Applying the Variational Principle to (1 + 1)-Dimensional Quantum Field Theories

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We extend the recently introduced continuous matrix product state variational class to the setting of (1 + 1)-dimensional relativistic quantum field theories. This allows one to overcome the difficulties highlighted by Feynman concerning the application of the variational procedure to relativistic theories, and provides a new way to regularize quantum field theories. A fermionic version of the continuous matrix product state is introduced which is manifestly free of fermion doubling and sign problems. We illustrate the power of the formalism by studying the momentum occupation for free massive Dirac fermions and the chiral symmetry breaking in the Gross-Neveu model.

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The variational principle is the basis for a tremendous number of highly successful calculational tools in many-body physics. Examples range from density functional theory [1] to Wilson's numerical renormalization group [2] and the density matrix renormalization group (DMRG) in condensed matter physics [3]. However, in relativistic quantum field theory (QFT) the variational principle has not met with the same success as in other areas of many-body physics. The core reasons for this were identified by Feynman [4], who in one of his last lectures summarized that (1) the variational principle is "too sensitive" to high frequencies, and (2) only the Gaussian ansatz combines extensivity with the ability to compute observable quantities efficiently and to high accuracy.

Recently a new class of variational wave functionals for (1 + 1)-dimensional QFTs has been introduced [5] based on the matrix product state construction [6], which lies at the heart of the success of the DMRG. Compelling evidence that continuous matrix product states (cMPSs) provide a powerful description of the quantum fluctuations of quantum fields has been presented in [5,7]. So far, cMPSs have been restricted to the approximation of ground states of nonrelativistic theories. An explicit specification of the ground state is not a common approach to study relativistic QFTs. Nevertheless, this formalism is well established (see [8] and references therein).

The DMRG [3] is, with the benefit of hindsight, a variational method within the class of matrix product states. Since its development, a better understanding of how quantum entanglement behaves in local quantum systems has led to an explosion in the development of variational wave functions for strongly interacting quantum systems. These wave functions, going well beyond Gaussian trial states, allow the accurate and efficient calculation of observable quantities. Thus Feynman's second objections can already be regarded as having been addressed, in the case where matrix product states are applied to quantum fields in conjunction with a lattice regulator [9]. By taking a continuum limit of the matrix product state class, the need for a lattice regulator was removed, allowing the definition of a variational class of non-Gaussian wave functionals directly for quantum fields.

In his closing remarks, Feynman speculated how best to overcome his second reservation and predicted that it should be possible to describe a global field state using a reduced set of local parameters, and he foresaw the role of the density matrix in such a description. It turns out that the density matrix in DMRG has precisely the properties envisaged by Feynman: it yields a local parametrization of the global properties of a state which is living on the boundary of the region of interest. The cMPSs inherit this holographic property: they are parametrized by the (nonequilibrium) dynamics of a boundary field theory of one lower geometric dimension [5,10]. The state of this auxiliary theory constitutes a compact description of the properties of the quantum field state outside the given region.

It is, however, less clear how the cMPS class will be able to escape Feynman's first objection, which is intrinsic to the variational principle and its attempt to find the "lowest" ground-state energy. This problem occurs in any theory with a large range of interacting energy scales, but is truly catastrophic in relativistic field theories. To lowest order, the ground state of a relativistic quantum field consists of the zero-point oscillations of all energy scales and is thus dominated by the infinite availability of high frequencies. In contrast, quantities of physical interest are related to the low-frequency modes. The variational principle will exploit all variational parameters to obtain the best description of the UV degrees of freedom at the expense of the relatively tiny energy penalty coming from the ill-described low frequencies. Whenever the variational parameters affect both the low and high frequencies, which is unavoidable in interacting theories but also true for free theories with a real space approach, this can lead to the paradoxical situation where the addition of variational parameters provides a *worse* approximation to physical quantities.

In this Letter we show how cMPSs naturally address Feynman's remaining criticism of the variational principle in relativistic QFT. In doing so we discover a new way to regulate QFTs and develop a powerful new way to numerically solve them.

