Qubit Lattice Approximation of some Quantum and Classical Physics Problems

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1 QLA for Nonlinear Schrodinger Equation

It is expected that quantum computers can provide exponential speedup over classical supercomputers for the solution of certain physics problems. We have been investigating the Qubit Lattice Approximation (QLA) for classical soliton collisions, for 2D and 3D quantum turbulence, and more recently for electromagnetic wave propagation in dielectric media. The QLA consists of a sequence of interleaved collision-streaming operators acting on a qubit set distributed on a lattice. The collision operators locally entangle the qubits at that particular lattice site, while the streaming operators move this entanglement throughout the lattice. The operators are so chosen that this discrete QLA will asymptotically converge to the desired continuum partial differential equations to second order in the lattice spacing Δx, as $\Delta x \to 0$.

We first applied the QLA to the propagation of soliton solutions to the Nonlinear Schrodinger equation (NLS) in 1D:

$$i\frac{\partial \psi}{\partial t} = \left(-\frac{\partial^2}{\partial x^2} + V + g|\psi|^2\right)\psi \tag{1}$$

where V is some external potential. Two qubits q_1, q_2 were introduced at each lattice site so that the wave function $\psi = q_1 + q_2$. The initial choice of the collision operator was the unitary $\sqrt{SWAP}$ matrix

$$\hat{C} = \frac{1}{2}\begin{bmatrix} 1-i & 1+i \\ 1+i & 1-i \end{bmatrix} \tag{2}$$

since $\hat{C}^4 = \hat{I}$, the identity operator. With the collision operator interleaving with the unitary streaming operator that shifts one qubit $+\Delta x$ and then after applying the collision operator a shift $-\Delta x$, we consider the unitary sequence with the streaming operator acting only on the first qubit q_1 :

$$\hat{L}_1 = \hat{C}\hat{S}_{1+}.\hat{C}\hat{S}_{1-}.\hat{C}\hat{S}_{1+}.\hat{C}\hat{S}_{1-} \tag{3}$$

One notes that if the unitary streaming and collision operators commuted then $\hat{L}_1 = \hat{I}$, the identity operator. Thus the non-trivial physics arises from the non-commutation of $\hat{C}$ and $\hat{S}_1$. Similarly for the unitary collision operator $\hat{C}$ interleaved with the corresponding streaming operator $\hat{S}_2$ acting on qubit q_2. By symmetrization, the QLA scheme becomes second order in Δx^2:

$$\hat{L}_{total} = \hat{L}_2^2.\hat{L}_1^2 \tag{4}$$

This scheme will recover the differential operators in the 1D NLS : $i\partial/\partial t$ and $\partial^2/\partial x^2$ under diffusion ordering $\Delta t = \Delta x^2 = O(\epsilon^2)$. To recover the nonlinear term $g|\psi|^2$ and any external potential V one can simply introduce the corresponding exponential operator so that the final second order discrete QLA for the 1D NLS, Eq. (1) is simply

$$\begin{bmatrix} q_1(t+\Delta t) \\ q_2(t+\Delta t) \end{bmatrix} = Exp\left[-\frac{1}{2}\epsilon^2(V+g|\psi|^2)\right]\hat{I}_{2\times 2}.\hat{L}_2^2.Exp\left[-\frac{1}{2}\epsilon^2(V+g|\psi|^2)\right]\hat{I}_{2\times 2}.\hat{L}_1^2.\begin{bmatrix} q_1(t) \\ q_2(t) \end{bmatrix} \tag{5}$$

