Quantum field theory and phylogenetic branching

LETTER TO THE EDITOR

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Abstract
A calculational framework is proposed for phylogenetics, using nonlocal quantum field theories in hypercubic geometry. Quadratic terms in the Hamiltonian give the underlying Markov dynamics, while higher degree terms represent branching events. The spatial dimension L is the number of leaves of the evolutionary tree under consideration. Momentum conservation modulo $\mathbb{Z}_2^{\times L}$ in $L \leftarrow 1$ scattering corresponds to tree edge labelling using binary L-vectors. The bilocal quadratic term allows for momentum-dependent rate constants—only the tree or trees compatible with selected nonzero edge rates contribute to the branching probability distribution. Applications to models of evolutionary branching processes are discussed.

PACS numbers: 87.23.Kg, 87.10.+e, 03.70.+k

Evolutionary processes are frequently represented as discrete or continuous time stationary Markov dynamics on some relevant set of system characters. Divergence events correspond to the initiation of two or more sibling processes, which each inherit the character probability distribution of the progenitor and then continue to evolve. It is the task of phylogenetic inference to deduce ancestral interrelationships given observed character probability distributions.

Although the individual ingredients for modelling such branching trees are quite well understood (see, e.g. [1, 2]), to date there is no overall *dynamical* picture for phylogenetics. In this letter we point out that existing tools from physics—namely, quantum field theory and quantum many-body theory—can provide both a theoretical perspective and a calculational framework. In this application the usual state space theory[1] must be interpreted in a stochastic context, for which there are well known transcriptions [3–5]. Below we sketch a general outline of our proposed model; details will be published in a separate paper.

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[1] This letter does not directly touch on more fundamental roles for quantum theory in 'quantum' biology, see for example [9, 10].

Consider a theory with a Hamiltonian of the general form $\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}_1(t)$, with

$$\mathcal{H}_0 = \sum_{x,y} \sum_{\alpha,\beta} \Psi^{\alpha\dagger}(x) \mathcal{M}_\alpha{}^\beta(x-y) \Psi_\beta(y)$$

$$\mathcal{H}_1(t) = \sum_{x,I} \delta(t - t_I) \left(\sum_\alpha W_\alpha^I \Psi^{\alpha\dagger}(x) \Psi_\alpha(x) - \sum_{\alpha,\beta,\gamma} V_{\alpha\beta}^{I\ \gamma} \Psi^{\alpha\dagger}(x) \Psi^{\beta\dagger}(x) \Psi_\gamma(x) \right) \tag{1}$$

for quantized fields $\Psi_\alpha(x)$ of type $\alpha = 1, \ldots, K$. The sum is taken over vertices of a unit hypercube $x, y \in \mathbb{Z}_2^{\times L}$, and the theory is manifestly translation invariant under $x \to x + a$, for $a \in \mathbb{Z}_2^{\times L}$. The interaction times t_I are temporally ordered as $0 = t_0 < t_1 < t_2 < \cdots < t_M < t_{M+1} = T$ where T is the total time for the evolution and $\mathcal{M}$ is the number of branchings that occur during this time. As will be seen below, cubic interaction terms generate branching events, with the additional quadratic terms necessary to ensure that the theory is overall probability conserving [3].

Quantization is imposed in such a way that the time evolution generated by the quadratic Hamiltonian $\mathcal{H}_0$ reproduces the standard Markov dynamics on each mode of the field. Consider the following expansions in momentum space $\mathbb{Z}_2^{\times L}$:

$$\mathcal{M}_\alpha{}^\beta(x-y) = \lambda(x-y) M_\alpha{}^\beta \qquad \lambda(z) = \sum_k \lambda(k) e^{i\pi k \cdot z}$$

$$\Psi_\alpha(x) = \sum_k e^{i\pi k \cdot x} c_\alpha(k). \tag{2}$$

Basis states of the system are Fock states of the form

$$|\alpha_1 k_1 \ \alpha_2 k_2 \ldots \alpha_N k_N\rangle = c_{\alpha_1}^\dagger(k_1) c_{\alpha_2}^\dagger(k_2) \ldots c_{\alpha_N}^\dagger(k_N)|0\rangle \tag{3}$$

where the vacuum is defined as usual by the property of being annihilated by the modes $c_\alpha(k)$. For the evolution of states $|P(t)\rangle$ under the time-independent Hamiltonian $\mathcal{H}_0$, the solution of Schrödinger's equation

$$\frac{\mathrm{d}}{\mathrm{d}t}|P(t)\rangle = -\mathcal{H}_0|P(t)\rangle \tag{4}$$

for evolution after time T, namely

$$|P(T)\rangle = e^{-\mathcal{H}_0 T}|P(0)\rangle \tag{5}$$

must be computed with the help of the canonical commutation relations of the field. At this stage it is only necessary to impose the *trilinear* condition [6]

$$\sum_k [c_\alpha^\dagger(k) c_\beta(k), c_\gamma(\ell)] = \delta^\alpha{}_\gamma c_\beta(\ell). \tag{6}$$

