

Some Comments on Unitary Qubit Lattice Algorithms for Classical Problems

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Abstract

A qubit lattice algorithm (QLA) for normal incidence of an rectangular electromagnetic pulse onto a dielectric slab is examined and shows that the transmission coefficient is indeed augmented over the Fresnel boundary value infinite plane wave result by the square root of the ratio of the refractive indices of the two media. For an oscillatory wave packet, this transmission coefficient is further increased. As the QLA is not fully unitary, due to one evolution operator being Hermitian, first steps are taken in correcting a similar problem of determining a fully unitary QLA for the Korteweg- de Vries equation. This is achieved by appropriate perturbation of the unitary collision angle.

1 Introduction

We have been investigating qubit lattice algorithms (QLA) for some time [1-20]. The aim of QLA is to develop a unitary interleaved sequence of collision-streaming operators which in the continuum limit reduces perturbatively to the desired differential equations describing the system of interest. The first step is to associate a basis set of qubits for the lattice, which on taking appropriate moments will recover the classical fields of interest. Some care is needed in making this identification, as seen in considering QLA for Maxwell equations (see Sec. 2 for details: only certain specific field bases can lead to unitary evolution). Quantum entanglement is essential if one is developing an algorithm for quantum computers. In our QLA, we typically have the unitary collision operator act on a qubit pair. We then can see immediately that QLA induces quantum entanglement. Indeed, consider a two qubit system with 2^2 basis elements ($|00\rangle, |01\rangle, |10\rangle, |11\rangle$), and a unitary 2×2 collision operator

$$C = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} \quad (1)$$

acting on the qubit subspace of ($|01\rangle, |10\rangle$). One of the post-collision qubit elements is

$$\cos \theta |01\rangle + \sin \theta |10\rangle.$$

Now this post-collision state cannot be represented by a tensor product of the 2^2 - basis, since the most general tensor product state is

$$a_0 b_0 |00\rangle + a_0 b_1 |01\rangle + a_1 b_0 |10\rangle + a_1 b_1 |11\rangle$$

for some coefficients $a_0 \dots b_1$. To eliminate the $|00\rangle$ -term, one must set either $a_0 = 0$ or $b_0 = 0$. This would eliminate either the state $|01\rangle$ or the state $|10\rangle$. States which cannot be represented in a tensor product basis of qubits are called entangled states. A maximally entangled state is achieved on taking $\theta = \pi/4$, and is known as a Bell state [21]

$$B_1 = \frac{|01\rangle + |10\rangle}{\sqrt{2}}$$

In trying to develop a QLA for the propagation of an electromagnetic pulse in a dielectric media, the QLA representation of Maxwell equations in 1 spatial dimension is typically more singular than in 2D. In particular, if one wishes to consider electromagnetic scattering from dielectric objects one must enquire into the thickness of the dielectric boundary layer to the length scale of the incident electromagnetic pulse as this will play an important role in the development of some of the QLA operators. This will be discussed at some length in Sec. 2. However, we will first discuss the choice of qubit representations for some choices will not be able to lead to fully unitary QLAs.

In Sec. 3 we discuss the problem of developing a fully unitary QLA for Maxwell equations, and consider some possible lines of attack by considering the QLA for the Korteweg-De Vries (KdV) soliton. It turns out that our initial QLA for KdV [1] required the introduction of a potential operator following the unitary collide-stream sequence of entangling the qubits and propagating that entanglement throughout the lattice. In the QLA evolution equation for the qubits, this potential operator is not unitary (it is Hermitian). In Sec 3 we shall develop new QLAs in which the effect of this potential operator is obtained by perturbing the unitary collision operator - thereby permitting a fully unitary QLA representation of the KdV equation.

