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A ground state Monte Carlo approach for study of dipolar systems with rotational degrees of freedom

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Abstract We have developed a path integral ground state Monte Carlo (PIGSMC) algorithm for quantum simulation of rotating dipolar molecules, using a highly accurate sixth-order algorithm. The method allows us to calculate unbiased estimates of ground state properties of dipolar molecules in a variety of geometries, with or without an external electric field. To demonstrate the capability of the approach, we calculate the orientational phase diagram of a one dimensional lattice system of rotating point dipoles in the absence of any external electric fields. We find that for finite lattice size, this system exhibits an order-disorder transition at finite dipolar interaction strength in contrast to the well-known orientational disorder of the corresponding one dimensional $O(3)$ quantum rotor models. Comparison of the quantum Monte Carlo results with a self-consistent field estimate of the phase transition shows the emergence of an ordered phase at non-zero dipolar strength, confirming the symmetry breaking role of the anisotropic dipole-dipole interaction.

1 Introduction

Ultracold molecules with a permanent electric dipole moment represent a potentially rich avenue for exploring many body physics. The interactions between molecules are dominated by the long ranged, anisotropic dipole-dipole interaction. Lattice systems of molecules, for example systems of dipoles in deep optical

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lattices of various geometries, have been suggested as means of realizing topo-
logical phases[1,2]. A number of theoretical studies have addressed the stability of
dipolar condensates of polarized dipoles in various geometries, using a variety of
methods[3,4,5]. However virtually all papers on dipolar condensates have assumed
the presence of strong external fields to orient the molecules and effectively sup-
press the rotational degrees of freedom, while the analyses of dipolar molecules
trapped in optical lattices typically operate in a regime where translational motion
is negligible[1]. The current work presents the first stage of a systematic analysis of
the phase diagrams of such trapped dipolar condensates, addressing the possibil-
ity of observing quantum phase transitions in these systems that are specifically
due to the orientational degrees of freedom. Our approach is to use a path inte-
gral ground state Monte Carlo (PIGSMC) method to simulate ensembles of dipo-
lar molecules. This method has the advantage over previously employed Monte
Carlo methods that with it we are able to calculate estimates for diagonal as well
as off-diagonal observables without introducing any bias due to the choice of trial
wavefunction employed. In the following, we summarize the general PIGSMC al-
gorithm, including how we achieve an accurracy of sixth order in the time step.
We then present first results for a model problem that demonstrates the capability
of the approach to capture novel orientational phase transitions of lattice-localized
dipolar molecules that result from the anisotropic nature of the dipolar interaction.

2 Method

In order to systematically study the effect of molecular rotation on the phases of
trapped dipolar molecules in a wide variety of situations (e.g., magneto-optical
traps, optical lattices, low temperature solid or plastic crystalline phases), we have
adapted the PIGSMC approach[7] to the study of molecules possessing both trans-
lational and rotational degrees of freedom. PIGSMC has been previously applied
to continuous systems with translational degrees of freedom only. We describe
the general PIGSMC approach for these systems here, although the first appli-
cation described in this work will be restricted to orientational phases of dipolar
molecules fixed on a lattice *i.e.* neglecting translational degrees of freedom. We
assume a Hamiltonian of the form $\hat{H} = \hat{T} + V(\mathbf{R})$ where T is the total kinetic en-
ergy operator of N particles and V is the potential energy between the N particles,
$V(\mathbf{R}) = \langle \mathbf{R}|V(\hat{R})|\mathbf{R}\rangle$, which depends on the coordinates for all degrees of freedom
of the system, i.e., $\mathbf{R}$, including rotational and (if present) translational degrees of
freedom. The PIGSMC method makes use of the fact that any trial state for a sys-
tem of N particles, $|\Psi_T\rangle$, with non-zero overlap with the true ground-state, $|\Psi_0\rangle$,
will decay to the ground state (ignoring normalization) under evolution in imagi-
nary time ($\tau = it/\hbar$)

$$|\Psi_0\rangle \propto \lim_{\varepsilon \to \infty} e^{-\varepsilon \hat{H}}|\Psi_T\rangle. \tag{1}$$

