in Table 1, in which the number of combinations in different $R = x_2^f/x_2^*$ ranges are established, where $x_2^f$ is the error obtained for the 1st best candidate, $x_2^*$ the one for the 2nd best candidate, with the definition of $x_2$ in Eq. (12). For each density, $R > 2$ holds for more than 50 $(m, s)$ combinations, and $R > 4$ for more than 47 combinations. Thus, the 1st candidate can be easily distinguished from the 2nd candidate.

In short, the correct $(m, s)$ combination can be easily obtained by simply fitting two main characteristic values of the RDF with an accuracy of 100%.

Table 1

<table>
<thead>
<tr>
<th>$\rho^*$</th>
<th>$R &gt; 2$</th>
<th>$R &gt; 4$</th>
<th>All</th>
</tr>
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<tbody>
<tr>
<td>0.8</td>
<td>51</td>
<td>51</td>
<td>51</td>
</tr>
<tr>
<td>0.9</td>
<td>51</td>
<td>51</td>
<td>51</td>
</tr>
<tr>
<td>1.0</td>
<td>51</td>
<td>51</td>
<td>51</td>
</tr>
<tr>
<td>1.1</td>
<td>50</td>
<td>50</td>
<td>51</td>
</tr>
<tr>
<td>1.2</td>
<td>51</td>
<td>48</td>
<td>51</td>
</tr>
<tr>
<td>1.3</td>
<td>50</td>
<td>47</td>
<td>51</td>
</tr>
</tbody>
</table>

In conclusion, we have validated a simple idea to measure pairwise interactions from simulation data is needed, although it of course does not offer a complete general solution.

In this paper, we established a simple connection between the characteristics of the first peak of the radial distribution function and the exponents of the Mie potential interaction for well-equilibrated configurations. Given a number of snapshots taken from an equilibrated ensemble created via the Mie potential with unknown exponents, we can directly determine the values of the exponents $(m, s)$ with excellent accuracy. This work offers two simple ways to determine the pairwise interaction by only using configuration snapshots, which are easily obtained in numerical simulations or experiments. Therefore, our strategy considerably simplifies the general inverse problem where a determination of the pair potential from simulation data is needed.

Conclusion

In this paper, we established a simple connection between the characteristics of the first peak of the radial distribution function and the exponents of the Mie potential interaction for well-equilibrated configurations. Given a number of snapshots taken from an equilibrated ensemble created via the Mie potential with unknown exponents, we can directly determine the values of the exponents $(m, s)$ with excellent accuracy. This work offers two simple ways to determine the pairwise interaction by only using configuration snapshots, which are easily obtained in numerical simulations or experiments. Therefore, our strategy considerably simplifies the general inverse problem where a determination of the pair potential from simulation data is needed, although it of course does not offer a complete general solution.

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a set of equilibrium configurations for a new system with unknown potential. In Method 2, an artificial neural network is trained at each density by using half of the samples, and the remaining samples are correctly predicted with an accuracy of 100% by the model, when the predicted \((m, n)\) are transformed into integer values. Both methods support the idea that easy and directly determinations of the pairwise interaction can be obtained by only using equilibrium snapshots. This idea can be readily extended to multicomponent systems, and will be valuable in both fundamental and applied research. This idea can also be applied to fundamental investigations of many-body interactions, such as coarse-grained pair potentials \([27,43,44]\) in multiscale simulations of complex fluids and biological systems and polymer systems. The extension to any possible pairwise potential interaction such as the Yukawa potential are in progress.

CRediT authorship contribution statement

Jianxiang Tian: MD simulations, Data curation, Writing – original draft, Writing – review & editing. Ludovic Berthier: MD simulations, Data curation, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Supplementary data

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References