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THE RANDOM BATCH METHOD FOR N-BODY QUANTUM DYNAMICS*

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Abstract

This paper discusses a numerical method for computing the evolution of large interacting system of quantum particles. The idea of the random batch method is to replace the total interaction of each particle with the $N-1$ other particles by the interaction with $p \ll N$ particles chosen at random at each time step, multiplied by $(N-1)/p$. This reduces the computational cost of computing the interaction potential per time step from $O(N^2)$ to $O(N)$. For simplicity, we consider only in this work the case $p = 1$ — in other words, we assume that N is even, and that at each time step, the N particles are organized in $N/2$ pairs, with a random reshuffling of the pairs at the beginning of each time step. We obtain a convergence estimate for the Wigner transform of the single-particle reduced density matrix of the particle system at time t that is both uniform in $N > 1$ and independent of the Planck constant $\hbar$. The key idea is to use a new type of distance on the set of quantum states that is reminiscent of the Wasserstein distance of exponent 1 (or Monge-Kantorovich-Rubinstein distance) on the set of Borel probability measures on $\mathbf{R}^d$ used in the context of optimal transport.

Mathematics subject classification: 82C10, 82C22 (65M75).
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1. Introduction

Consider the quantum Hamiltonian for N identical particles with unit mass located at positions $x_1, \cdots, x_N \in \mathbf{R}^d$:

$$\mathcal{H}_N := \sum_{m=1}^{N} -\frac{1}{2}\hbar^2 \Delta_{x_m} + \frac{1}{N-1} \sum_{1 \le l < n \le N} V(x_l - x_n)\,, \tag{1.1}$$

where $\hbar$ is the reduced Planck constant. The N- particles in this system interact via a binary (real-valued) potential V assumed to be even, bounded and sufficiently regular (at least of class

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$C^{1,1}$ on $\mathbf{R}^d$). The coupling constant $\frac{1}{N-1}$ is chosen in order to balance the summations in the kinetic energy (involving N terms) and in the potential energy (involving $\frac{1}{2}N(N-1)$ terms).

We seek to compute the solution $\Psi_N \equiv \Psi_N(t,x_1,\cdots,x_N) \in \mathbf{C}$ of the Schrödinger equation

$$i\hbar\partial_t\Psi_N(t,x_1,\cdots,x_N) = \mathcal{H}_N\Psi_N(t,x_1,\cdots,x_N)\,, \quad \Psi_N\big|_{t=0} = \Psi_N^{in} \tag{1.2}$$

where $t \geq 0$ is the time while $x_m \in \mathbf{R}^d$ is the position of the mth particle. When solving (1.2), the computation is exceedingly expensive due to the smallness of $\hbar$ which demands small time steps Δt and small mesh sizes of order $\hbar$ for the convergence of the numerical scheme, due to the oscillation in the wave function Ψ_N with frequency of order $1/\hbar$ (see [2,18]). On top of this, any numerical scheme for (1.2) requires computing, at each time step, the sum of the interaction potential for each particle pair in the N-particle system, i.e. the sum of $\frac{1}{2}N(N-1)$ terms. For large values of N, the cost of this computation, which is of order $O(N^2)$, may become significant at each time step. The purpose of the Random Batch Method (RBM) described below is precisely to reduce significantly the computational cost of computing the interacting potential from $O(N^2)$ to $O(N)$.

Throughout this paper, we assume for simplicity that $N \geq 2$ is an even integer. Let $\sigma_1,\sigma_2,\cdots,\sigma_j,\cdots$ be a random sequence of mutually independent permutations distributed uniformly in $\mathfrak{S}_N$. Each permutation $\sigma \in \mathfrak{S}_N$ defines a partition of $\{1,\cdots,N\}$ into $N/2$ batches of two indices (pairs) as follows:

$$\{1,\cdots,N\} = \coprod_{k=1}^{N/2}\{\sigma(2k-1),\sigma(2k)\}.$$

Pick a time step $\Delta t > 0$, set

$$\mathbf{T}_t(l,n) := \begin{cases} 1 & \text{if } \{l,n\} = \left\{\sigma_{[\frac{t}{\Delta t}]+1}(2k-1),\sigma_{[\frac{t}{\Delta t}]+1}(2k)\right\} \text{ for some } k = 1,\cdots,\dfrac{N}{2}\,, \\ 0 & \text{otherwise,} \end{cases}$$

and consider the time-dependent Hamiltonian

$$\mathcal{H}_N(t) := \sum_{m=1}^{N} -\frac{1}{2}\hbar^2\Delta_{x_m} + \sum_{1\leq l<n\leq N}\mathbf{T}_t(l,n)V(x_l-x_n). \tag{1.3}$$

In other words, at each time step, the particle labels $m = 1,\cdots,N$ are reshuffled randomly, then grouped pairwisely, and the potential applied to the mth particle by the system of $N-1$ other particles is replaced with the interaction potential of that particle with the other — *only one in this case* — particle in the same group (batch).

The motivation of the RBM is that the computation of the solution $\widetilde{\Psi}_N \in \mathbf{C}$ of the time-dependent, random batch Schrödinger equation

$$i\hbar\partial_t\widetilde{\Psi}_N(t,x_1,\cdots,x_N) = \mathcal{H}_N(t)\widetilde{\Psi}_N(t,x_1,\cdots,x_N)\,, \quad \widetilde{\Psi}_N\big|_{t=0} = \widetilde{\Psi}_N^{in} \tag{1.4}$$

is much less costly than computing the solution Ψ_N of the N-body Schrödinger (1.2) for large values of N. Clearly, for each time step the cost of computing the interaction potential is reduced from $O(N^2)$ to $O(N)$. We remark that the computational cost of reshuffling the N labels is $O(N)$ by Durstenfeld's algorithm [11]. Of course, one needs to prove that (1.4) is a "good approximation of Ψ_N" for a sufficiently small time-step Δt.

Our goal in the present paper is to show that the RBM converges in some sense as $\Delta t \to 0$, with an error estimate that is both

(a) independent of N, and

(b) uniform in $\hbar \in (0,1)$.