Approximations of ground state expectation values can be expressed in terms of
the imaginary time propagator and the trial state

$$\langle \hat{O} \rangle = \frac{\langle \Psi_T|e^{-\beta \hat{H}/2}\hat{O}e^{-\beta \hat{H}/2}|\Psi_T\rangle}{\langle \Psi_T|e^{-\beta \hat{H}}|\Psi_T\rangle}, \tag{2}$$

for sufficiently long imaginary time β. The ground state wavefunction is then related to the trial wavefunction through the relationship (ignoring normalization)

$$\Psi_0(\mathbf{R}) = \int d\mathbf{R}'\, G(\mathbf{R},\mathbf{R}';\beta/2)\Psi_T(\mathbf{R}'), \tag{3}$$

where the integration kernel is

$$G(\mathbf{R},\mathbf{R}';\beta/2) = \langle\mathbf{R}|e^{-\beta\hat{H}/2}|\mathbf{R}'\rangle, \tag{4}$$

which is the imaginary time evolution operator in the coordinate representation and

$$\Psi_{T(0)}(\mathbf{R}) = \langle\mathbf{R}|\Psi_{T(0)}\rangle \tag{5}$$

is the trial (ground state) wavefunction. This allows us to write down the general expectation value (assuming $\Psi_T(\mathbf{R})$ is real)

$$\langle\hat{O}\rangle = \int d\mathbf{R}_1\, d\mathbf{R}_2\, d\mathbf{R}_2'\, d\mathbf{R}_3\, \Psi_T(\mathbf{R}_1)G(\mathbf{R}_1,\mathbf{R}_2;\beta/2)$$
$$\times O(\mathbf{R}_2,\mathbf{R}_2')G(\mathbf{R}_2',\mathbf{R}_3;\beta/2)\Psi_T(\mathbf{R}_3). \tag{6}$$

with the coordinate representation of the operator $\hat{O}$

$$O(\mathbf{R},\mathbf{R}') = \langle\mathbf{R}|\hat{O}|\mathbf{R}'\rangle. \tag{7}$$

Here we have allowed for the possibility that the path is broken at the center by including an extra index $\mathbf{R}_2'$. This allows the sampling off-diagonal quantities, *e.g.* for ^{4}He this method has been employed to calculate the off-diagonal elements of the one-body density matrix[8]. In the first application presented below, we employ $\mathbf{R}_2 = \mathbf{R}_2'$ which corresponds to sampling quantities corresponding to operators that are diagonal in the coordinate representation.

Evaluation of the integral in eq. (6) is made possible by the relationship

$$G(\mathbf{R},\mathbf{R}';\beta) = \int d\mathbf{R}''\, G(\mathbf{R},\mathbf{R}'';\beta/2)G(\mathbf{R}'',\mathbf{R}';\beta/2) \tag{8}$$

which allows us to employ approximations to the imaginary time evolution operator valid for short imaginary time by breaking the path into M intervals of length $\tau = \beta/M$. The resulting integral

$$\int d\mathbf{R}_1\, d\mathbf{R}_2\, \ldots\, d\mathbf{R}_M \Psi_T(\mathbf{R}_1)G(\mathbf{R}_1,\mathbf{R}_2;\tau)$$
$$\times G(\mathbf{R}_2,\mathbf{R}_3;\tau)\times\cdots\times G(\mathbf{R}_{M/2-1},\mathbf{R}_{M/2};\tau)O(\mathbf{R}_{M/2},\mathbf{R}_{M/2}')$$
$$\times G(\mathbf{R}_{M/2}',\mathbf{R}_{M/2+1};\tau)\times\cdots\times G(\mathbf{R}_{M-1},\mathbf{R}_M;\tau)\Psi_T(\mathbf{R}_M) \tag{9}$$

can be evaluated by making the association between the quantum system and a classical linear polymer which can be simulated using standard Metropolis Monte Carlo methods[19].

The above exposition is completely general and applicable to both rotational and translational degrees of freedom, i.e., $\mathbf{R}$ denotes a general set of molecular coordinates. In this first work we focus on the rotational degrees of freedom alone:

extension to analysis of both rotations and translations together will be made in future work. Here we therefore implement an "any order" short time approximation to the imaginary time propagator[11] for the rotational motion of all dipoles. The general expression for this any order propagator for a given Hamiltonian is

$$\hat{G}_{2n}(\tau) = \sum_{i=1}^{n} c_i (\hat{G}_2(\tau/k_i))^{k_i} + O(\tau^{2n+1}) \tag{10}$$

where $\hat{G}_2(\tau)$ is the well known second order propagator

$$\hat{G}_2(\tau) = e^{-\tau V(\hat{R})/2} e^{-\tau \hat{T}} e^{-\tau V(\hat{R})/2}. \tag{11}$$