2 QLA for Maxwell Equations

2.1 Qubit-Electromagnetic field representation

Consider a simple dielectric non-magnetic medium with the constitutive equations

$$\mathbf{D} = \epsilon \mathbf{E}, \quad \mathbf{B} = \mu_0 \mathbf{H}. \tag{2}$$

Treating $\mathbf{u} = (\mathbf{E}, \mathbf{H})^T$ as the fundamental fields, and $\mathbf{d} = (\mathbf{D}, \mathbf{B})^T$ the derived fields, Eq. (2) can be written in matrix form

$$\mathbf{d} = \mathbf{W} \mathbf{u} \tag{3}$$

where \mathbf{W} is a Hermitian 6×6 matrix

$$\mathbf{W} = \begin{bmatrix} \epsilon_{3 \times 3} & 0 \\ 0 & \mu_0 \mathbf{I}_{3 \times 3} \end{bmatrix} \tag{4}$$

with $\mathbf{I}_{3 \times 3}$ the 3×3 identity matrix. and \mathbf{T} is the transpose operator. The curl-curl (source-free) Maxwell equations $\nabla \times \mathbf{E} = -\partial \mathbf{B} / \partial t$, and $\nabla \times \mathbf{H} = \partial \mathbf{D} / \partial t$ are just

$$i\frac{\partial \mathbf{d}}{\partial t} = \mathbf{M}\mathbf{u} \quad (5)$$

where, under standard boundary conditions, the curl-matrix operator \mathbf{M} is Hermitian

$$\mathbf{M} = \begin{bmatrix} 0_{3 \times 3} & i\nabla \times \\ -i\nabla \times & 0_{3 \times 3} \end{bmatrix} \quad (6)$$

Since \mathbf{W} is invertible, Eq. (5) can be written in terms of the basic electromagnetic fields $\mathbf{u} = (\mathbf{E}, \mathbf{H})$

$$i\frac{\partial \mathbf{u}}{\partial t} = \mathbf{W}^{-1}\mathbf{M}\mathbf{u} \quad (7)$$

In continuum applications, one typically treats the two Maxwell divergence equations $\nabla \cdot \mathbf{B} = 0$ and $\nabla \cdot \mathbf{D} = 0$ as initial conditions. From the curl-curl equations we see that they will then be satisfied for all time.

2.1.1 homogeneous dielectric medium

If one is dealing with a homogeneous dielectric medium (e.g., a vacuum), then the constitutive matrix \mathbf{W} is a constant and trivially commutes with the curl-operator \mathbf{M} . As a result, the product of the two Hermitian matrices, $\mathbf{W}^{-1}\mathbf{M}$ is itself Hermitian, and Eq. (7) gives a unitary evolution of the electromagnetic fields $\mathbf{u} = (\mathbf{E}, \mathbf{H})^T$ used as a basis for the qubit field.

2.1.2 inhomogeneous dielectric media

However, when the matrix \mathbf{W} is spatially dependent, then $\mathbf{W}^{-1}\mathbf{M} \neq \mathbf{M}\mathbf{W}^{-1}$ and $\mathbf{W}^{-1}\mathbf{M}$ is not Hermitian. Under these conditions, a qubit representation of the electromagnetic fields $\mathbf{u} = (\mathbf{E}, \mathbf{H})^T$ will not yield a unitary evolution of these qubits. However Koukoutsis et. al. [24] have shown how to determine the so-called Dyson map from the fields \mathbf{u} to a new field representation \mathbf{U} such that the resultant representation in terms of the new field \mathbf{U} will result in a unitary evolution of these fields. Indeed, it can be shown [24], that the Dyson map

$$\mathbf{U} = \mathbf{W}^{1/2}\mathbf{u} \quad (8)$$

will yield a unitary evolution equation for \mathbf{U} with

$$i\frac{\partial \mathbf{U}}{\partial t} = \mathbf{W}^{-1/2}\mathbf{M}\mathbf{W}^{-1/2}\mathbf{U} \quad (9)$$

as the matrix operator $\mathbf{W}^{-1/2}\mathbf{M}\mathbf{W}^{-1/2}$ is Hermitian.

