Rearranging the Exponential Wall for Large N-Body Systems

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(Received 5 February 2010; published 7 July 2010)

The work required to solve for the fully interacting N boson wave function, which is widely believed to scale exponentially with N, is rearranged so the problem scales order by order in a perturbation series as N^0. The exponential complexity reappears in an exponential scaling with the order of our perturbation series allowing exact analytical calculations for very large N systems through low order.

DOI: 10.1103/PhysRevLett.105.020402 PACS numbers: 03.65.Ge, 02.10.Xm, 31.15.xh, 31.15.xp

Introduction.—Recently it has been shown that the solution to the general quantum mechanical N-body problem, for both fermions [1,2] and bosons [3], is quantum Merlin Arthur (QMA) hard where the complexity class QMA is an extension of the complexity class nondeterministic polynomial time (NP) to the quantum domain [4]. This means that these problems, in the worst case scenarios, are unlikely to have efficient algorithms for their solution even on quantum computers.

In practice, the required resources on a classical computer (computational time, memory, etc) for an essentially exact solution scale exponentially with N [5], the number of particles, often doubling for every particle added. With current numerical resources, this problem ''hits a wall'' around $N = 10$ (within a factor of 2 for systems without symmetry) [6]. This intractability, called the ''exponential wall'', is manifested in various ways depending on the method. For example, the number of basis configurations for modest systems can increase exponentially, yielding matrices for which storage and accurate manipulation are impossible. Exponential behavior can appear in the number of grid points required to describe the quantum wave function. Monte Carlo simulations involving fermions see an exponential growth of the statistical error due to the ''sign problem'' resulting in exponentially long simulation times.

Despite decades of research, no polynomial solution has been found for these problems. Numerous approximations have been proposed in fields such as quantum chemistry, condensed matter, nuclear physics, and atomic physics which try to capture the essential physics while circumventing the exponential N scaling of the exact solution. These methods typically truncate a perturbation series in the case of many-body perturbation theory [7–9] or sample only part of the Hilbert space. Examples of the latter include the correlated basis methods which perform calculations in a subset of correlated states [10,11]. The renormalization group method of Wilson judiciously selects states kept at each iteration [12]. Coupled cluster methods truncate an exact expansion for the wave function in a way that is size-extensive [13]. Monte Carlo simulations are performed in polynomial time for bosons by sampling only the important part of the Hilbert space [14–16]. Density functional methods [6,17,18] use various models to approximate the energy as a functional of the density.

Determining the full quantum wave function, however, is important for understanding and controlling the quantum world which depends on a detailed understanding of the microscopic interactions of quantum particles. The interconnectedness of the quantum world associates with every alternative a complex amplitude—not a probability. This interconnectedness gives rise to the exponential growth of numerical complexity for an exact solution and is responsible for the richness of quantum phenomena such as entanglement (the basis of quantum computing), quantum interferometry (the basis of ultrasensitive detection and a route to quantum control), and superfluidity (which is not yet fully understood on the microscopic level). Approximations in N-body methods must be carefully made to preserve this interesting physics.

While the exponential wall will continue to be scaled by advances in numerical resources, such as the advent of quantum computers [19], it is sensible to ask if analytical mathematical techniques could be used to greater advantage to soften the wall or to reconfigure the problem to shift some of the work into an analytical regime that remains robust as N increases.

Such an approach to solve for a fully-interacting wave function for the N-body problem for identical bosons is being developed [20–22]. This approach, which truncates a perturbation series, uses analytical mathematical techniques, namely, group theory and graphical techniques, to shift work away from numerical computation for a single N to analytical work valid for all N (N is a parameter), and so remains robust as N increases. Despite its analytic nature, this method can obtain an exact solution at each order for a completely general interaction. The series is invariant under the $N!$ operations of a point group isomorphic with the symmetric group S_N. The full quantum N-body problem, as represented by this series, scales as N^0. However, we show in this Letter that the exponential complexity of the problem reappears in an exponential wall that scales with the order of the perturbation series, moving the work from numerical effort that scales expo-

nentially with N to analytic work that scales exponentially with order. Essentially the problem has been restructured so the effort is spent obtaining exact results analytically through low order for all N, rather than obtaining results that approximate the exact solution (i.e. to higher order) for a single N.

