Quantum Simulation of Phylogenetic Trees

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Introduction: In the last two decades quantum mechanics has found itself in a situation that could be characterized as an epistemological exodus. It has expanded its scope and applicability into new fields, such as information theory, the theory of computation, and even biology, and has addressed fundamental problems and procedures of these fields, by means of its physical-mathematical conceptual and computational apparatus\textsuperscript{3,4}. What were previously accepted as quantum paradoxes and oddities, like quantum entanglement, have turned out to be the keys to constructing novel computational and communicational algorithms, providing the means for launching a new quantum technology. In this vein, this paper puts forward a novel application of the means for launching a new quantum technology.

Quantum simulations constructing probability tensors of biological multi-taxon in phylogenetic trees are proposed, in terms of positive trace preserving maps, describing evolving systems of quantum walks with multiple walkers. Basic phylogenetic models applying on trees of various topologies are simulated following appropriate decoherent quantum circuits. Quantum simulations of statistical inference for aligned sequences of biological characters are provided in terms of a quantum pruning map operating on likelihood operator observables, utilizing state-observable duality and measurement theory.

\textit{Notation}: Let the character set be $\Sigma = \{0, 1, \ldots, N - 1\} = \{0\} \cup \Sigma^*$. Here 0 is considered to be the “null” or no character symbol. Introduce the Hilbert space of character states $H \approx l_2(\Sigma) = \text{span}\{i\}; i \in \Sigma\}$, of dimension $\dim H = |\Sigma|$, and consider the space $\text{Lin}(H)$ of linear operators acting on $H$. Exemplars are the complete set of projectors $\hat{P}_i = |i\rangle \langle i|$, $i \in \Sigma$, the shift operator $h|j\rangle = |i + N\rangle$ (so that $h^N = 1$), and the space of density matrices $\mathcal{D}(H) \subset \text{Lin}(H)$. A classical (discrete) probability distribution is represented as a vector $(p_0, p_1, p_2, \ldots p_N - 1)$, and the corresponding quantum stochastic system is represented by a diagonal density matrix $\rho = \sum_{i \in \Sigma^*} p_i \hat{P}_i \in \mathcal{D}(H)$; for biological applications we will always assume $p_0 = 0$ (so that in practice the sum runs only over characters $i \in \Sigma^*$).

On bipartite systems, the unitary control-not operator $U_{cn} \in \text{Lin}(H \otimes H)$ defined as $U_{cn} = \sum_{i \in \Sigma^*} p_i \hat{P}_i \otimes h^k$, acts as $U_{cn}|i\rangle \otimes |j\rangle = |i\rangle \otimes |i + N\rangle$.

Splitting, cladogenesis, speciation: The splitting operation $\Delta$ for given 1-taxon matrix $p = \sum_{i \in \Sigma^*} p_i \hat{P}_i$, is implemented by the adjoint action of $U_{cn}$

$$\Delta \rho = U_{cn}(\rho \otimes \hat{P}_0)U_{cn}^\dagger = \sum_{i,j \in \Sigma^*} p_{ij} \hat{P}_i \otimes \hat{P}_j, \quad (1)$$

where $p_{ij} = p_i \delta_{ij}$, so $\Delta \rho$ is identified with a two-taxon density matrix. The control-not gate embedded in various positions in $s$-fold products of character spaces, e.g. $1^\otimes s - k - 1 \otimes U_{cn} \otimes 1^\otimes s - k - 1$, provides the way to construct $s$-taxon phylogenetic trees of various topologies\textsuperscript{5,6}.