Thus one could start to build a QLA based on the electromagnetic fields

$$\mathbf{U} = \left(\epsilon^{1/2}\mathbf{E}, \mu_0^{1/2}\mathbf{H} \right)^T \quad (10)$$

or under the rotation matrix

$$\mathbf{L} = \frac{1}{\sqrt{2}} \begin{bmatrix} I_{3 \times 3} & iI_{3 \times 3} \\ I_{3 \times 3} & -iI_{3 \times 3} \end{bmatrix} \quad (11)$$

one could base a QLA on the field representation $\mathbf{U}_{\text{RSW}} = \mathbf{L}\mathbf{U}$ where

$$\mathbf{U}_{\text{RSW}} = \frac{1}{\sqrt{2}} \begin{bmatrix} \epsilon^{1/2} \mathbf{E} + i\mu_0^{1/2} \mathbf{H} \\ \epsilon^{1/2} \mathbf{E} - i\mu_0^{1/2} \mathbf{H} \end{bmatrix}. \quad (12)$$

This is nothing but the unitary evolution of the Riemann-Silberstein-Weber (RSW) vector - a representation used to represent Maxwell equations from the early 1920's [25-27]. The theory can be readily extended to diagonal tensor dielectric media, with (assuming non-magnetic materials) the 6-qubit representation \mathbf{Q} of the field

$$\mathbf{U} = \left(n_x E_x, n_y E_y, n_z E_z, \mu_0^{1/2} \mathbf{H} \right)^T = \mathbf{Q} \quad (13)$$

\mathbf{n} is the vector (diagonal) refractive index, with $\epsilon_x = n_x^2 \dots$ and we work in Cartesian coordinates.

2.2 2D QLA for x - y dependent propagation of Maxwell Equations

From Eqs. (9) and (13), Maxwell equations for 2D x-y spatially dependent fields written in terms of the 6- \mathbf{Q} vector components

$$\begin{aligned} \frac{\partial q_0}{\partial t} &= \frac{1}{n_x} \frac{\partial q_5}{\partial y}, & \frac{\partial q_1}{\partial t} &= -\frac{1}{n_y} \frac{\partial q_5}{\partial x}, & \frac{\partial q_2}{\partial t} &= \frac{1}{n_z} \left[\frac{\partial q_4}{\partial x} - \frac{\partial q_3}{\partial y} \right] \\ \frac{\partial q_3}{\partial t} &= -\frac{\partial(q_2/n_z)}{\partial y}, & \frac{\partial q_4}{\partial t} &= \frac{\partial(q_2/n_z)}{\partial x}, & \frac{\partial q_5}{\partial t} &= -\frac{\partial(q_1/n_y)}{\partial x} + \frac{\partial(q_0/n_x)}{\partial y} \end{aligned} \quad (14)$$

This representation is unitary.

One QLA representation focusses on recovering Eq. (14) perturbatively. One can thus consider developing the representation dimension by dimension. In particular we introduce the following unitary collision operator with collision angles θ_1 and θ_2 (to be specified later):

$$C_X = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & o \\ 0 & \cos \theta_1 & 0 & 0 & 0 & -\sin \theta_1 \\ 0 & 0 & \cos \theta_2 & 0 & -\sin \theta_2 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \sin \theta_2 & 0 & \cos \theta_2 & 0 \\ 0 & \sin \theta_1 & 0 & 0 & 0 & \cos \theta_1 \end{bmatrix} \quad (15)$$

and the unitary collision operator

$$C_Y = \begin{bmatrix} \cos \theta_0 & 0 & 0 & 0 & 0 & \sin \theta_0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos \theta_2 & 0 & \sin \theta_2 & 0 \\ 0 & 0 & -\sin \theta_2 & \cos \theta_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ -\sin \theta_0 & 0 & 0 & 0 & 0 & \cos \theta_0 \end{bmatrix} \quad (16)$$

with collision angles θ_0 and θ_2 . The unitary streaming operator S_{14}^{+x} shifts qubits q_1 and q_4 one lattice unit in the $+x$ direction, while leaving the remaining 4 qubits alone. We finally need to introduce the (nonunitary) external potential operators

$$V_X = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & o \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -\sin \beta_2 & 0 & \cos \beta_2 & 0 \\ 0 & \sin \beta_0 & 0 & 0 & 0 & \cos \beta_0 \end{bmatrix} \quad (17)$$

and

$$V_Y = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \cos \beta_3 & \sin \beta_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ -\sin \beta_1 & 0 & 0 & 0 & 0 & \cos \beta_1 \end{bmatrix} \quad (18)$$

for particular angles β_0 , β_1 and β_2 .