The S_N invariant perturbation expansion.—The S_N invariant perturbation expansion is obtained using the inverse spatial dimension, $\delta = 1/D$, as the perturbation parameter. The choice of parameter is important because it leads to a maximally symmetric structure at zeroth order. As $\delta \to 0$, i.e. $D \to \infty$, a system of N particles assumes a structure in which every particle is equidistant and equiangular from every other particle, a maximal symmetry impossible to achieve in lower dimensions. The point group of this configuration is isomorphic with the symmetric group of N particles, S_N; thus the tensor blocks needed at each order in the series must be invariant under the $N!$ operations of this point group. This severe symmetry restriction results in ''small'' finite basis sets that do not grow with N, are complete at each order, and allow for an exact solution at each order using group theory and graphical techniques. As N increases, the group theory and graphical techniques ''hold their own'' resulting in an N^0 scaling. (The basis elements remain invariant under the $N!$ operations of S_N, a number which grows as N grows putting increasing restrictions on the set.) Group theory is used to separate the N scaling problem away from the interaction dynamics allowing the N scaling to be treated as a straight mathematical issue. Once this mathematical work, which involves significant analytical effort, has been completed at a given order, it never has to be repeated again for a new interaction or a different N, i.e., the problem scales as N^0.

The perturbation series is developed by expanding the dimensionally scaled, Jacobian-weighted Hamiltonian, wave function, and energy in powers of $\delta^{1/2}$ to give

$$\bar{H} = \bar{H}_\infty + \delta^{1/2}\bar{H}_{-1} + \delta\sum_{j=0}^{\infty}(\delta^{1/2})^j\bar{H}_j,$$

$$\Phi(\bar{r}_i, \gamma_{ij}) = \sum_{j=0}^{\infty}(\delta^{1/2})^j\Phi_j, \tag{1}$$

$$\bar{E} = \bar{E}_\infty + \delta^{1/2}\bar{E}_{-1} + \delta\sum_{j=0}^{\infty}(\delta^{1/2})^j\bar{E}_j,$$

where

$$\bar{H}_\infty = \bar{E}_\infty, \tag{2}$$

$$\bar{H}_{-1} = \bar{E}_{2n-1} = 0, \tag{3}$$

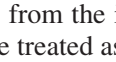
$$\bar{H}_0 = -\tfrac{1}{2}\,{}^{(0)}_{2}G_{\nu_1,\nu_2}\partial_{\bar{y}'_{\nu_1}}\partial_{\bar{y}'_{\nu_2}} + \tfrac{1}{2}\,{}^{(0)}_{2}F_{\nu_1,\nu_2}\bar{y}'_{\nu_1}\bar{y}'_{\nu_2} + {}^{(0)}_{0}F, \tag{4}$$

$$\bar{H}_1 = -\frac{1}{2}\,{}^{(1)}_{3}G_{\nu_1,\nu_2,\nu_3}\bar{y}'_{\nu_1}\partial_{\bar{y}'_{\nu_2}}\partial_{\bar{y}'_{\nu_3}} - \frac{1}{2}\,{}^{(1)}_{1}G_{\nu}\partial_{\bar{y}'_{\nu}} + \frac{1}{3!}\,{}^{(1)}_{3}F_{\nu_1,\nu_2,\nu_3}\bar{y}'_{\nu_1}\bar{y}'_{\nu_2}\bar{y}'_{\nu_3} + {}^{(1)}_{1}F_{\nu}\bar{y}'_{\nu}. \tag{5}$$

The $\bar{y}'$ vectors refer to internal displacement coordinates, $\bar{r}'$ and γ', with γ' the internal displacement angle cosine between two particles; the F tensors involve derivatives of the effective potential while G tensors involve kinetic energy terms. The superprescripts on the $\boldsymbol{F}$ and $\boldsymbol{G}$ tensors denotes the order in $\delta^{1/2}$. The subprescripts denote the rank of the tensors. The indices, ν, run from 1 to $N(N+1)/2$.

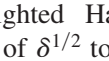
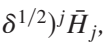
The perturbation equations have been solved exactly for N particles through first order [20–22] using an S_N invariant basis of tensor elements called binary invariants. These tensors have rank R, dimension $[N(N+1)/2]^R$ and are composed of $[N(N+1)/2]^R$ elements, either 1's or 0's planted in the tensor so the tensor is invariant under the $N!$ operations of S_N. The set of binary invariants span the tensor space at each order in the series and thus form a complete basis at each order. Each binary invariant can be represented by an unlabeled multiloop graph (with no unattached vertices). This facilitates the enumeration and determination of this tensor basis [20].