Phyletic evolution, anagenesis: For an $s$-taxon density matrix $\rho = \sum_{i_1, \ldots, i_s \in \Sigma^*} p_{i_1} \ldots \hat{P}_{i_s} \otimes \ldots \hat{P}_i$, a suitable local unitary $U = \bigotimes_{i=1}^s U_i \in \text{Lin}(H)^{\otimes s}$, formalizes the phyletic evolution of taxa, when its action is composed with the $s$-fold product of the local diagonalizing map $\mathcal{E}_d$, where $\mathcal{E}_d(\cdot) = \sum_{k \in \Sigma^*} \hat{P}_k(\cdot) \hat{P}_k$, is the completely positive trace preserving (CPTP) map that projects out the diagonal part of a matrix\textsuperscript{7}, that is a decoherent map.
Thus we have $\rho \rightarrow \bar{\rho} \equiv E_d^{\otimes s}(U \rho U^\dagger)$, where

$$
\bar{\rho} = \sum_{i_1, \ldots, i_s \in \Sigma^*} \bar{p}_{i_1 \ldots i_s} \hat{P}_{i_1} \otimes \cdots \otimes \hat{P}_{i_s},
$$

(2)

and

$$
\bar{p}_{i_1 \ldots i_s} = \sum_{j_1, \ldots, j_s \in \Sigma^*} p_{j_1 \ldots j_s} (M_1 \otimes \cdots \otimes M_s)_{i_1 j_1; \ldots; i_s j_s}.
$$

(3)

Abbreviating the adjoint action of an operator as $Ad S(\cdot) \equiv S(\cdot) S^\dagger$, we say that the map $E_d^{\otimes s}(Ad U)$ thus induces a general doubly-stochastic transformation in the probability tensor. The Hadamard or entry-wise product of matrices defined as $(A \otimes B)_{ij} = A_{ii} B_{jj}$, has been used, to obtain the Markov matrices $M_i = U_i \circ U_i^\dagger$, which will drive evolution on edges of a model phylogenetic tree. Below, we make particular choices of $U$ to reflect different types of phylogenetic models. Fig. 1 summarizes the preceding discussion by showing a four taxon tree and its simulating quantum circuits.

Phylogenetic evolution and quantum walks: It has long been appreciated that faithful modeling of trait evolution in phylogenetics is problematic. As has been remarked, “...Brownian motion is a poor model, and so is Ornstein-Uhlenbeck”. We here present a novel proposal for the stochastic phyletic evolution of traits via quantum simulation employing QWs (see reference[14]), operating locally on density matrices along edges of trees. This is set up as follows. Introduce in additional to character Hilbert space $H$ (the “walker” space), at each node of phylogenetic tree an auxiliary “coin” Hilbert space $H_c \approx l_2(C) = span(|+\rangle, |−\rangle)$, and projectors $P_{\pm} \in Lin(H_c)$. Evolution now proceeds on joint “walker” and “coin” states $|\psi_c \otimes \rho\rangle$ via a standard QW conditional unitary operator $V = (P_+ \otimes h + P_- \otimes h^\dagger)U \otimes 1$, acting from $H_c \otimes H$ to itself. One “step” of such a QW is realized by the map on the “walker” density matrix, viz. $\rho \rightarrow E_{V,k}(\rho) := Tr_c V^k (\rho_c \otimes \rho) V^{k\dagger}$, followed by diagonalization with $E_d$. For s taxon, $E_{V,k} \equiv (E_d^{\otimes s} \circ E_{V,2})$. For example for the two-taxon case, with $k = 2$ and coin initially in a pure state $|\psi_c\rangle = |c\rangle |c\rangle$ with $|c\rangle = |+\rangle$ or $|−\rangle$, we obtain $E_{V,2}(\rho) = \sum_{m,n} \bar{p}_{mn} P_m \otimes P_n$, with components $\bar{p}_{mn} = \sum_{a,b} p_{m-a,b-n} q^{(c)}_a q^{(c)}_b$, where $q^{(c)}_a := \sum_{\gamma,\alpha,\zeta} M_{\gamma,\alpha-c} M_{\gamma-\alpha,c} \geq 0$, is a probability distribution (that is, $q^{(c)}_a > 0$, $\sum_a q^{(c)}_a = 1$), determined by the coin tossing unitary $U$ via the Hadamard product $M = U \circ U^\dagger$. The tensor $\bar{\rho}$ so obtained, and its multi-taxon generalizations, are objects of quantum simulations. Also the diagonalizing map $E_d$ can be cast in the form of a CPTP map, i.e. $E_d(\rho) = \sum_{k \in \Sigma^*} \bar{P}_k \rho \bar{P}_k = \sum_{k \in \Sigma^*} q_k U_k \rho U_k^\dagger$ with each $q_k = 1/|\Sigma|$, thanks to the non-uniqueness of the operator sum representation, with unitaries $U_k$ related to projectors by discrete Fourier transform, $U_k = \sum_{i} \omega^{kl} \hat{P}_i$ and $\omega = \exp(i2\pi/|\Sigma|)$. Below, similar quantum prescriptions will be given to the structural maps of standard evolutionary models.