Unfortunately this exponential QLA representation breaks overall unitarity of the algorithm. However if one resorts to the following unitary collision operator

$$\hat{C}_{unit} = \begin{bmatrix} cos\,\theta(x) & -i\,sin\,\theta(x) \\ -i\,sin\,\theta(x) & cos\,\theta(x) \end{bmatrix} \tag{6}$$

with (real) $\theta(x)$ defined by

$$\theta(x) = \frac{\pi}{4} - \frac{\epsilon^2}{8}\left[V + g|\psi|^2\right] \tag{7}$$

one recovers a fully unitary QLA for 1D NLS. The extension to 3D NLS is immediate by tensor product in the $y-$ and $z-$ directions. This then permits the examination of quantum turbulence of the ground state wave function of a Bose-Einstein condensate since the Gross-Pitaevski equation is nothing but the 3D NLS equation. Of course, even though we now have a fully unitary QLA it is very difficult to directly encode it on a quantum computer because of the nonlinearity $|\psi|^2$. The no-cloning theorem that one cannot make a copy of a wave function that is unknown puts to rest any easy implementation on a quantum computer. Currently the study of how to incorporate nonlinearities into a linear quantum mechanic framework is a very important research area. On the otherhand, these nonlinear QLA's are ideally parallelized on classical supercomputers since the collision operator acts only on on-site qubits and the streaming operator is simply a shift operation on these entangled qubits. In 2016, the QLA for a spin-1 BEC running on a 5120^3 spatial lattice achieved 1.174 PetaFlops at 94.1% parallel efficiency on 524 288 cores on the IBM $Mira$ supercomputer at Argonne. A classical computer has no problems handling the quadratic noninearity.

2 QLA for Lorenz and Ordinary Differential Equation Systems

In NLS we noticed that the streaming operator gives rise to the continuum spatial derivatives. Hence if we wished to develop a QLA for just time evolving systems, one would need only a suitably chosen collision operator. For example, the Lorenz equations are a set of 3 ordinary differential equations for the time evolution of coupled modes with terms mimicking the Fourier transformed Navier -Stokes equation with its quadratic nonlinearities and viscous damped modes :

$$\frac{dx}{dt} = \sigma(y-x) \quad \frac{dy}{dt} = \rho x - x.z - y \qquad \frac{dz}{dt} = x.y - \beta\, z \tag{8}$$

Clearly the collision operator will be non-unitary because of the dissipative terms. σ, ρ and β are parameters and with suitable choices yields chaotic attractors.

3 QLA for Maxwell Equations in Dielectric Media

Finally we are developing QLA for electromagnetic propagation in dielectric media. One first finds that a simple use of the electric and magnetic fields $\mathbf{E}, \mathbf{H}$ as base variables does not give rise to a unitary system in inhomogeneous media. In particular, if one has a non-Hermitian matrix equation

$$i\frac{\partial \psi}{\partial t} = \hat{D}\psi \quad , \quad \hat{D} \neq \hat{D}^{\dagger} \tag{9}$$

with a quadratically conserved Hermitian operator $\hat{Q} = \hat{Q}^{\dagger}$ with inner product $< \psi|\hat{Q}|\psi >= const.$. then a Dyson map $\hat{\rho}$ exists with $\hat{Q} = \hat{\rho}^{\dagger}.\hat{\rho}$ and wave function $\Phi = \hat{\rho}\psi$ satisfying the explicit Hermitian system

$$i\frac{\partial \Phi}{\partial t} = \hat{\rho}\hat{D}\hat{\rho}^{-1}\Phi \tag{10}$$

This use of a Dyson map does lead theoretically to a unitary representation in terms of the fields $(n_x E_x, n_y E_y, n_z E_z, \mu_o^{1/2}\mathbf{H})$ but finding its implementation in a unitary QLA is not straightforward. $n_x, ...$ are the refractive indices along the principal axes of the tensor dielectric medium.

The QLA simulations for 2D scattering from tensor dielectric objects yielded very interesting results. In particular, if there is a sharp (but continuous) refractive index gradient from the background vacuum then one finds from this initial value simulation strong multiple interference effects from the reflections within the dielectric object. These waves will then be transmitted into the background vacuum region and could be detected.