While Feynman's argument is valid both for bosonic and fermionic theories, we focus on fermionic theories where the Dirac sea picture can be exploited. We now define the fermionic cMPS class as

$$|\chi\rangle = \mathrm{Tr}_{\mathrm{aux}}[\mathcal{P}e^{\int_{-\infty}^{+\infty} dx Q\otimes \mathbb{1} + \sum_{\alpha} R_\alpha \otimes \hat{\psi}_\alpha^\dagger(x)}]|\Omega\rangle, \qquad (1)$$

where $\hat{\psi}_\alpha^\dagger(x)$ are field operators creating fermions of type α at position x with anticommutation relations $\{\psi_\alpha^\dagger(x), \psi_\beta^\dagger(y)\} = 0$ and $\{\psi_\alpha^\dagger(x), \psi_\beta(y)\} = \delta_{\alpha,\beta}\delta(x-y)$, Q and R_α are $D\times D$ matrices acting on the auxiliary system, $\mathrm{Tr}_{\mathrm{aux}}$ denotes a partial trace over the auxiliary system, and $\mathcal{P}e$ denotes the path ordered exponential. While Q and R_α can be position dependent, we focus on a translational-invariant setting where they are not. Both the calculational rules, as well as the physical interpretation for bosonic cMPSs can be found in [5,10] and only differences resulting from the anticommutation relations will be highlighted. In the relativistic scenario, the two field operators $\hat{\psi}_\alpha^\dagger$ ($\alpha = 1, 2$) in Eq. (1) represent the two components of the Dirac spinor. The state $|\chi\rangle$ will approximate the ground state of a relativistic QFT by acting with the field creation operators on the state $|\Omega\rangle$, for which all levels are empty ($\hat{\psi}_\alpha|\Omega\rangle = 0$).

Let us now describe physical properties of this variational class. It is a non-Gaussian class that is both extensive and allows the exact evaluation of the expectation values of local operators; e.g., we obtain (we henceforth use the summation convention on repeated indices)

$$\mathrm{Im}\langle\chi|\hat{\psi}_\alpha^\dagger\sigma^y_{\alpha\beta}\frac{d\hat{\psi}_\beta}{dx}|\chi\rangle = \mathrm{Im}[\sigma^y_{\alpha\beta}\langle l|[Q, R_\alpha]_- \otimes \bar{R}_\beta|r\rangle],$$

for the kinetic energy density, where, in order to obtain real coefficients, we have chosen the convention $\alpha^x = \sigma^y$ and $\beta = \sigma^z$ for the Dirac matrices. The D^2 component vectors $\langle l|$ and $|r\rangle$ are, respectively, the left and right eigenvectors of the transfer matrix $T = Q\otimes\mathbb{1} + \mathbb{1}\otimes\bar{Q} + R_\alpha\otimes\bar{R}_\alpha$, corresponding to eigenvalue zero [5,10]. We focus on the kinetic energy density as it is the dominant term in the UV region, which is the region responsible for divergences and for Feynman's criticism. As long as the $D\times D$ matrices Q and R_α have finite entries, this expression will be finite and is thus regularized.

A better understanding of this regularization is gained by looking at the momentum occupation in a cMPS: $\langle\chi|\hat{\psi}_\alpha^\dagger(k)\hat{\psi}_\beta(k')|\chi\rangle = \delta(k-k')n_{\alpha,\beta}(k)$ [11]. The momentum occupation number $n_{\alpha,\beta}(k)$ is the Fourier transform of $C_{\alpha\beta}(x)$, where

$$C_{\alpha,\beta}(x) = \begin{cases} \langle l|(\mathbb{1}\otimes\bar{R}_\alpha)e^{x\tilde{T}}(R_\beta\otimes\mathbb{1})|r\rangle, & x<0 \\ \langle l|(R_\beta\otimes\mathbb{1})e^{x\tilde{T}}(\mathbb{1}\otimes\bar{R}_\alpha)|r\rangle, & x>0, \end{cases}$$

and $\tilde{T} = Q\otimes\mathbb{1} + \mathbb{1}\otimes\bar{Q} - R_\alpha\otimes\bar{R}_\alpha$, where the last minus sign originates from the Fermi statistics of the particles. There will not be any disconnected contribution, as we require $\langle\chi|\hat{\psi}_\alpha|\chi\rangle = 0$. The behavior of $n_{\alpha,\beta}(k)$ for large k is determined by the continuity and differentiability of $C_{\alpha,\beta}$, in particular, around $x = 0$, which is the only point where differentiability is not trivially guaranteed. Since $C_{\alpha,\beta}(x)$ is a continuous function its Fourier transform decays as $n_{\alpha\beta}(k) \le \mathcal{O}(k^{-2})$ for $|k|\to\infty$. Continuity of the derivative of $C_{\alpha,\beta}(x)$ at $x = 0$ requires

$$\langle l|\{R_\beta, R_\gamma\}\otimes\{\bar{R}_\alpha, \bar{R}_\gamma\}|r = 0, \quad \forall\ \alpha, \beta, \qquad (2)$$

which satisfied by choosing all matrices R_α nilpotent and anticommuting. The second derivative of $C_{\alpha,\beta}(x)$ at $x = 0$ is then automatically continuous, from which one can conclude that $n_{\alpha,\beta}(k) \le \mathcal{O}(k^{-4})$ for $|k|\to\infty$. While a faster decrease of the momentum occupation number imposes additional constraints on the matrices Q and R_α the current behavior already ensures a finite kinetic energy. The region in momentum space where the k^{-4} decay behavior sets in defines a soft momentum cutoff Λ.