Phylogenetic evolutionary models and quantum maps: Next we exploit the above considerations in specific cases of standard phylogenetic models, namely the so-called group-based models (see references[14]): Jukes-Cantor (JC), Kimura two-parameter (K2), Kimura three-parameter (K3), and the binary symmetric model (B), as well as the Felsenstein model (F) [14]. Firstly we give in each case a direct Kraus representation of the quantum map $E_\tau \equiv E_d \circ E_\tau$. This is followed by a QW formulation using, as above, an additional ancillary “coin” space. Let $X$, $Z$ denote the usual single qubit not and phase gates (the Pauli matrices $\sigma_z$, $\sigma_x$ respectively) and $U_{kl} = X^k \otimes X^l$, for $k, l = 0, 1$. The following propositions are verified by direct calculation for operators in $l_2(\Sigma^*)$ acting on $\rho = \sum_{m \in \Sigma^*} p_m \hat{P}_m$.

**Proposition K:** Let $|\Sigma^*| = 4$ and $\tau \in \{K3, K2, JC\}$. We have

$$
E_\tau(\rho) = \sum_{k,l} \lambda^{(\tau)}_{kl} U_{kl} (\rho) U^\dagger_{kl} = \sum_{m \in \Sigma^*} (M_\tau p_m) \hat{P}_m,
$$

$$
M_\tau(a, b, c) = \sum_{k,l} \lambda^{(\tau)}_{kl} U_{kl} \circ U_{kl}^\dagger = \sum_{k,l} \lambda^{(\tau)}_{kl} X^k \otimes X^l.
$$

(4)

The weights $\lambda^{(\tau)}_{kl}$ and corresponding model Markov matrices $M_\tau$ are defined as follows. For generic parameters define the weights $\lambda^{(\tau)}_{kl}(a, b, c)$ as $\lambda_{00} = 1-a-b-c$, $\lambda_{10} = a$, $\lambda_{01} = b$, $\lambda_{11} = c$, and take the corresponding convex sum $M(a, b, c)$. Then $\lambda_{kl}^{(3K)} = \lambda_{kl}(a, b, c)$, $M_{3K} = M(a, b, c)$, $\lambda_{kl}^{(2K)} = \lambda_{kl}(a, b, b)$, $M_{2K} = M(a, a, b)$, and finally $\lambda_{kl}^{(JC)} = \lambda_{kl}(a, a, a)$, $M_{JC} = M(a, a, a)$.

**Proposition K’:** The CPTP map $E_\tau$ has, in addition to the operator sum representation above, also a QW like representation $E_\tau(\rho) = Tr_V V_T (\rho_c \otimes \rho) V_T^\dagger$, in terms of a unitary dilation $V_T = (\sum_k P_k \otimes P_k \otimes U_k) U_T \otimes 1$ which acts on a composite coin-walker space $H_c \otimes H$, with four-dimensional ancillary space. Here $V_T$ is a control-coin $U_{kl}$ operator. For a coin density matrix with spectral decomposition $\rho_c = \sum_{k} \mu_k |c_k\rangle \langle c_k|$, the coin-tossing unitary $U_T$ should satisfy $(k l) U_T \circ U^*_{T l} = c^{(\tau)}_{kl}$, with $|c\rangle = \sum_{k} \mu_k |c_k\rangle$ a stochastic vector. Also $U_{kl} = e^{i\theta_{kl}}$, where $\theta_{kl} = \frac{1}{2} \pi - (k+l) |1\rangle \langle 1| + kX \otimes 1 + lX \otimes 1$.