The coefficients c_i are given by

$$c_i = \prod_{j \neq i} \frac{k_i^2}{k_i^2 - k_j^2} \tag{12}$$

with $\{k_i\} \in \mathbb{Z}$ and can be chosen freely but it is most often convenient to choose a commensurate sequence since then the free particle propagators, $e^{-\tau \hat{T}}$, can be factored out[11]. In the current study we employ a sixth-order implementation of this propagator with $\{k_i\} = \{1, 2, 4\}$, which is given in the coordinate representation by[11]

$$G_6(\mathbf{R}_1, \mathbf{R}_5; 4\tau) = G_0(\mathbf{R}_1, \mathbf{R}_2; \tau) G_0(\mathbf{R}_2, \mathbf{R}_3; \tau) G_0(\mathbf{R}_3, \mathbf{R}_4; \tau) G_0(\mathbf{R}_4, \mathbf{R}_5; \tau)$$
$$\times \left(\frac{64}{45} e^{-\tau(V(\mathbf{R}_1)/2 + V(\mathbf{R}_2) + V(\mathbf{R}_3) + V(\mathbf{R}_4) + V(\mathbf{R}_5)/2)} \right.$$
$$\left. - \frac{4}{9} e^{-\tau(V(\mathbf{R}_1) + 2V(\mathbf{R}_3) + V(\mathbf{R}_5))} + \frac{1}{45} e^{-2\tau(V(\mathbf{R}_1) + V(\mathbf{R}_5))} \right), \tag{13}$$

where $G_0(\mathbf{R}, \mathbf{R}'; \tau)$ is the free particle propagator.

The free rotor imaginary time propagator for a single rigid rotor for an imaginary time interval τ, which forms part of the short time propagator, is well known and given by[10]

$$G_0^{(1)}(\mathbf{n}, \mathbf{n}'; \tau) = \langle \mathbf{n} | e^{-\tau \hat{H}_r} | \mathbf{n}' \rangle = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l(\mathbf{n} \cdot \mathbf{n}') e^{-\tau \hbar^2 Bl(l+1)}, \tag{14}$$

where $\mathbf{n}$ is the orientation of the rotor, $P_l(x)$ are the Legendre Polynomials, and $\hat{H}_r$ is the familiar rigid rotor Hamiltonian $\hat{H}_r = B\hat{L}^2$ in which B is the rotational constant $1/2I$. For greater computational efficiency, the rotational propagator was tabulated on a fine grid at the beginning of the simulation and interpolation between these values was carried out during the simulation. The summation over l was from zero up to a sufficiently large l_{max} which varies with the small time step, τ, but can be experimented with before the simulation until a suitable accuracy is achieved. The free rotor density matrix for a system of N particles is given by the product of single particle density matrices

$$G_0(\Omega, \Omega'; \tau) = \prod_{i=1}^{N} G_0^{(1)}(\mathbf{n}, \mathbf{n}'; \tau) \tag{15}$$

where Ω represents all of the orientational degrees of the N rotors.

The sampling of rotational and translational configurations was accomplished by utilizing methods previously employed in rigid body diffusion Monte Carlo[12] and path integral studies of van der Waals complexes and molecular impurities in helium clusters[13]. We found it convenient to use unit quaternions to sample orientations[12]. Quaternions are the four component analog of complex numbers

$$\mathbf{q} = a + b\hat{i} + c\hat{j} + d\hat{k}, \tag{16}$$

with a non-commutative multiplication rule[14]. A quaternion may be regarded as a combination of a scalar, a, with a 3-vector (b,c,d), leading to a convenient form of representation for rigid body rotations. Thus, a unit quaternion representing a rotation by angle α about the direction $\mathbf{v}$ is given by $\mathbf{q} = \cos(\alpha/2) + \sin(\alpha/2)\mathbf{v}$ which can be translated to a rotation matrix through the relationship[18]

$$\bar{R} = \begin{pmatrix} a^2 + b^2 - c^2 - d^2 & 2bc - 2ad & 2bd + 2ac \\ 2bc + 2ad & a^2 - b^2 + c^2 - d^2 & 2cd - 2ab \\ 2bd - 2ac & 2cd + 2ab & a^2 - b^2 - c^2 + d^2 \end{pmatrix} \tag{17}$$