Consider, for example, separable states such as

$$|p(k_1, t)\rangle \otimes |p(k_2, t)\rangle \otimes \cdots \otimes |p(k_N, t)\rangle \tag{7}$$

representing a number of processes evolving in parallel, with each $|p(k, t)\rangle$ a single-particle state corresponding to a probability distribution for characters of an individual process,

$$|p(k, t)\rangle = \sum_\alpha p_\alpha(k, t)|\alpha k\rangle. \tag{8}$$

With (2), (6), *either* fermionic *or* bosonic quantization lead to the time evolution of (7) such that the probability distribution of each individual mode is given by the solution of the appropriate classical master equation,

$$p_\alpha(k, T) = (e^{-\lambda(k)T \cdot M})_\alpha{}^\beta p_\beta(k, 0) \equiv U(k)_\alpha{}^\beta p_\beta(k, 0). \tag{9}$$

Turning to the full, time-dependent Hamiltonian $\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}_1(t)$, (5) must be replaced by the time-ordered exponential

$$|P(T)\rangle = \mathbb{T}\mathrm{e}^{-\int_0^T \mathrm{d}t\mathcal{H}(t)}|P(0)\rangle \qquad (10)$$

which in turn is expressible in the usual way as sums of multiple integrals of time-ordered products $\cdots \mathcal{H}(t')\mathcal{H}(t'') \cdots$. Consider in particular the $L \leftarrow 1$ process, and its evolution kernel representing the corresponding probability distribution of characters. Choose the distinct outgoing momenta in some ordering to be the simple binary vectors $(0, 0, \ldots, 1)$, $(0, \ldots, 1, 0), \ldots$, and $(1, 0, \ldots, 0)$ respectively. Since momentum conservation modulo $\mathbb{Z}_2^{\times L}$ must hold by translation invariance, this fixes the incoming momentum to be the maximal value $(1, 1, \ldots, 1)$. The probability distribution is then a sum over all terms generated by the expansion of the time ordered exponential. Contributions from admissible tree diagrams are enumerated by labelling edges with momenta k, with vertices for interaction times t_I having one incoming and two outgoing momenta k, k', k''. Along edges, the probability distribution $p_\alpha(k, t)$ evolves via (9) for the appropriate time intervals $\Delta_{JI} = (t_J - t_I)$ for $I < J$, so that the effective rate constant is $\kappa(k) \equiv \lambda_k \Delta_{JI}$. At vertices, momentum conservation ensures that a particular character type splits with appropriate sharing of the probability and type between the two subsequent edges (with momenta such that $k = k' + k''$). A plausible description of the divergence event is $V_{\alpha\beta}^{I\ \gamma} \equiv \delta_\alpha{}^\gamma \delta_\beta{}^\gamma$, which means that the two sibling processes commence evolution on their respective edges with characters distributed identically to that of their progenitor. Clearly, the model admits further generalization to nondiagonal or even trilocal or time-smeared interaction terms. Note that the additional diagonal quadratic terms in $\mathcal{H}_1(t)$ are necessary to ensure that the theory is overall probability conserving [3] but do not contribute to the tree diagrams under consideration. The question of *which* tree or trees contribute to $L \leftarrow 1$ scattering is encoded in the bilocal form of $\mathcal{H}_0$ (see (1)). Only momenta k corresponding to nonzero rate constants λ_k are allowed. For computation based on a given tree, it is thus possible to choose nonzero rate constants λ_k for selected momenta corresponding to the binary edge labelling unique to that tree's topology [2].

As an illustration, consider the case $L = 3$, $M = 2$. Nonzero rate constants for the model (1) are chosen for the root and leaf momenta $\vec{7} = (111)$, $\vec{1} = (001)$, $\vec{2} = (010)$ and $\vec{4} = (100)$ respectively, together with a *single* additional momentum $\vec{6} = (110)$ (see figure 1). Write $\mathcal{H}_1(t) = \mathcal{V}^1\delta(t - t_1) + \mathcal{V}^2\delta(t - t_2)$. The time-ordered exponential in (10) may be written as a product,

$$\mathbb{T}\mathrm{e}^{-\int_0^T \mathrm{d}t\mathcal{H}(t)} = \mathbb{T}\mathrm{e}^{-\int_{2^+}^T \mathrm{d}t\mathcal{H}(t)} V_2 \mathbb{T}\mathrm{e}^{-\int_{1^+}^{2^-} \mathrm{d}t\mathcal{H}(t)} V_1 \mathbb{T}\mathrm{e}^{-\int_0^{1^-} \mathrm{d}t\mathcal{H}(t)} \qquad (11)$$