**Proposition B:** Let $|\Sigma^*| = 2$. The map $E_d \circ E_B$, where $E_B(\rho) = (1-a)\rho + aX \rho X^\dagger$, simulates the binary
symmetric model $M_B(a) = (1-a)1 + aX$ acting as
$\rho = \sum_{m \in \Sigma^*} p_m \tilde{P}_m \rightarrow \sum_{m \in \Sigma^*} (M_B p)_m \tilde{P}_m$. □

**Proposition B’** The “control flip” map $E_B$ is unitarized in composite coin-walker space with a two-dimensional ancillary space as, $E_B(\rho) = Tr e V_B(\rho_c \otimes \rho) V_B^\dagger$, with the starting coin state $\rho_c = |1\rangle \langle 1|$, and $V_B = \sqrt{a}1 \otimes 1 + \sqrt{1-a}Y \otimes X$, and $Y = ZX$.

**Remark:** In the QW picture, the weight parameters $A_{kl}^{(r)}$ determine non-uniquely, via the unistochastic matrix $U_r \circ U^*_r$, the coin-tossing matrix $U_c$, which in turn determines the $U$-quantization of the underlying classical walk with evolution matrix $V_d = \sum_{kl} P_{kl} \otimes P_l \otimes U_{kl}$.

For the Felsenstein model (F), quantum simulation requires the following ingredients. The model’s stationary distribution $(\pi_1, \pi_2, \pi_3, \pi_4)$, $\sum \pi_i = 1$, is to be used to introduce the observable $1_\pi := 4 \sum \pi_i P_i$, with Kraus operators $F_{ij} = \sqrt{\pi_j} |i\rangle \langle j|$, $j \in \Sigma = \{1, 2, 3, 4\}$ obeying the resolution relation $\sum_{ij} F_{ij}^\dagger F_{ij} = 41_\pi$. Again let $\rho = \sum_{m \in \Sigma^*} p_m \tilde{P}_m$. By direct calculation we obtain:

**Proposition F:** The quantum map implementing the Felsenstein model $\rho \rightarrow E_F(\rho)$ is given by

$$E_F(\rho) = (1 - a) \frac{1}{p_\pi} \sum_{i,j} F_{ij}^\dagger \rho F_{ij} + a \rho,$$

(5)

where $p_\pi = Tr(\sum_{i,j} F_{ij}^\dagger F_{ij} \rho) = Tr(\frac{1}{p_\pi} \rho)$ is a normalization constant, and the model’s stochastic matrix is obtained as $M_F = (1 - a) \sum_{i,j} F_{ij} \otimes F_{ij} + a 1$.

In the framework of quantum measurement theory, simulation of the Felsenstein model is interpreted as follows. There are two observables: $1_\pi$ as above, and also $1^n_{\pi}$ defined analogously in terms of the complementary probability distribution $(\pi_1^#, \pi_2^#, \pi_3^#, \pi_4^#)$, with $1 \equiv 1_\pi + 1^n_{\pi}$ forming a non-orthogonal decomposition of unity. These observables are measured by means of the so-called instrumenta, which are the two families of Kraus generators: the $\{F_{ij}^\pi\}_{i,j=0}$ as above, and the analogous $\{F_{ij}^{#\pi}\}_{i,j=0}$ defined in terms of $\pi^#$ rather than $\pi$ (see e.g. [15]). The measurement probabilities of the observables $1_\pi$ and $1^\#_{\pi}$ in the system are $p_\pi = Tr(1_{\pi} \rho)$, and $p_{\pi} = Tr(1^\#_{\pi} \rho)$, and the action of quantum map $E_F$ on the density matrix $\rho$ gives the post-measurement density matrix for a non-efficient quantum measurement for observable $1_\pi$ of finite strengtha. The complementary measurement of $1^\#_{\pi}$ is not used. In the uniform limit $\pi_j = \frac{1}{4}$ then $1_\pi = 1$, $1^\#_{\pi} = 0$ and $p_{\pi} = 1$, and the model reduces to the JC model.