Let us now illustrate how Feynman's first objection manifests itself for the cMPS ansatz. The problem is situated in a cMPS's ability to describe a change of scale $x\mapsto cx$, $c>0$, by an equivalent transformation $Q' = cQ$ and $R'_\alpha = \sqrt{c}R_\alpha$. This transformation does not change $\langle l|$ and $|r\rangle$. Thus the kinetic energy per unit length will simply be multiplied by a factor c^2. However, in contrast to the nonrelativistic case, the relativistic kinetic energy is not a positive definite operator and can acquire a negative expectation value. If $|\chi\rangle$ is a cMPS for which this is the case, the kinetic energy can be lowered by making a scale change with $c>1$. Any variational approach will then try to push $c\to\infty$, in order to approximate the divergent kinetic energy of the exact solution. Correspondingly, the momentum occupation changes to $n'_{\alpha,\beta}(k) = n_{\alpha,\beta}(k/c)$ and the intrinsic cutoff determined by n' is given by $\Lambda' = c\Lambda$.

This change of scale will be accompanied by a worse description of the low-frequency region, as predicted by Feynman. The reason is that a cMPS can only accurately describe states with a finite amount of entanglement. The maximal entanglement entropy in a $1D$ system with energy gap Δ and energy cutoff Λ will roughly be given by $S\sim\log(\Lambda/\Delta)$, and a cMPS with D proportional to $\mathcal{O}(\exp(S))$ should suffice to provide a good description [12]. If D is too low, compromises will be made in that part of the frequency spectrum which contributes least to the ground-state energy, i.e., the low-frequency region. In nonrelativistic systems, the cutoff is related to the particle density. In a relativistic field theory there is no physical cutoff, only the intrinsic momentum cutoff Λ of the cMPS. Given some cMPS which already fills negative-energy levels up to Λ, the variational procedure will lower the energy, not by improving the filling, but by shifting the cutoff to $\Lambda' = c\Lambda$ with $c \to \infty$. For every finite D, all low-energy modes will eventually fall into the region that is poorly described. This is schematically illustrated in Fig. 1. If the cMPS actually succeeds in letting c run to infinity, the description at any observable energy will be completely off.

However, a solution is now straightforward as we can prevent c from running to infinity by imposing a constraint on the matrices Q and R_α: Eq. (1) indicates that Q has the dimension of momentum, while R_α has the dimension of the square root of a momentum, constraining the norm of Q and R_α prevents c from running and regularizes the resulting theory by introducing a scale, i.e., a dimensionful parameter, into the system, similar to what happens in analytical regularization techniques or lattice regularization. In the following, we will constrain the norm of the commutator $[Q, R_\alpha]$ by fixing the expectation value of $(d\hat{\psi}^\dagger/dx)\,(d\hat{\psi}/dx)$ [13]. Hereto, we add this term to the Hamiltonian with a Lagrange multiplier $1/\Lambda$, i.e., $\hat{H}_{\text{cutoff}} = \Lambda^{-1}\int dx (d\hat{\psi}^\dagger/dx)(d\hat{\psi}/dx)$. This apparently arbitrary choice is motivated by the requirement that the constraint needs to penalize high values of the momentum k, to which $[Q, R_\alpha]$ is related by the calculational rules of cMPS. H_{cutoff} will give a k^2 contribution in momentum space, which is low enough to ensure a finite result in combination with a momentum occupation that decays as k^{-4}. It is, however, strong enough to penalize high-frequency modes, even the ones that give a contribution $-|k|$ to the (kinetic) energy. It also respects the chiral symmetry of the kinetic energy term. It does of course break relativistic invariance, which is inevitable when introducing a momentum cutoff in a Hamiltonian framework. We would like to stress that our approach is not specific to this term. We expect that any norm constraint respecting the symmetries of the system should also be sufficient.