We now consider the following unitary sequence of interleaved collision-streaming operators:

$$\mathbf{U}_X = S_{25}^{+x} \cdot C_X^\dagger \cdot S_{25}^{-x} \cdot C_X \cdot S_{14}^{-x} \cdot C_X^\dagger \cdot S_{14}^{+x} \cdot C_X \cdot S_{25}^{-x} \cdot C_X \cdot S_{25}^{+x} \cdot C_X^\dagger \cdot S_{14}^{+x} \cdot C_X \cdot S_{14}^{-x} \cdot C_X^\dagger \quad (19)$$

and

$$\mathbf{U}_Y = S_{25}^{+y} \cdot C_Y^\dagger \cdot S_{25}^{-y} \cdot C_Y \cdot S_{03}^{-y} \cdot C_Y^\dagger \cdot S_{03}^{+y} \cdot C_Y \cdot S_{25}^{-y} \cdot C_Y \cdot S_{25}^{+y} \cdot C_Y^\dagger \cdot S_{03}^{+y} \cdot C_Y \cdot S_{03}^{-y} \cdot C_Y^\dagger \quad (20)$$

with the discrete time advancement of the 6-qubit \mathbf{Q} given by

$$\mathbf{Q}(t + \delta t) = V_Y \cdot V_X \cdot \mathbf{U}_Y \cdot \mathbf{U}_X \cdot \mathbf{Q}(t) \quad (21)$$

To recover the desired Maxwell equations (14) perturbatively, one introduces a small parameter ϵ as the spatial lattice shift unit (assuming a square $x - y$ lattice), and the unitary collision angles

$$\theta_0 = \frac{\epsilon}{4n_x} \quad , \quad \theta_1 = \frac{\epsilon}{4n_y} \quad , \quad \theta_2 = \frac{\epsilon}{4n_z} \quad (22)$$

Finally, the nonunitary external potential angles need to be defined as

$$\beta_0 = \epsilon^2 \frac{\partial n_y / \partial x}{n_y^2} \quad , \quad \beta_1 = \epsilon^2 \frac{\partial n_x / \partial y}{n_x^2} \quad , \quad \beta_2 = \epsilon^2 \frac{\partial n_z / \partial x}{n_z^2} \quad , \quad \beta_3 = \epsilon^2 \frac{\partial n_z / \partial y}{n_z^2} \quad (23)$$

Indeed, using Mathematica to evaluate Eq. (21), one obtains in the continuum spatial limit the desired Maxwell equations to errors of ϵ^4

$$\begin{aligned} \frac{\partial q_0}{\partial t} &= \epsilon^2 \delta t \frac{1}{n_x} \frac{\partial q_5}{\partial y}, & \frac{\partial q_1}{\partial t} &= -\epsilon^2 \delta t \frac{1}{n_y} \frac{\partial q_5}{\partial x}, & \frac{\partial q_2}{\partial t} &= \epsilon^2 \delta t \frac{1}{n_z} \left[\frac{\partial q_4}{\partial x} - \frac{\partial q_3}{\partial y} \right] \\ \frac{\partial q_3}{\partial t} &= -\epsilon^2 \delta t \frac{\partial(q_2/n_z)}{\partial y}, & \frac{\partial q_4}{\partial t} &= \epsilon^2 \delta t \frac{\partial(q_2/n_z)}{\partial x}, & \frac{\partial q_5}{\partial t} &= -\epsilon^2 \delta t \left(\frac{\partial(q_1/n_y)}{\partial x} + \frac{\partial(q_0/n_x)}{\partial y} \right) \end{aligned} \quad (24)$$

i.e., under diffusion ordering, $\epsilon^2 \delta t \approx O(1)$, one recovers the continuum Maxwell equations to errors $O(\epsilon^2)$.