and then used to transform the orientational vector for a particle. Because rotations about the dipole moment do not change its orientation, the rotational axis $\mathbf{v}$ was constrained to be perpendicular to the orientation $\mathbf{n}$. To prevent redundancies in the transformations, the angle was constrained to lie within the interval $[0, \pi)$ and these angles sampled from a truncated Gaussian distribution

$$P(\alpha) \propto \begin{cases} \dfrac{2}{\sqrt{2\pi\sqrt{2\hbar^2 B\tau}}} e^{-\alpha^2/4\hbar^2 B\tau} & \text{if } 0 \le \alpha < \pi \\ 0 & \text{otherwise.} \end{cases} \tag{18}$$

To increase the efficiency of sampling paths, the well-known multilevel bisection scheme[19] was employed.

In the proof of principle application shown below, the focus is on orientational ordering of dipoles fixed at points of a regular lattice in one dimension. To demonstrate the power of this method for simulating strongly interacting systems when high quality trial wavefunctions are not available we employed a constant trial wavefunction ($\Psi_T(\mathbf{R}) = 1$) which is equivalent to the wavefunction for a set of dipoles in their ground rotational states (s-state) and is the exact ground state wavefunction in both the limit when the dipolar interaction goes to zero and when the molecular rotation constant goes to infinity. We note that it is possible to obtain accurate results with constant trial wavefunctions also for problems involving translational degrees of freedom[8,9] and we therefore expect the PIGSMC method to be useful even when good trial wavefunctions are difficult to obtain, as is expected to be the case when systems with both translational and rotational degrees of freedom must be considered on equal footing.

3 Application to orientational ordering transitions

In the current application we consider a model in which three dimensional dipoles are fixed on a one dimensional lattice oriented along $\mathbf{x}$, without any external field.

The Hamiltonian describing this system of N dipoles in the absence of an external aligning field is

$$\hat{H} = B \sum_{i=1}^{N} \hat{L}_i^2 + \frac{C_{dd}}{4\pi} \sum_{j<i} \frac{1}{r_{ij}^3} \left(\hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j - 3(\hat{\mathbf{n}}_i \cdot \hat{\mathbf{r}}_{ij})(\hat{\mathbf{n}}_j \cdot \hat{\mathbf{r}}_{ij}) \right) \tag{19}$$

where $\hat{\mathbf{r}}_{ij}$ is the unit vector pointing along the direction from rotor i to rotor j, $\hat{\mathbf{n}}_i$ is the vector orientation of the dipole moment of rotor i and C_{dd} is the dipole-dipole coupling constant which would be $C_{dd} = d^2/\varepsilon_0$ in the case of diatomic molecules with a permanent electric dipole moment, d being the electric dipole moment of the molecular species under consideration. The ratio

$$g = \frac{C_{dd}}{4\pi\hbar^2 B r_{\text{lat}}^3}, \tag{20}$$

where r_{lat} is the nearest neighbor lattice spacing, provides a measure of the interaction strength and will be used to scale the relative contributions of potential and kinetic terms. Since these dipoles are three-dimensional, each $\hat{\mathbf{n}}_i$ is a three component vector. This model is thus a generalization of the well-known $O(3)$ quantum rotor model which, in one dimension, does not possess an ordered phase at any finite value of interaction strength[15]. In the model under consideration in this work the $O(3)$ symmetry of the rotors has been broken by the anisotropic component of the interaction term (the last term in eq. (19), which favors "head-to-tail" orientation of the dipoles. It has been shown that the replacement of the nearest neighbor interaction with an interaction which scales as $1/r^3$ in the $O(3)$ quantum rotor does not significantly impact the phase diagram of such a system in one dimension[6]. Consequently any new physics we may find from eq. (19) will be solely attributable to the anisotropy of the dipole-dipole interaction potential.

It is also useful to compare this dipolar lattice model with the quantum Ising model, i.e., the Ising model in a transverse field, since the symmetry broken ground states of both of these models are related through a $\mathbb{Z}_2$ symmetry[15]. The quantum Ising model in one dimension has a second order phase transition between a paramagnetic phase and a phase with long range magnetic order, at a finite value of the interaction strength.