**Quantum estimation of likelihood:** Our general framework also encompasses the quantum estimation of model-based tree likelihoods (F), whose numerical calculation and optimization provides a major tool for phylogenetic inference (for computational heuristics see e.g. [15, 16]). Likelihood evaluation has been demonstrated to be a computationally NP-hard problema, and it is therefore desirable to put forward a quantum simulation equivalent. In the usual formulation (F), likelihood vectors are initialized at the pendant nodes (leaves) of a tree, and are then computed recursively back to the root node, the final result being a scalar quantity, the tree likelihood.

The key operation is that of pruning, that is, of arriving at the likelihood for a parent node, say $A$, by combining a pair of daughter likelihoods, say $B$, $C$, from nodes which root two sub-trees. Explicitly, likelihoods for daughter nodes $B$, $C$ are combined to give the parent likelihood $L_A = (\sum_{i \in \Sigma} M_{B,C}^i(t_{BC}))$, where $M_{B,C}^i(t_{BC})$ are stochastic matrices depending on branch lengths $t_{BC}$ specified by the evolutionary model employed.

Next, an alignment of $s$ taxa over $A$ sites is considered. If the characters at site $l$ of the alignment are $i_1^{(l)}, i_2^{(l)}, \ldots, i_s^{(l)}$, then likelihoods for the tips of the tree (leaf nodes) are initialized to $L_k^{(l)} = \delta(k, i_k^{(l)})$. The pruning map is applied recursively at all cherries, and then higher up the tree, to arrive at the total tree likelihood $L^{(r)}_{tr} = (L_k^{(r)})^{s}_{k=1}$ which is finally averaged over the assumed stationary distribution $(\pi_i)$ of the model to obtain site $l$’s likelihood $L_k^{(l)} = \sum_{i \in \Sigma} \pi_i L_k^{(l)}$. For the entire alignment, the tree (log) likelihood is then $L(T; w^*) = \max_w \log H_{l=1}^T L_k^{(l)}$, where $T$ denotes the tree topology and $w^*$ the optimal model (weight) parameters.

In the quantum simulation introduced here, likelihoods are regarded as quantum observables, that is operators in $Lin(H)$, dual to density operators under the trace inner product (see above). The likelihood operator at node $A$ has components $\hat{L}_A = L_A(i|i) = \mathbb{P}(i|i)$, where $\mathbb{P}(i|i)$ is the conditional probability of character $i$ at $\Sigma^*$. For parameters $t = (T, w)$. Here $A = 1, 2, \ldots, s$ are leaf nodes and $A = s + 1, \ldots, 2s - 2$, internal (ancestral) nodes. Consider parent and daughter nodes $A$, $B$ and $C$, with respective likelihood operators $\hat{L}_A$, $\hat{L}_B$ and $\hat{L}_C$. Operators for daughter nodes $B$, $C$ are combined using the analog of pruning, the quantum pruning map $\mu : Lin(H) \otimes Lin(H) \rightarrow Lin(H)$ that provides the parent operator $\hat{L}_A = \mu(\hat{L}_B \otimes \hat{L}_C)$, where $\mu = Tr_B \circ Ad_U_{dc} \circ \mathbf{E}_{dd} \circ Ad(U_B \otimes U_C)$. The map $\mu$
uses stochastic matrices $M^x(t_x) = U_x \circ U_x^*$, depending on branch lengths $t_x$ for $x = A, B$, as given by the model employed, and the collective “diagonalizing map” $\mathcal{E}_{Bpd}(\cdot) = \sum_k \widehat{P}_k \otimes \widehat{P}_k (\cdot) \widehat{P}_k \otimes \widehat{P}_k$. Fig. 2 presents a quantum circuit realizing map $\mu$. By using its embedding $\mu_{r,r+1} = id^{s-r-1} \otimes \mu \otimes id^{s-r}$ for various values of $r$ according to the topology of the binary tree, the pruning map $\mu$ is applied recursively to all cherries, and then higher up the tree.

