

Cold Molecules in a Synthetic Dimension

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We examine a system of molecules in one real space dimension and one ‘synthetic’ dimension of rotational states. These molecules occupy one real site and can move between rotational states, while also interacting with one another via dipole interactions, or angular momentum exchange between adjacent sites. The system is simulated using a world-line quantum Monte Carlo model to examine a phase change at different dipole interaction strengths for a much larger system size than previously explored. The current status of this ongoing work is described.

I. EXPERIMENTS WITH COLD ATOMS AND MOLECULES

For many years, physicists in the field of atomic, molecular, and optical (AMO) physics have done experiments using cold atoms. These atoms are cooled to nano-kelvin temperatures with laser cooling techniques and used in experiments to probe a variety of fundamental physical phenomena [1]. Cold temperatures allow quantum mechanical properties to dominate the experimental systems. From investigating many body quantum problems, to probing high energy questions in the search for dark matter, such experiments have provided the opportunity for advancement in many fields of physics.

Possibilities for new science also emerge in the frontier of ultra-cold molecules given that molecules are the building blocks for materials [2]. Molecules are more difficult to cool than atoms because of their many more rotational and vibrational degrees of freedom. In the past few years, first diatomic and now polyatomic molecules have been cooled and used to study molecular quantum interactions as well as condensed matter systems.

A. Quantum Simulation

One category of experiments done in AMO is that of quantum simulation. These are experiments in which atoms or molecules are manipulated such that condensed matter systems can be studied through analogous physics. Often, these experiments are done by forming an optical lattice with interfering laser light that represents a crystal structure in a material. An example of this is demonstrated in figure 1 where atoms and their interactions in the optical lattice represent electrons and their interactions within a crystal. In an optical lattice, one can control the amplitude and frequency of the lasers used and thus also the potential in which atoms sit and the spacing between them [1]. Thus, quantum simulation

has an advantage in parameter control over condensed matter experiments when looking at the same system.

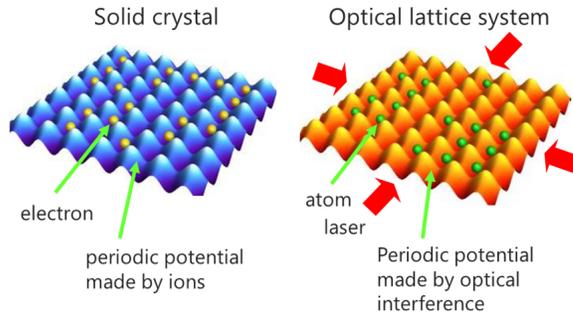


FIG. 1. As pictured here, cold atom systems in optical lattices (right) can be used to simulate condensed matter systems (left). Interfering lasers create a potential landscape in which atoms interact as electrons would in the potential landscape of a crystal. Such a scheme provides direct control over parameters such as lattice spacing and potential depth. *image credit: Kozuma Laboratory, Tokyo Institute of Technology*

One disadvantage when using quantum simulation techniques is that the lattice created is not as large as physical crystal lattices which can be approximated to be infinite. Thus, finite size effects can at times limit the insight that AMO experiments provide.

B. Synthetic Dimensions

Quantum simulations can also be used to study problems not in real space but in different, ‘synthetic’ dimensions, such as momentum space. One or more synthetic dimensions can be used in combination with a real space dimension to actualize a given Hamiltonian. In figure 2, one can see an example of a lattice which uses one synthetic dimension and one real dimension to simulate a two dimensional lattice. Synthetic dimensions can allow an experimental apparatus to simulate experiments with higher dimensionality, and in some cases can allow them to address the problem of finite system size limitations.

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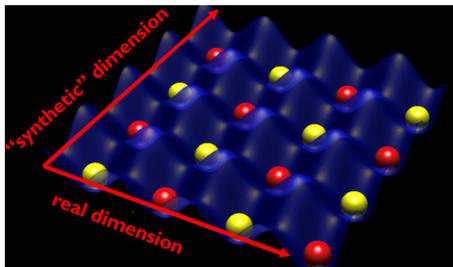


FIG. 2. An example is given of how a synthetic dimension can be used with a real dimension to increase the dimensionality of a system. This ‘synthetic’ dimension can be any parameter useful to the experiment, and so the potential wells in this axis are not in real space. *image adapted from:* Porto Laboratory, Joint Quantum Institute

The use of rotational states in molecules as a synthetic dimension is the focus of this paper. One can use a one-dimensional row of stationary molecules along with their rotational states to create a two-dimensional lattice. Such a system uses the rotational states of molecules for experimental advantage despite the associated disadvantages for molecular cooling. This system addresses system size limitations that plague typical AMO quantum simulations because molecules have hundreds of rotational states.