3 QLA for KdV without external non-unitary potential operators

The KdV equation is an important nonlinear equation and has been derived in considering the evolution of shallow water waves. Interestingly, it [33] has also been associated with the Fermi-Pasta-Ulam-Tsingou simulations of the 1950's which were undertaken computationally to study the expected equipartition of the system's energy in set of coupled nonlinear oscillators. Instead, in the parameter regime they considered, Fermi et. al. found recurrence of initial conditions. The general KdV equation for arbitrary positive constants a and b

$$\frac{\partial \psi}{\partial t} + a \psi \frac{\partial \psi}{\partial x} + b \frac{\partial^3 \psi}{\partial x^3} = 0$$

is exactly integrable. One of its solutions is the right traveling soliton with speed c - a free parameter

$$\psi(x, t) = \frac{3c}{a} \operatorname{sech}^2 \left(\frac{1}{2} \sqrt{\frac{c}{b}} [x - ct] \right)$$

Since the KdV equation is a scalar equation for the real function $\psi(x, t)$ one need only to employ 2 qubits / lattice site. First we shall reconsider the QLA for KdV with the use of an external potential to model the nonlinear term in KdV. The collision operator is nothing but Eq. (1) with maximal entanglement angle $\theta = \pi/4$. We denote the operator S_{0+} to be the streaming operator that translates the qubit q_0 one lattice unit in the $+x$ -direction. To eliminate the 2nd order spatial derivative one must choose the interleaved sequence of collision-stream unitary operators carefully. In particular the following sequence will generate a second order QLA for the KdV equation

$$Q(t + \Delta t) = V_{\text{pot}} \cdot S_{0+} C \cdot S_{1-} C^T \cdot S_{0-} C \cdot S_{1+} C^T \cdot S_{0-} C^T \cdot S_{1+} C \cdot S_{0+} C^T \cdot S_{1-} C \cdot Q(t)$$

where the 2-qubit function $Q = (q_0 q_1)^T$, and the superscript T is the transpose operation. The external potential V_{pot} is the Hermitian matrix

$$V_{\text{pot}} = \begin{bmatrix} \cos \alpha & -\sin \alpha \\ -\sin \alpha & \cos \alpha \end{bmatrix} \quad \text{with} \quad \alpha = \epsilon^3 m[x].$$

In the continuum limit, one recovers

$$\frac{\partial \psi}{\partial t} + \epsilon^3 \left(m[x] \cdot \psi(x, t) + \frac{1}{2} \frac{\partial^3 \psi}{\partial x^3} \right) = 0 + O(\epsilon^5)$$

on defining $\psi = q_0 + q_1$. With the choice of $m[x] = \partial \psi / \partial x$ we have a second order accurate QLA for KdV. Note that the QLA of Eq. (26) is not fully unitary because of the non-unitary property of the external potential operator V_{pot} .

3.1 Fully unitary QLAs for KdV

QLAs are not unique in recovering the desired physics models to second order accuracy. Here, we will present two QLAs, both having the same unitary collision operator, but with different streaming sequences on the two qubits. Indeed, using Mathematica, it can be shown that the following QLA

$$Q(t + \Delta t) = S_{0-} C_1 \cdot S_{0+} C_1 \cdot S_{1+} C_1 \cdot S_{1-} C_1^T \cdot S_{0-} C_1^T \cdot S_{0+} C_1^T \cdot S_{1+} C_1^T \cdot S_{1-} C_1 \cdot Q(t)$$

with unitary collision operator C_1

$$C_1 = \begin{bmatrix} \cos \alpha_1 & \sin \alpha_1 \\ -\sin \alpha_1 & \cos \alpha_1 \end{bmatrix} \quad \text{with} \quad \alpha_1 = \epsilon^2 m_1[x].$$

leads in the continuum limit to

$$\frac{\partial \psi_1}{\partial t} + \epsilon^3 \left(4m[x] \cdot \frac{\partial \psi_1}{\partial x} + \frac{1}{2} \frac{\partial^3 \psi_1}{\partial x^3} \right) = 0 + O(\epsilon^5)$$

so that the choice of $m[x] = \psi_1$ will recover KdV.