4 Results

The path length, β, for these simulations was 20.0 Hartree^{-1} with a short time step, τ, of 1.32×10^{-1} Hartree^{-1}. The simulation was carried out with a finite number of dipoles, each located at fixed, evenly spaced positions in a periodic box. We employed the nearest image convention for calculating the potential energy of the system. While the dipole-dipole interaction does extend beyond the nearest neighbors we control for this effective cutoff at half the periodic box length by running simulations with system sizes ranging from 6 to 64 dipoles. The behavior of the system depends only upon the value of the dimensionless parameter g and not on any of the individual parameters B, C_{dd}, and r_{lat}. For the purpose of this study, B and r_{lat} were therefore set to convenient values and only C_{dd} was varied.
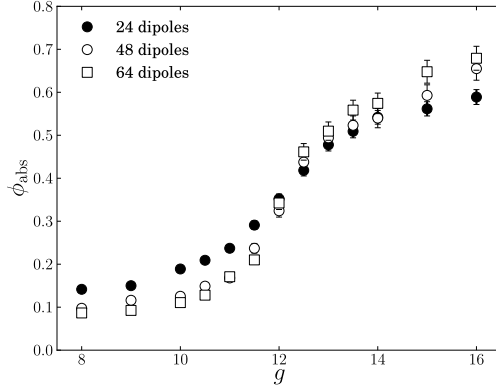
Fig. 1 The order parameter ϕ_{abs} (eq. (22), for a system of rotating dipoles in linear chains of various lengths N, interacting via the dipole-dipole interaction, eq. (19). Note that this measure is always positive and thus statistical fluctuations lead to a small but non-zero value of ϕ_{abs} even when g is zero and the signed order parameter ϕ is statistically zero.

For this model the limit in which the interaction strength is much greater than $\hbar^2 B$ constitutes a classical limit in which the rotational kinetic energy goes to zero. In this classical limit the anisotropic dipole-dipole interaction potential results in a specific ordering with all of the dipoles aligned along **x**. A convenient order parameter characterizing this classical phase is

$$\phi = \left\langle \frac{1}{N} \sum_{i=1}^{N} n_i^x \right\rangle, \tag{21}$$

the average dipolar polarization along the x-axis. ϕ has a maximum magnitude of 1 for an N particle system, corresponding to all dipoles oriented in the same direction, and is equal to zero in the disordered phase (where the expectation value of each of the components of $\hat{\mathbf{n}}_i$ is zero). There are two symmetry related ordered phases, corresponding to all dipoles being oriented along **x** in the positive or negative direction. This results in two possible signed extremal values of ϕ in the ordered phase (1 and -1), and the possibility of spontaneous symmetry breaking. However, since the physics in the two sectors is the same, in order to study the disorder to order transition without regard to the choice of specific direction of order, it is more convenient to evaluate the polarization order parameter ϕ_{abs},

$$\phi_{\text{abs}} = \left\langle \left| \frac{1}{N} \sum_{i=1}^{N} n_i^x \right| \right\rangle, \tag{22}$$

which is always greater than or equal to zero and allows reduction of the statistical error associated with sampling the two equivalent sectors.

The order parameter ϕ_{abs} for our simulations is plotted in Fig. 1. It is evident that for a finite number of dipoles, there is an order-disorder transition between $g = 11.0$ and 12.0. While it is not possible to determine the precise location of
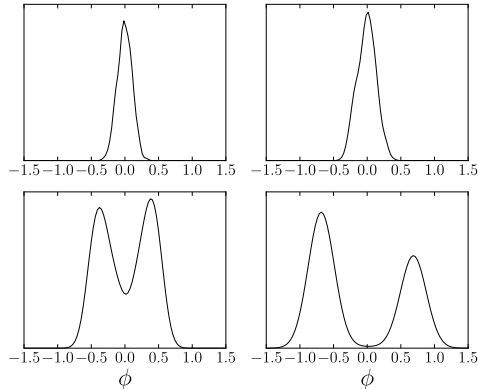
Fig. 2 Gaussian kernel density estimates of the distribution of the order parameter ϕ at $g = 8.0$ (top left), 10.0 (top right), 12.0 (bottom left), and 16.0 (bottom right) for 64 dipoles, with a gaussian bandwidth of $h = 0.2782$. The lack of trimodal distributions and the displacement of the maxima suggests that the finite size phase transition is not a first order transition. Note that the kernel density estimates should be symmetric: the asymmetry seen here derives from the fact that in such a large system the probability of inversion of all dipoles is low so that a very large number of independent simulations are required to achieve full convergence.