II. HAMILTONIAN AND EXPECTED DYNAMICS

In a Scientific Reports paper published in 2018 [3] and a Phys Rev A paper in 2019 [4], groups at Rice University and at the University of Illinois at Urbana-Champaign propose a molecule experiment that utilizes one synthetic dimension as shown in figure 3, where t is the strength of the hopping term for a molecule between rotational states in the synthetic dimension, and V is the strength of dipolar interaction, or angular momentum exchange between adjacent molecules. In order to conserve angular momentum, this exchange is restricted to directly swapping rotational states, and for simplicity in addressing these transitions with lasers, it is also restricted to adjacent rotational states.

The system was studied using exact diagonalization techniques, mean field approximation [3], and matrix product state [4]. The Hamiltonian that describes this system of molecules follows.

$$\hat{H} = \sum_{i=0}^{M_{real}-1} \sum_{n=1}^{N_{rot}-1} \left[-t_n \left(\hat{c}_{n-1,i}^\dagger \hat{c}_{n,i} \right) - V_n \left(\hat{c}_{n-1,i}^\dagger \hat{c}_{n,i} \hat{c}_{n,i-1}^\dagger \hat{c}_{n-1,i-1} \right) \right] + h.c. \quad (1)$$

A phase, dubbed ‘quantum string’, was found to emerge when the ratio of V/t was negative or greater

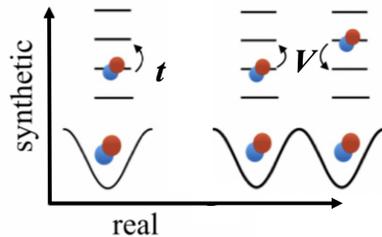


FIG. 3. This image is a visualization of the Hamiltonian in equation 1. There is one molecule per real site, which moves between its synthetic rotational states with hopping term t . Angular momentum can be exchanged with strength V , only by molecules in adjacent real states and adjacent rotational states. *image credit:* [4]

than 2 as seen in figure 4. A similar ‘quantum surface’ is found when extending the proposed lattice to three-dimensions, where two of these are real dimensions, and one is a synthetic dimension of rotational states.

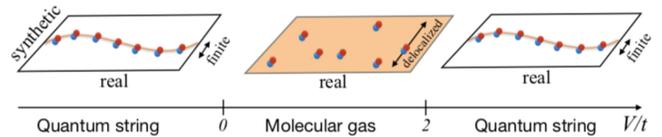


FIG. 4. This figure demonstrates the dependence of the phase on the ratio of V/t . At negative values and large positive values of V/t , a ‘quantum string’ forms, and the dipolar term in the Hamiltonian dominates interactions. *image credit:* [4]

While such current strategies have predicted this phase and looked at particular approximations, the exact system has not been studied for large system sizes because the computation time for exact diagonalization techniques scales as 2^N where N is the number of lattice sites. Thus, the potential of using rotational states in molecules for a synthetic dimension to increase system sizes in AMO experiments has not been fully examined. Quantum Monte Carlo techniques, which will be presented later, scale as N^2 and allow us to study larger system sizes and encompass the potential benefits of such an experiment.

III. EXACT DIAGONALIZATION

While the Hamiltonian in equation 1 has already been studied using exact diagonalization techniques, the same studies are replicated for comparison to quantum Monte Carlo (QMC) calculations. This code will be used to check the QMC code for small system sizes and will also be used to demonstrate the differences between results predicted for phases of different lattice sizes.