For dispersive media, the constitutive equations involve convolution integrals. Consider a cold magnetized plasma medium. Working with a vacuum representation permits us to incorporate the plasma inhomogeneities into the source terms for ion and electron conductivity currents $\mathbf{J_{ci}}, \mathbf{J_{ce}}$. The unitary evolution of the 12-vector field $\Phi = \epsilon_0^{-1/2}\left[\epsilon_0\mathbf{E} \quad c^{-1}\mathbf{H} \quad \omega_{pi}^{-1}\mathbf{J}_{ci} \quad \omega_{pe}^{-1}\mathbf{J}_{ce}\right]^T$

$$\Phi(t+\delta t) = Exp\left[-i\delta t\hat{D}_H\right]\Phi(t) \tag{11}$$

where $\hat{D}_H$ is a Hermitian operator and c is the speed of light in vacuum, and ω_{pj} the plasma frequency for ions (i) and electrons (e). This Hermitian operator $\hat{D}_H$ can be split into its Hermitian components

$$\hat{D}_H = \hat{D}_{vac} + \hat{D}_{\omega_{pe}} + \hat{D}_{\omega_{pi}} + \hat{D}_{\omega_{ce}} + \hat{D}_{\omega_{ci}} \tag{12}$$

and one can use the leading order Trotterization on the exponential of this operator sum to finish with a product of individual unitary operators. One could then reduce these large matrices into simpler 2×2 unitary gates for future implementation into a QLA code.

Finally, we comment on how dissipation can be handled using ideas from quantum information science (QIS). Collisions and other dissipative mechanisms will lead to a non-unitary evolution system of equations of the form

$$i\frac{\partial \Phi}{\partial t} = \left[\hat{D}_0 - i\hat{\Gamma}\right]\Phi \quad , \quad \hat{D}_0 = \hat{D}_0^{\dagger} \quad , \quad \hat{\Gamma} = \hat{\Gamma}^{\dagger}. \tag{13}$$

In some simple cases the matrix representation of the collisional terms is diagonal. QIS would view Eq. (13) as referring to an open quantum system S whose density matrix $\rho_S(t)$ evolves through the so-called Kraus operators $\hat{K}_\mu$

$$\rho_S(t) = \sum_\mu \hat{K}_\mu\, \rho_S(0)\hat{K}_\mu^{\dagger} \quad \text{with} \quad \sum_\mu \hat{K}_\mu\, \hat{K}_\mu^{\dagger} = I. \tag{14}$$

Using the leading order Suzuki-Trotter approximation one can separate out the non-unitary term:

$$exp\left[-i\delta t(\hat{D}_0 - i\hat{D}_{diss})\right] = exp\left[-i\delta t\hat{D}_0\right].exp\left[-\delta t\hat{D}_{diss}\right] + O(\delta t^2) \tag{15}$$

Interpreting the classical dissipation as the observable result of the interaction between the quantum represented lossless system and an unspecified environment, we have

$$\rho_{aug}(\delta t) = e^{-i\delta t\hat{D}_0}.\rho_{diss}(t).e^{i\delta t\hat{D}_0} \tag{16}$$

with

$$\rho_{diss}(\delta t) = \hat{K}_0.\rho(0).\hat{K}_0^\dagger + \hat{K}_1.\rho(0).\hat{K}_1^\dagger \tag{17}$$

and the Kraus operators

$$\hat{K}_0 = e^{-\delta t\hat{\Gamma}} \quad , \quad \hat{K}_1 = \begin{bmatrix} 0 & \sqrt{I - \hat{\Gamma}^2} \\ 0 & 0 \end{bmatrix} \tag{18}$$

For the system-environment system this total system undergoes unitary evolution in the dilated space, with

$$\hat{U}_{diss} = \begin{bmatrix} \hat{K}_0 & -\hat{K}_1^\dagger \\ \hat{K}_1^\dagger & \hat{\mathcal{X}}\hat{K}_0\hat{\mathcal{X}}. \end{bmatrix} \tag{19}$$

where $\hat{\mathcal{X}}$ is the extension of the Pauli-$\hat{X}$ operator to appropriate dimensions. This unitary operator can then be decomposed into simple gates.