this transition in the thermodynamic limit without a more thorough investigation of finite size scaling effects, it is clear from the information available that the transition occurs for a finite value of the interaction strength, in contrast to the behavior of the $O(3)$ quantum rotor model, for which in one dimension there is no phase with long ranged order[15]. More insight into the nature of the phase transition is revealed by analysis of the distribution of the signed order parameter[16] ϕ. Gaussian kernel density estimates[17] are plotted in Fig. 2, displaying a single peak in the disordered phase and two peaks at $\pm|\phi|$. We see no evidence for coexistence between the ordered and disordered phases, which would be signaled by three peaks of changing weight in the distribution of ϕ throughout the transition region. Note that we did not bias the simulation by a trial function that could force the system to stay in one of the two phases. This suggests that the order-disorder transition in these dipolar systems is a higher order phase transition. This comes as no surprise since the broken symmetry ground states are related through $\mathbb{Z}_2$ symmetry akin to the quantum Ising model, which itself possesses a second order phase transition from a disordered paramagnetic state to an ordered ferromagnetic state in one dimension at zero temperature[15]. The asymmetry of the distribution in the symmetry-broken phase is simply a consequence of the fact that Monte Carlo sampling of both ordered phases slows down with increasing system size. In the thermodynamic limit the system is no longer ergodic and may remain in one phase for an indefinite time. This could be easily overcome by introducing a orientation swap move that simultaneously reorients all dipoles in their opposite direction, leading to a symmetric ϕ distribution. However, since the two phases are completely equivalent, there is no need for such a move here.
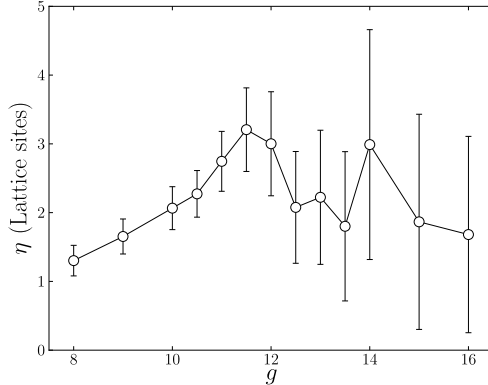
Fig. 3 Correlation length η extracted from exponential decay of $C(r)$, plotted as a function of interaction strength, g, for a system of 64 dipoles. Despite the increasing error bars for large g, a peak near $g = 11.5$ is clearly visible, signaling the phase transition from a disordered phase at low g and an ordered phase at high g.

We have also calculated the spatial correlation function between two dipoles at lattice points x and x'

$$C(|x - x'|) = \langle n^x(x)n^x(x') \rangle - \phi^2. \tag{23}$$

We found that spatial correlations decay approximately exponentially with distance, characterized by a correlation length η. For a higher order phase transition, this correlation length should diverge at the phase transition. Fig. 3 shows the behavior of η for a system of 64 dipoles over a range of interaction strengths g spanning the phase transition: the peak between $g = 11$ and $g = 12$ is consistent with such a divergence, broadened by finite size effects. Fig. 3 also shows that in the ordered phase, the error bars become prohibitively large. In the ordered phase, our trivial choice for the trial wavefunction $\Psi_T(\mathbf{R}) = 1$, corresponding to noninteracting molecules in the rotational ground state, is clearly a poor approximation for the alignment found in the ordered phase. The behavior of the statistical uncertainty for large g therefore suggests that in principle our PIGSMC simulations could be made more efficient by introducing a well-optimized trial wavefunction. However, in this work we deliberately refrained from using a trial wavefunction to demonstrate that the PIGSMC simulations of rotational degrees of freedom are feasible also without a trial wavefunction. This is important for more complicated Hamiltonians, e.g. dipoles on a higher-dimensional lattice, where constructing a trial wavefunction, that is guessing the ordering in the ordered phase, is no longer trivial.