In figure 5, the probability for a molecule to occupy

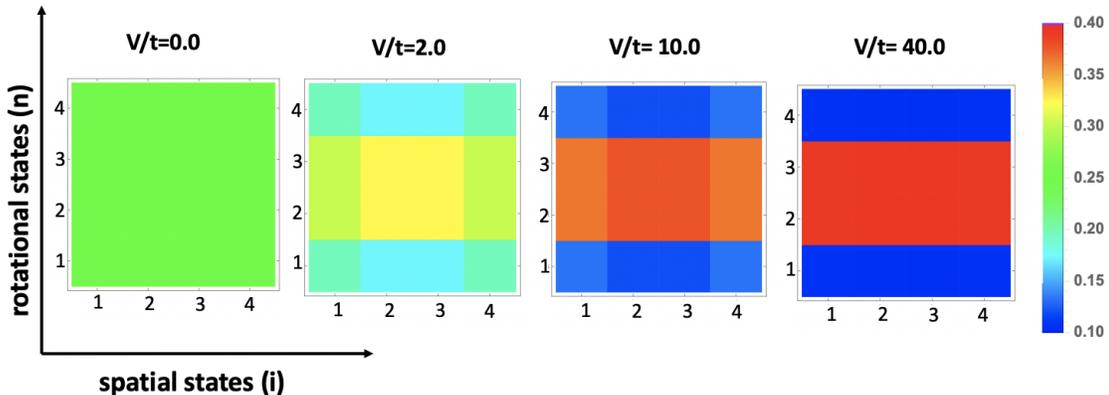


FIG. 5. We use exact diagonalization techniques to demonstrate the occupation probability for increasing values of V/t in a four by four lattice. Warmer colors show a higher probability and cooler colors show a lower probability as indicated in the scale to the right. A two-state-wide ‘quantum string’ is seen to form as values of V/t increase.

each site in a four by four lattice is graphed for different ratios of V/t . One can see a ‘quantum string’, made of two rotational sites, emerging and becoming more pronounced for larger values of V/t as predicted.

IV. MONTE CARLO METHODS

Monte Carlo methods allow us to do what we can call ‘computer experiments’. This emphasizes the idea that the output of a Monte Carlo algorithm replicates properties of a system at thermal equilibrium, and that these methods allow researchers to probe problems that do not have analytic solutions [5]. A Monte Carlo simulation, like nature, provides configurations that we can ‘measure’, where each configuration has a particular probability of occurring. While Monte Carlo methods do incorporate randomness, they have a rigorous mathematical basis which creates rules that, when followed, allow a configuration i to evolve to a configuration j with the correct probability [5]. These rules include ergodicity, which requires a non-zero probability for every configuration to be reached from every other configuration. Another rule requires the algorithm to satisfy ‘detailed balance’, where a probability, T_{ij} , of evolving state i to state j , is chosen such that when a configuration i evolves to a configuration j , it satisfies

$$T_{ji}p_i = T_{ij}p_j \quad (2)$$

where p_n is the probability of a state n . One algorithm that obeys these rules is the Metropolis algorithm, which is used in the rest of this paper. The Metropolis algorithm accepts a change of configuration from i to j with probability one if $p_j/p_i > 1$ and with probability p_j/p_i if $p_j/p_i < 1$.

A. Monte Carlo Steps

In practice, the steps in a Monte Carlo simulation take the current configuration, and suggest a change to that configuration. This change is either accepted or rejected according to an algorithm which satisfies the rules discussed in the previous section. This process is repeated until equilibrium is reached, and then measurements can be made of desired quantities.

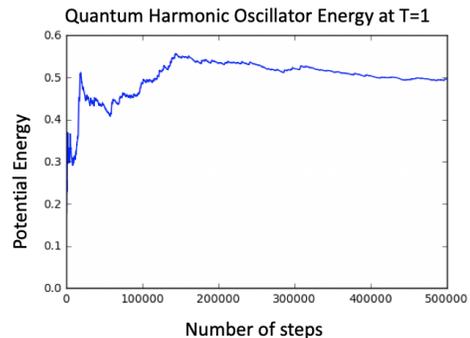


FIG. 6. The measurement is presented from a quantum Monte Carlo algorithm for the potential energy of a quantum harmonic oscillator for up to 500,000 steps. One can visualize here how a Monte Carlo simulation reaches equilibrium.

In figure 6, one can see a Monte Carlo simulation for the potential energy of a quantum harmonic oscillator, which begins at an arbitrary energy value and then takes steps until it nears equilibrium beginning around 200,000 steps. As is visible in this graph, this is not a monotonic process. After around 200,000 steps, one could measure the system and take an average of measurements in order to obtain a predicted value for the potential energy.