Another fully unitary QLA that recovers KdV has the following interleaved sequence of unitary collision-streaming operators:

$$Q(t + \Delta t) = C_1 S_{0-} \cdot C_1 S_{1+} \cdot C_1 S_{0-} \cdot C_1 S_{1+} \cdot C_1^T S_{0+} \cdot C_1^T S_{1-} \cdot C_1^T S_{0+} \cdot C_1^T S_{1-} \cdot Q(t)$$

C_1 is the same collision operator as in Eq. (30), and in the continuum limit yields

$$\frac{\partial \psi_1}{\partial t} + \epsilon^3 \left(-4m[x] \cdot \frac{\partial \psi_1}{\partial x} + \frac{1}{2} \frac{\partial^3 \psi_1}{\partial x^3} \right) = 0 + O(\epsilon^5)$$

so that the choice of $m[x] = -\psi_1$ will recover a KdV.

The implementation of these fully unitary algorithms may not necessarily be straightforward as the perturbation parameter ϵ introduced into the Mathematica algorithm requires a perturbation in the collision angle of $O(\epsilon^2)$, Eq. (30), while the continuum limit has scaling proceeds as $O(\epsilon^3)$. In previous QLA for nonlinear physics, the order of the function ψ controlled the ϵ -factor.

4 SUMMARY

The development of a fully unitary QLA for plasma physics [34-37] in particular is of considerable interest as they are readily encodable on future error-correcting quantum computers. In developing QLAs for plasma physics we have taken the tack of first concentrating on Maxwell equations in dielectric media. Our current QLAs for Maxwell equations are not fully unitary. However, it has been proven that there does exist a unitary representation for Maxwell equation in dielectric media - and it is thus a question of determining that unitary representation. Our current QLAs have employed a sequence of interleaved collide-stream unitary operators that recover in the continuum limit the spatial and time derivatives on the electromagnetic fields (see, e.g, Eqs. (19) and (20)). The derivative terms on the refractive index are currently recovered by introducing two potential operators - one of them is unitary, but the other is Hermitizn.

Earlier, we tested the accuracy of the QLA representation by determining such a representation for the KdV equation - particularly since the 2-collision problem has an exact theoretical solution for all times, even during the transient times when the solitons overlap. However for QLA [1] one needs only one potential operator following the interleaved sequence of unitary collision-streaming operators, but that potential operator was Hermitian. In this paper, we have looked for QLAs that will recover KdV but now totally unitary by incorporating a perturbation on the collision angle to eliminate the need for the non-unitary potential operator. Two such QLAs are presented. Since the non-unitary potential has exactly the same form for KdV as for Maxwell equations, it is hoped that such an approach on augmenting the collision angle will lead to a fully unitary QLA for Maxwell equations.

We have also presented here some more evidence that there is a fundamental difference between the initial value to boundary value approach for electromagnetic field propagation at dielectric interfaces. The standard textbook boundary value approach assumes the existence of infinite plane waves at the interface - the incident, the transmitted and the reflected plane waves. From the dielectric discontinuity, one recovers Fresnel conditions on the respective wavelengths, speeds and amplitudes. No transients effects can be handled. As is well known from the Sommerfeld-Brillouinn calculations that for an event there must be nothing and then something. Such an approach is found in QLA where we launch an electromagnetic pulse and then solve the QLA representation of Maxwell equations as an initial value problem. The mathematical expediency of a δ -function interface is

replaced by a sharp but continuous dielectric boundary layer. There is no need for the introduction of internal boundary conditions, and one can follow the transient effects of a spatially limited pulse. While the QLA recovers all the Fresnel jump conditions - except that it predicts the transmitted to incident electric fields be augmented by a factor of $\sqrt{n_2/n_1}$ over Fresnel. Earlier QLA simulations worked with various single-maximum pulse geometries and many different dielectric n_1 and n_2 . Here we considered a rectangular pulse to facilitate an easy back of the envelope calculation of the Poynting flux. QLA is found to conserve energy very accurately - even during that transient times in which the pulse is overlapping the two regions. When one considers an oscillating finite-extent wave packet, results indicate that the ratio of transmitted to incident fields is enhanced even more than in the single-maximum pulse. This will be considered in a future paper.

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