We now illustrate our arguments by applying them to relativistic fermionic QFTs. Note that we have given a central role to the kinetic energy term, which dominates the UV regime, and that the approach is insensitive to the nature of the additional terms in the Hamiltonian, whether they are quadratic or interacting. However, we would first like to test our approach with an exactly solvable model and consider free massive Dirac fermions with Hamiltonian density

$$\hat{h}_D = -\frac{i}{2}\hat{\psi}^\dagger(x)\sigma^y\frac{d\hat{\psi}}{dx}(x) + \text{H.c.} + m\hat{\psi}^\dagger(x)\sigma^z\hat{\psi}(x),$$

with Dirac matrices chosen as described above, and m the fermion mass. Because the cutoff term acts trivially on the spinor components, it will not mix the particle and antiparticle levels of the Dirac Hamiltonian. Adding $\hat{H}_{\text{cutoff}}$ to $\hat{H}_D$ will only introduce a sharp cutoff for the negative (antiparticle) energy levels at $k_{\text{cutoff}} = \Lambda(1 + \mathcal{O}(m^2/\Lambda^2))$. The cMPS ansatz will not be able to reproduce this sharp cutoff because it decays as k^{-4}. To test the accuracy of the description of low-frequency region, we have calculated the momentum occupation of the exact positive (particle) and negative (antiparticle) levels. With $\hat{\psi}_\pm(k)$ annihilating a particle from the exact negative (positive) energy level at momentum k [14], we define

$$\langle\hat{\psi}_+^\dagger(k)\hat{\psi}_+(k')\rangle \sim n^{++}(k), \qquad \langle\hat{\psi}_-^\dagger(k)\hat{\psi}_-(k')\rangle \sim n^{--}(k),$$
$$\langle\hat{\psi}_+^\dagger(k)\hat{\psi}_-(k')\rangle \sim n^{+-}(k), \qquad \langle\hat{\psi}_-^\dagger(k)\hat{\psi}_+(k')\rangle \sim n^{-+}(k),$$

where the proportionality factor $\delta(k - k')$ has been omitted for brevity. The exact solution has $n^{--}(k) = 1$ all the way up to k_{cutoff}, after which $n^{--}(k) = 0$ for $|k| > k_{\text{cutoff}}$, and $n^{++}(k) = n^{+-}(k) = 0$, $\forall\, k$. Results are shown in Fig. 2 and were obtained using the cMPS ansatz where Q and R_α act on an auxiliary Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^D$. The first two two-dimensional Hilbert spaces accommodate auxiliary fermions which are used to impose the anticommutation relations Eq. (2) on R_α. The optimal matrices were determined using an evolution in imaginary time. It is clear from these results that the low-energy behavior is approximated very well for the massive Dirac theory, and the accuracy greatly increases by increasing D. As anticipated, the cutoff behavior is approximated less well.

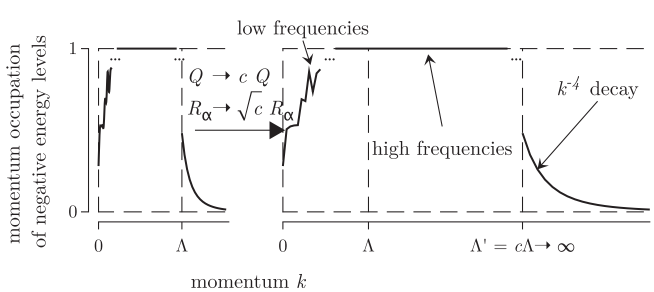

FIG. 1. Hypothetical momentum distribution of an optimal cMPS for a free fermionic theory: high-frequency degrees of freedom are well approximated up to a cutoff Λ, after which the momentum occupation decays as k^{-4}. Also shown is the effect of a scale transformation.

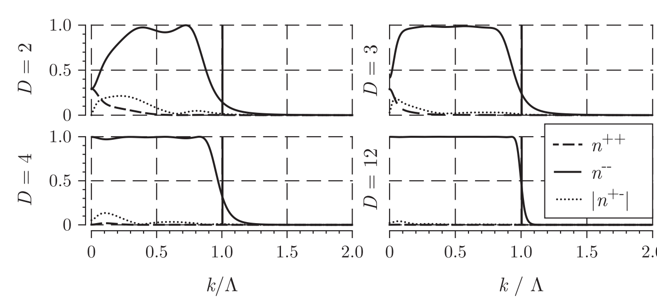

FIG. 2. Momentum occupation of the antiparticle levels $n^{--}(k)$, the particle levels $n^{++}(k)$ and the mixing $|n^{+-}(k)|$ in a cMPS approximation of the Dirac field with mass $m/\Lambda = 1/10$. The auxiliary space of the cMPS is $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^D$. The vertical line indicates the position of the exact cutoff.