B. Quantum Monte Carlo

In order to address quantum mechanical systems with classical Monte Carlo methods, one must map an n dimensional quantum problem to an $n+1$ dimensional classical problem [6]. The formalism that allows for this mapping comes from Feynman's path integral formulation of quantum mechanics which provides a connection to classical statistical mechanics [6]. This formulation of quantum mechanics describes a particle as sampling all possible paths when traveling between two locations in time and space, and generalizes the classical use of action. Using tools provided by a Euclidean or imaginary time approach, one can write the partition function

$$Z = \langle x_f | e^{-H\tau/\hbar} | x_i \rangle \sim \int e^{-S(x)/\hbar} dx \quad (3)$$

where $S(x)$ can be written as

$$S = \int_0^T d\tau \left(\frac{1}{2} m_0 \left[\frac{dx}{d\tau} \right]^2 + V(x) \right). \quad (4)$$

Here, imaginary time $\tau = it$, where t is classical time. We see that this integral sums over imaginary time which is equivalent to inverse temperature. Quantum Monte Carlo simulations are performed at a finite temperature T corresponding to a finite β . Paths are sampled in imaginary time with different probabilities for each path. After many iterations, an equilibrium state is reached and pertinent quantities can be measured.

1. World-line Quantum Monte Carlo

For bosonic systems, there is a direct generalization from Monte Carlo simulations to quantum Monte Carlo systems as described above. However, the anti-commutative nature of fermionic operators complicates quantum Monte Carlo for fermionic systems [7]. Here we focus on World-line quantum Monte Carlo (WLQMC), a method that addresses this problem particularly for Hamiltonians in one real dimension and one imaginary time dimension.

WLQMC requires splitting the Hamiltonian that is being studied into commuting pieces that sum to the full Hamiltonian. Thus, if different pieces of the Hamiltonian act on a fermionic world-line at different time steps, a Hamiltonian that is split into two pieces can be represented as a checkerboard, demonstrated in figure 7. Shaded squares determine areas in which fermions can interact in space and time on each time slice [7]. As a result, when moves are made to sample different configurations, or when equivalently, world-lines are 'pulled', world-lines can diagonally cross shaded squares but remain on the edge of unshaded squares. The probability for a move to be made is the product of the four matrix elements corresponding to the populations of the pertinent

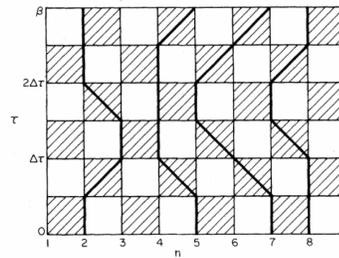


FIG. 7. Here, a world-line quantum Monte Carlo algorithm is visualized. The vertical axis, τ , represents inverse temperature and the horizontal axis, n , represents spatial steps. The shaded squares represent two commuting pieces of a Hamiltonian in one real dimension and one time dimension. The bold lines represent fermionic 'world-lines' which are pulled across white squares to sample all paths. *image credit:[7]*

square in the checkerboard. Sampling different configurations according to these rules allows for every configuration to be reached, and each path to contribute to the weighted sum. Thus, an equilibrium can be reached.

V. WLQMC FOR MOLECULES IN ROTATIONAL STATES

We used WLQMC to examine the Hamiltonian presented in equation 1, describing molecules in one spatial dimension and one synthetic dimension of rotational states. As previously explained, WLQMC is most used for fermionic systems whose world-lines can be represented in one real space dimension, and one inverse temperature dimension. At first glance, this criterion does not seem to apply to the Hamiltonian. However, each molecule only occupies one position in real space and cannot exchange location. This allows us to draw individual checkerboards for each molecule which can move only between rotational sites. Thus, the world-line for each molecule remains in a separate rotational space-inverse temperature plane even as it is pulled to sample all configurations.