where V_I are time-ordered exponentials for small intervals δ_I covering t_I. These have the form $1 - \mathcal{H}_0\delta_I - \mathcal{V}^I + \cdots$, the higher-order terms being ordered monomials in $\mathcal{H}_0$ and $\mathcal{V}_I$ multiplied by nested δ-function integrals. In the limit $\delta_I \to 0$,

$$\mathbb{T}\mathrm{e}^{-\int_0^T \mathrm{d}t\mathcal{H}(t)} = \mathrm{e}^{-\mathcal{H}_0(T - t_2)}(1 - \mathcal{V}^2 + \cdots)\mathrm{e}^{-\mathcal{H}_0(t_2 - t_1)}(1 - \mathcal{V}^1 + \cdots)\mathrm{e}^{-\mathcal{H}_0 t_1}. \qquad (12)$$

Clearly the contribution to the $3 \leftarrow 1$ scattering probability associated with the tree of figure 1 is, as required, the unique nonzero term arising from inserting intermediate states in the above with the correct intermediate edge momenta, giving finally

$$\langle \alpha_{\vec{1}}\vec{1}\ \alpha_{\vec{2}}\vec{2}\ \alpha_{\vec{4}}\vec{4}\ |\mathrm{e}^{-\mathcal{H}_0(T - t_2)}\mathcal{V}^2\mathrm{e}^{-\mathcal{H}_0(t_2 - t_1)}\mathcal{V}^1\mathrm{e}^{-\mathcal{H}_0 t_1}|p(\vec{7}, 0)\rangle = \sum U(\kappa_{\vec{2}})_{\alpha_{\vec{2}}}{}^{\beta_{\vec{2}}} U(\kappa_{\vec{4}})_{\alpha_{\vec{4}}}{}^{\beta_{\vec{4}}} V_{\beta_{\vec{2}}\beta_{\vec{4}}}^2{}^{\gamma_{\vec{6}}}$$

$$\times U(\kappa_{\vec{6}})_{\gamma_{\vec{6}}}{}^{\beta_{\vec{6}}} U(\kappa_{\vec{1}})_{\alpha_{\vec{1}}}{}^{\beta_{\vec{1}}} V_{\beta_{\vec{1}}\beta_{\vec{6}}}^1{}^{\beta_{\vec{7}}} \cdot U(\kappa_{\vec{7}})_{\beta_{\vec{7}}}{}^{\alpha_{\vec{7}}} p_{\alpha_{\vec{7}}}(\vec{7}, 0).$$

In phylogenetics, the probability distributions or dispersion tensors of characters of interest are given directly from observations. Whether these are compatible with calculations for a
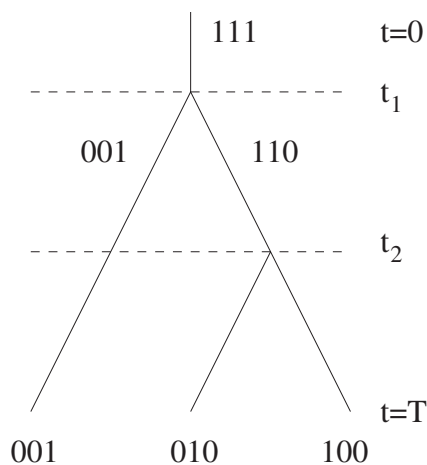
Figure 1. Binary labelling scheme for a tree on three leaves ($L = 3$) with branching events at intermediate times t_1, t_2. Nonzero rate constants for the model (1) are chosen for the root and leaf momenta $\vec{7} = (111)$, $\vec{1} = (001)$, $\vec{2} = (010)$ and $\vec{4} = (100)$ respectively, together with a *single* additional momentum $\vec{6} = (110)$.

specific tree remains a question of statistics. Our model (1) relates phylogenetic inference for evolutionary processes to a scattering problem for the associated quantum field theory. Each 'particle' represents a species and 'particle scattering' corresponds to speciation events. Tree diagrams in the theory correspond literally to possible branching trees describing ancestral relationships amongst observed species.

The overall framework provided by giving a definite dynamical model for the branching process has potentially wide applicability. At the formal level, for example recent work using Fourier–Hadamard inversion techniques for phylogenetic reconstruction in molecular phylogenetics [7, 8] has a natural interpretation in our model in terms of working with position states rather than in the momentum representation. Calculationally, quantities such as correlations between various character states are straightforward to compute in terms of expectation values of appropriate operators as in applications in statistical physics [3–5]. As already mentioned the picture can be extended by embellishment of various features, such as vertex decorations. It is also possible to effect a separation of the underlying substitution model into a systematic part reflecting different substitution frequency types, and a more random Poissonian background, and to calculate the effects of the latter perturbatively. Details of the model, and prospects for such extensions, will be published in a separate paper.

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