For example, the graphs needed at zeroth and first order for the kinetic energy terms are:

$\mathbb{G}_{rr} = \{$  $\}$, $\mathbb{G}_{\gamma r} = \{$  $\}$, (6)

$\mathbb{G}_{\gamma\gamma} = \{$  $\}$ (7)

$\mathbb{G}_r = \{$  $\}$, $\mathbb{G}_\gamma = \{$  $\}$ (8)

$\mathbb{G}_{rrr} = \{$  $\}$
$\mathbb{G}_{\gamma rr} = \{$ $\}$
$\mathbb{G}_{\gamma\gamma r} = \{$ $\}$
$\mathbb{G}_{\gamma\gamma\gamma} = \{$  $\}$, (9)

grouped according to the number of straight edges (γ) and loop edges (r). Each of the above graphs denotes a binary invariant. Explicit expressions for these binary invariants may be found in an EPAPS document [20]. Proof that the binary invariants are a complete basis at each order can be found in Ref. [21].

Since the Hamiltonian, $\bar{H}_0$, of the lowest-order wave function has the form of an $[N(N+1)/2]$-dimensional coupled harmonic oscillator, it may be solved by transforming to normal modes using the FG method familiar from quantum chemistry [23]. The normal modes transform under irreducible representations (irreps.) of S_N, and thus the frequencies are highly degenerate. For a confined system of N identical bosons, there are just five distinct frequencies and five types of normal modes which will describe the dominant motions if higher-order terms are

not too large. There are two one-dimensional $[N]$ irreps. denoted by $\mathbf{0}^+$, $\mathbf{0}^-$, two $N-1$ dimensional $[N-1,\,1]$ irreps. denoted by $\mathbf{1}^+$, $\mathbf{1}^-$, and one $N(N-3)/2$ dimensional $[N-2,\,2]$ irrep denoted by $\mathbf{2}$.

The higher-order terms in the series are derived using this normal mode basis, $\mathbf{q}'$. Writing the many-body wave function, Φ as

$$\Phi(\mathbf{q}') = (1 + \delta^{1/2}\hat{\Delta}_1 + \delta\hat{\Delta}_2 + \delta^{3/2}\hat{\Delta}_3 + O(\delta^2))\Phi_0(\mathbf{q}'), \tag{10}$$

where Φ_0 is the zeroth-order state, then $\hat{\Delta}_1$ satisfies

$$[\hat{\Delta}_1, \bar{H}_0]\Phi_0 = \bar{H}_1\Phi_0. \tag{11}$$

After applying the linear transformation to normal modes to the higher-order terms in the expansion of $\bar{H}$ in Eq. (1), each of the higher-order terms, $\bar{H}_j$, is a polynomial in the normal modes and their derivatives. Defining G_V and F_V to be the G and F tensors in the normal coordinate basis, the first-order Hamiltonian is

$$\bar{H}_1 = -\frac{1}{2}[{}^{(1)}_{3}G_V]_{\nu_1,\nu_2,\nu_3}\bar{q}'_{\nu_1}\partial_{\bar{q}'_{\nu_2}}\partial_{\bar{q}'_{\nu_3}} - \frac{1}{2}[{}^{(1)}_{1}G_V]_{\nu}\partial_{\bar{q}'_{\nu}} + \frac{1}{3!}[{}^{(1)}_{3}F_V]_{\nu_1,\nu_2,\nu_3}\bar{q}'_{\nu_1}\bar{q}'_{\nu_2}\bar{q}'_{\nu_3} + [{}^{(1)}_{1}F_V]_{\nu}\bar{q}'_{\nu}. \tag{12}$$

To solve Eq. (11), we note that since $\Phi_0(\mathbf{q}')$ is a Gaussian, the derivatives in $\bar{H}_1$ and $\bar{H}_0$ "bring down" normal coordinates from the exponent so that $\bar{H}_1$ effectively becomes a third-order polynomial of only odd powers in $\mathbf{q}'$. Therefore, the first-order many-body wave function is obtained by multiplying the lowest-order wave function by $\hat{\Delta}_1$, a polynomial in $\mathbf{q}'$: $\Phi_1(\mathbf{q}') = (1 + \delta^{1/2}\hat{\Delta}_1)\Phi_0(\mathbf{q}')$.

Exponential growth with order.—Although the number of basis elements does not scale with N, it does grow with increasing order. This growth is a measure of the complexity of the problem. To measure this growth, we need to determine the number of binary invariants as a function of order. Since binary invariants can be represented by graphs, determining the number of binary invariants is equivalent to enumerating the number of unlabeled multiloop graphs that have no unattached vertices (i.e., vertices that do not connect to an edge). While it is not very difficult to determine the number of such graphs at zeroth order (seven graphs) or at first order (25 graphs) by manually drawing possible graphs and throwing out any new candidates that are isomorphic to previous graphs, this task becomes challenging even at second order where there are 79 new graphs.