In this way we arrive at the tree likelihood operator $\hat{L}_{tr}$, which then is contracted with model’s stationary density matrix $\rho^x = \sum_i \pi_i \hat{P}_i$, to yield as a measurement result the site $l$ likelihood $L^{(l)} = Tr(\hat{L}_{tr}^x \rho^x) = \left\langle \hat{L}_{tr}^x, \rho^x \right\rangle$. For the entire alignment, the tree (log) likelihood is (c.f. the identity $Tr(AB)Tr(CD) = Tr(A \otimes C)(B \otimes D)$)

$$L = \max_w \log \prod_{l=1}^L \left\langle \hat{L}_{tr}^x, \rho^x \right\rangle = \max_w \log Tr(\otimes_{l=1}^L \hat{L}_{tr}^x \rho^x),$$

where $\rho_A \equiv (\rho^x)^{\otimes L}$ is the product of $L$ stationary density matrices.

In fact this Heisenberg-like picture of updating the observables (likelihoods), and finally contraction with the stationary density matrix to derive site and eventually alignment likelihoods, can be converted to a Schrödinger-like picture, using the observable-state duality, exemplified here by the trace cyclic property. Firstly note that the pruning map can be expressed as $\mathcal{E}_{Bpd}(\cdot) = \sum_{k \in \Sigma} q_k^B \Ad \widehat{P}_k (\cdot)$, a probabilistic diagonalizing map, with probabilities $q_k^B = \nu^{-1} \langle k | U B \widehat{L} B U_B^\dagger | k \rangle$. As the roles of $\widehat{L} B$ and $\widehat{L} C$ can be exchanged above with appropriate modification, ($\mathcal{E}_B$ becomes $\mathcal{E}_C$ etc), we note that $\mu$ is proportional to a stochastic map either way, and by duality it can be made to act on density matrices instead of likelihood operators. This is also true for embedded pruning maps $\mu_{r,r+1}$, i.e. they will also be proportional to maps $\mathcal{E}_{B^{(r)},B^{(r+1)}}$ for the appropriate current likelihood $\widehat{L} B$ etc. Then the tree likelihood operator $\hat{L}_{tr}^{(l)}$, obtained by composing pruning maps, will eventually be described by pruning a final cherry, say with nodes $B_f$ and $C_f$, i.e. $\hat{L}_{tr}^{(l)} = \nu_f^{-1} \mathcal{E}_{B_f} (\hat{L} C_f)$, $\nu_f = Tr \hat{L} B_{(f)}$. Then the likelihood at site $l$ is obtained as $L^{(l)} = \nu_f^{-1} Tr(\mathcal{E}_{B_f} (\hat{L} C_f) \rho_x) = \nu_f^{-1} Tr(\hat{L} C_f \mathcal{E}_{B_f} (\rho_x))$, where the dual map $\mathcal{E}_{B_f}^\dagger$ of $\mathcal{E}_{B_f}$ acting on the density matrix is introduced. This situation is extended similarly to the likelihood of the entire alignment by assigning additional site indices $l$ to each likelihood operator, e.g. $\hat{L}_{tr} B$ and $\hat{L}_{tr} C$, as well as trace coefficients $\nu_f^{(l)}$ etc, to obtain $L(T; w^*) = \max_{w^*} \log \prod_{l=1}^L (\nu_f^{(l)})^{-1} Tr(\hat{L}_A (\otimes_{l=1}^L \mathcal{E}_{B_{tr}}^{(l)}) \rho_A)$.

Here $\hat{L}_A \equiv \otimes_{l=1}^L (\hat{L} C_f^{(l)})$ is the product of $L$ different likelihood operators, corresponding to final cherries of the respective trees, employed to construct tree likelihoods. Note that $\otimes_{l=1}^L \mathcal{E}_{B_{tr}}^{(l)}$ is a collective factorized map that can be expressed in terms of a unitary dilation, and this would in principle be implemented by a Hamiltonian quantum model.

In conclusion, this study lays the groundwork for simulating, by quantum mechanical means, the probability tensors of multi-taxon systems, and for estimating the maximal likelihood of a phylogenetic alignment. With the tools developed here, prominent among problems for future investigations would be for example a quantum computational simulation of Steel’s conjecture and its resolution.

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