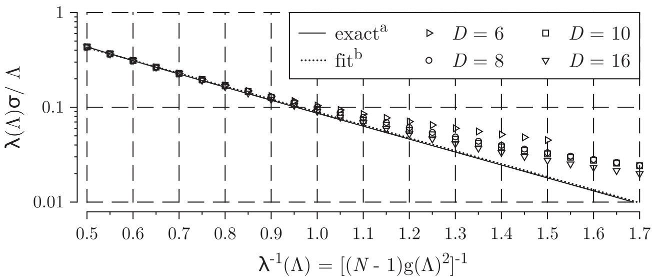

FIG. 3. Expectation value of $\sigma = \langle\chi|\hat{\psi}^\dagger\sigma^z\hat{\psi}|\chi\rangle$ in the Gross-Neveu model as function of $\lambda(\Lambda)$ for $N = \infty$. The solid line is the exact result $|\lambda\sigma|/\Lambda \approx 2e^{-\pi/\lambda}$ and follows from Eq. (3). The dotted line shows a fit of the form $c_1 e^{-c_2/\lambda}$ to the numerical results for $\lambda^{-1} \leq 1$ at $D = 16$ and results in $c_2 = 3.142^{+0.047}_{-0.047}$ and $c_1 = 2.057^{+0.074}_{-0.072}$.

As a final proof of principle, we study a theory with interactions. One of the most important models for one-dimensional relativistic fermions is the Gross-Neveu model, as it shares many features with QCD [15], including asymptotic freedom and spontaneous breaking of chiral symmetry. The Hamiltonian density for the N-flavor Gross-Neveu model is given by

$$\hat{h}_{\text{GN}} = -\frac{i}{2}\hat{\psi}^\dagger_a\sigma^y\frac{d\hat{\psi}_a}{dx} + \text{H.c.} - \frac{g^2}{2}:(\hat{\psi}^\dagger_a\sigma^z\hat{\psi}_a)^2:,$$

where the x dependence of the field operators has been omitted for brevity and there is an implied summation over the flavor index $a = 1, 2, \ldots, N$. One must not forget to apply normal ordering when deriving an interacting Hamiltonian from the coherent-state path integral of a relativistic fermionic QFT. Since we add $\hat{H}_{\text{cutoff}}$, in which Λ is our regularization parameter, we know that the coupling constant g will have to depend on Λ in order to have a consistent theory. The theory is completely determined by specifying the parameters N and $\lambda(\Lambda) = g(\Lambda)^2(N-1)$. In the $N \to \infty$ limit, we can solve this problem exactly, and we obtain the well-known result for $\sigma = \langle\chi|\hat{\psi}^\dagger\sigma^z\hat{\psi}|\chi\rangle$

$$\frac{\pi}{\lambda} = \int_0^{k_{\text{cutoff}}}\frac{dk}{\sqrt{\lambda^2\sigma^2 + k^2}} \tag{3}$$

where $k_{\text{cutoff}} \approx \Lambda(1 + \mathcal{O}(|\lambda\sigma|^2/\Lambda^2))$. This indicates that the cutoff fixing term $\hat{H}_{\text{cutoff}}$ has no effect other than what it is meant to be doing, i.e., introducing a cutoff.

As a variational ansatz we employ a product state of cMPSs across the different fermion flavors, which can also be optimized over with the imaginary time evolution algorithm. Because the exact ground state has $\mathcal{S}_N$ flavor symmetry [and actually O($2N$) symmetry], we can thus use the same cMPS for every flavor. This amounts to a Hartree-Fock approximation of the theory, where the self interaction of the flavor is treated exactly, and the self-consistent mean-field approach is only applied to the interactions between different flavors.

Numerical results for σ as function of λ for $N = \infty$ are illustrated in Fig. 3. The discrepancies between the exact solution and the cMPS approximation are clearly finite-D effects. They become more pronounced as $\lambda\sigma/\Lambda$ gets smaller, since $\lambda\sigma$ is precisely the mass gap in the $N = \infty$ limit. By fitting an exponential, we obtain absolute scaling of the data, where we reproduce the coefficient in the exponential, which is related to the first coefficient in the β function of the coupling constant, with a relative accuracy of about 1%. A detailed analysis of the result both for $N = \infty$ and finite N will be presented elsewhere.

In this Letter we have argued that cMPSs offer a new way to regularize quantum field theories and are, as a variational class, not susceptible to Feynman's objections. Our approach is free of fermion doubling and sign problems.

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