Research in graphical enumeration has derived generating functions for general graphs on p points with q edges [24–26]. These studies include graphs with isolated vertices that do not correspond to our binary invariants. At a given order, j, the maximum rank, q, of the F and G tensors is $q = j + 2$ corresponding to graphs with $j + 2$ straight or loop edges. The number of vertices can run from 1 to $2q$ as can be confirmed for the graphs in Eq. (9). Thus, at each order j, we need to count the number of unlabeled multiloop graphs with $q = j + 2$ edges and $p = 1, 2, \ldots, 2q$ attached vertices. A little thought will demonstrate that the number of ways that q lines can be distributed among p unlabeled vertices if $p \geq 2q$ and unattached vertices are allowed (i.e., the graphs of Fulling *et al.*, Ref. [24].) is the same as the sum of graphs with q edges and p vertices as p runs from 1 to $2q$ with no unattached vertices (our case). For example, consider the case of one edge and four vertices ($p = 4$, $q = 1$). There are two graphs to consider:  and  – the same number of one-edge graphs in Eq. (8), which includes all graphs with no isolated vertices for one edge ($q = 1$) and one vertex ($p = 1$) plus the graphs for one edge and two vertices. Thus, we require $p \geq 2q$ and choose $p = 2q$ since Fulling's algorithm is quicker to execute when $p = 2q$. The resulting data are shown in the Table I. When we consider a log plot of the data in Table I, see Fig. 1, the data lie almost exactly along a straight line. A least-squares fit gives: $\log(N_G) = 1.221\,85q - 0.518\,622$, with a residual of only $1.666\,95 \times 10^{-4}$. We conclude that the number of binary invariants scales exponentially with the rank of the tensor implying an exponential scaling with the order of the pertubation series. Thus although we are able to handle arbitrarily large-N systems, we are limited in the order to which we can develop the series. We hit an "exponential complexity wall" with order. If the slope for $\log(N_G)$ were small, then we could develop the series solution to large order, but since the slope is of order unity, deriving low orders is the only practical proposition.

Conclusions.—Without approximations, the required computational resources to effectively solve the quantum N-body problem, either fermions or bosons, scales exponentially with N [5], limiting essentially exact solutions to systems with surprisingly low N [6]. Indeed, it has been shown recently, in the worst case scenarios, the quantum

TABLE I. The number of graphs (= number of binary invariants) vs the number of edges (=rank of tensor).

q (=rank of tensor)	Number of Graphs, $N_{\mathbb{G}}$ (=number of binary invariants)
1	2
2	7
3	23
4	79

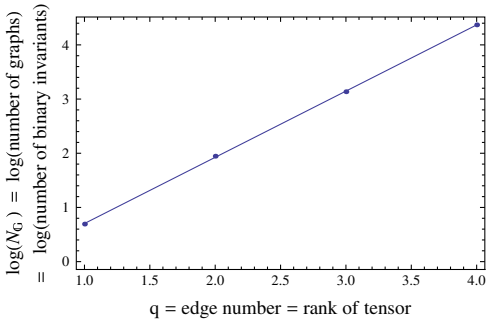


FIG. 1 (color online). log (number of graphs) vs number of edges ≡ log(number of binary invariants) vs rank of tensor.

N-body problem is unlikely to have efficient algorithms for solution even on quantum computers [1–3].

The use of powerful analytic tools such as the group theory of the symmetric group and graphical techniques to tackle the quantum N-body problem is a logical step to take whether numerical resources are sufficient or not. Transferring numerical effort to analytic effort will pay off in stability, efficiency, and in physical intuition.

While the exponential wall will always yield to sufficient symmetry, real quantum systems, of course, do not in general possess enough symmetry to make a big difference. Our method forces maximal symmetry by using a perturbation series that is invariant under $N!$ operations of the S_N group. The S_N group does the "heavy lifting" to allow a direct transformation from microscopic two-body interactions to the macroscopic motions of the normal modes regardless of the strength of the interaction. The rearrangement of the exponential wall described in this paper opens up the possibility of exact analytic solutions for large N systems through low order and thus could be an important route for obtaining an understanding of the microscopic basis for the behavior of large N systems.

We gratefully acknowledge continued support from ARO.

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