We compare the results of the quantum Monte Carlo simulations with a self-consistent field analysis in which the field-free Hamiltonian was replaced with a single-site Hamiltonian corresponding to non-interacting dipoles in an external field, *i.e.*,

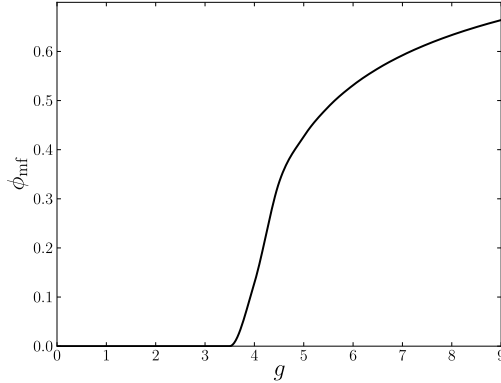$$H_{\mathrm{scf}} = B\sum_i L_i^2 + \sum_i V(\hat{\mathbf{n}}_i) \tag{24}$$

Fig. 4 Orientational order parameter ϕ_{mf}, eq. (21), from mean field analysis for a system of 32 dipoles in a linear chain, calculated with $l_{\max} = 4$. The mean field calculation predicts a phase transition from a disordered phase to an ordered phase at $g = 3.8$ and shows no finite size effects, in contrast to the Monte Carlo simulations.

with self-consistent potential

$$V(\hat{\mathbf{n}}_i) = \frac{C_{dd}}{4\pi} \sum_{j \neq i} \frac{1}{r_{ij}^3} \left(\hat{\mathbf{n}}_i \cdot \left\langle \hat{\mathbf{n}}_j \right\rangle - 3\hat{n}_i^x \left\langle \hat{n}_j^x \right\rangle \right). \qquad (25)$$

$\left\langle \hat{\mathbf{n}}_j \right\rangle$ and hence $V(\hat{\mathbf{n}}_i)$ are determined self consistently by diagonalizing H_{scf} for each rotor in the basis of spherical harmonics with $l \leq l_{\max}$, where $l_{\max}$ is chosen to be sufficiently large. The order parameter eq. (21) is plotted as a function of g in Fig. 4. We see that, in contrast with the location of the phase transition at an interaction strength value g lying between 11.0 and 12.0 that is indicated by the quantum Monte Carlo results, the mean field analysis shows instead a phase transition already at $g_c = 3.8$. As with the classical Ising model in two dimensions (which is isomorphic to the quantum Ising model in one dimension[15]) the mean field analysis captures the qualitative behavior of the phase diagram but underestimates the transition interaction strength because quantum fluctuations are not fully accounted for in the mean field approximation.

5 Conclusions

We have developed a PIGSMC code for the study of systems with rotational degrees of freedom and have demonstrated its use for the study of a system of dipoles at fixed lattice points. While this first application is a relatively simple system, the present analysis clearly reveals the role of the anisotropy of the dipole-dipole interaction in inducing orientational order. We have shown that one dimensional systems of dipoles without translational degrees of freedom and in the absence of an external electric field undergo an order-disorder phase transition. This transition occurs for values of the dimensionless constant g_c near 11.5. Assuming

realistic molecular values of $\hbar B$ on the order of 10 GHz and d on the order of 3 debye would imply that a lattice spacing smaller than 3 nm would be required in order to reach the critical value g_c. While this is outside the current realm of applicability of typical optical lattice experiments, where the optical lattice spacing is on the order of 300 nm so that adjacent dipoles are separated by 300 nm in the case of unit filling[1], when multiple dipoles can inhabit the same lattice site the distances between molecules will necessarily be much smaller and the interaction strength correspondingly much larger. Investigation of this regime for trapped dipolar molecules will require incorporation of translational motion at the same level as the rotational motion, as described in Section 2.

We expect that the PIGSMC method will be useful for further studies of the quantum ground state of dipolar systems, with its ability to calculate in an efficient manner all properties of the ground state of many body dipolar systems whilst sampling rotational degrees of freedom without the need to introduce a trial wavefunction. Another related realm in which this technique might prove useful is in the study of quantum effects in plastic crystalline phases[20]. These are phases of matter in which there is no orientational order but yet there is still translational ordering. Simple classical models of such systems possess a variety of different crystalline phases[21]. Finite temperature quantum Monte Carlo studies have shown that quantum effects are important in orientational ordering phenomena in molecular crystals[10,22]. The study of crystalline systems of dipolar molecules at low temperatures may therefore be expected to reveal a rich phase diagram when subjected to external electric fields.

Generalization of our PIGSMC approach to include both translational and rotational motion is underway. This will allow study of dipolar gases with analysis of translational and rotational degrees of freedom on equal footing. The method can then be used to study high density systems of dipoles with more realistic interaction potentials that accurately model the short range interaction and include higher order multipole contributions.

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