As described in the previous section, the Hamiltonian was split into commuting parts. In this case, due to the angular momentum exchange available between molecules in adjacent sites, the Hamiltonian was split into the following four pieces, where we define $\frac{H_{i,n}}{2} = -\frac{t_n}{2} (\hat{c}_{n-1,i}^\dagger \hat{c}_{n,i}) - \frac{V_n}{2} (\hat{c}_{n-1,i}^\dagger \hat{c}_{n,i} \hat{c}_{n,i-1}^\dagger \hat{c}_{n-1,i-1}) + h.c.$

$$\hat{H}_1 = \sum_{i \text{ odd}} \sum_{n \text{ odd}} \frac{H_{i,n}}{2}$$

$$\hat{H}_2 = \sum_{i \text{ odd}} \sum_{n \text{ even}} \frac{H_{i,n}}{2}$$

$$\hat{H}_3 = \sum_{i \text{ even}} \sum_{n \text{ odd}} \frac{H_{i,n}}{2}$$

$$\hat{H}_4 = \sum_{i \text{ even}} \sum_{n \text{ even}} \frac{H_{i,n}}{2}$$

We note that $\hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \hat{H}_4 = \hat{H}$, as is necessary, and that each piece commutes with the others. For each molecule, its world-line moves in a checkerboard (figure 8) made of the four pieces of the Hamiltonian, where the fermion can interact on shaded squares but not on unshaded squares. Although the checkerboard for each

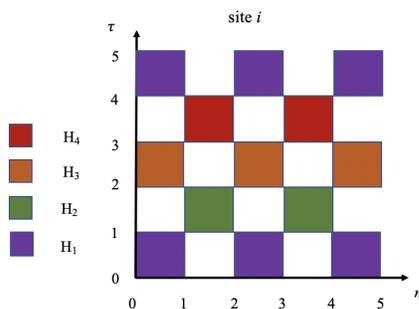


FIG. 8. Checkerboard for a single spatial site, which will contain one world-line, or one molecule. Here, n represents rotational states, and τ represents imaginary time steps.

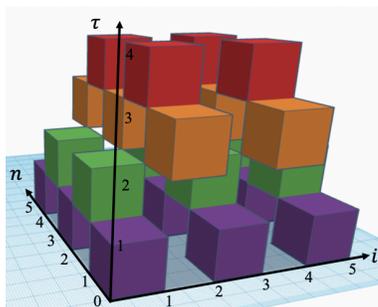


FIG. 9. Commuting pieces of the Hamiltonian are depicted in 3D where n is rotational states, i is spatial states, and τ is imaginary time slices. The colors corresponding to \hat{H}_m are determined by the key in figure 8. Fermionic world-lines are confined to slices in the real space i direction and can only exchange angular momentum with whichever molecule may share the adjacent box corresponding to the given time slice.

molecule appears identical, and each molecule remains in one spatial site, the dipolar term does connect adjacent molecules. Therefore, for example, \hat{H}_1 may connect site

i to site $i - 1$, but then it will connect another site j to site $j + 1$ depending on the parity of the state. As a result, the slices that confine the molecules form boxes which one can depict in three dimensions as in figure 9. While molecules are confined to world-lines on their respective faces, angular momentum can be exchanged between sites connected by a box.

The matrix probabilities, analogous to the T_{ij} in equation 2, for a state to change correspond to the changing occupation on boxes adjacent to the one or two world-lines that move depending on whether the hopping term or the dipolar term acts to reach a new configuration. If only the hopping term acts, only one world-line moves and 4 adjacent boxes are affected. If the dipolar term acts, two world-lines in adjacent sites will move. The two world-lines that switch positions on opposite faces of one box either share 1 or 3 additional adjacent boxes. In this algorithm, therefore, there can be 4, 5, or 7 matrix elements that change with one move. As previously mentioned, each change is accepted or rejected based upon its probability determined by the product of the matrix elements being discussed, using the Metropolis algorithm.

VI. CURRENT STATUS

This is an ongoing project that the author is continuing with Professor Richard Scalettar. Data have not yet been acquired from the WLQMC algorithm, and we are troubleshooting the code. Despite this, results from the exact diagonalization code, such as those for energy at different ratios of V/t in figure 10, promise to be useful for comparison with results to be acquired from the WLQMC code.

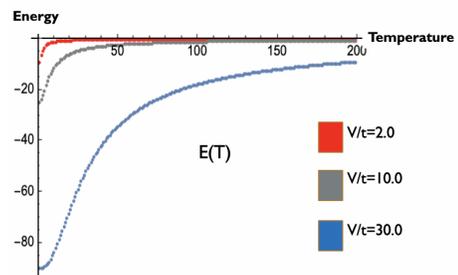


FIG. 10. After the algorithm is completed, we will compare the world-line quantum Monte Carlo results to exact diagonalization results for different lattice sizes and different measured quantities. Pictured here are exact diagonalization results for Energy vs Temperature.

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