Hamiltonian truncation methods in QFT

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Based on works with S. Rychkov, J. Elias-Miro
How to extract quantitative predictions about a strongly-coupled, non-integrable quantum field theory in any $d$?

Long-term goal: numerical solution of QCD in 4 dimensions

*Lattice Monte Carlo methods* have been developed for decades. Alternative: variational methods.

In this talk: “Hamiltonian truncation” method to extract the *spectrum* of a non-perturbative QFT
Rayleigh-Ritz methods in QM are efficient to find the low-energy spectrum

\[ H = H_0 + V \]

Compute \( H \) in basis of eigenstates of \( H_0 \)

\[
H_0|i\rangle = E_i|i\rangle \\
H_{ij} = E_i\delta_{ij} + \langle i|V|j\rangle
\]

Truncate to \( i \leq N_{\text{max}} \) and diagonalize \( H_{ij} \). Extract numerical eigenvalues \( \mathcal{E}_{RR} \).

Ideally take the limit \( N_{\text{max}} \to \infty, \mathcal{E}_{RR} \to \mathcal{E} \).
Example: Anharmonic oscillator

\[ H_0 = \frac{1}{2} \left( p^2 + x^2 \right), \quad V = x^4 \]

- Exponential convergence
- \( \epsilon_{RR} - \epsilon \) from above (min-max theorem).
Integrable or solvable Hamiltonian plus (local) deformations

\[ H = H_0 + \sum_i g_i \int V_i(x) \]

How to compute the observables in the IR?

- Gapped?
- Spontaneous symmetry breaking?
- Spectrum and S-matrix
Consider deforming a CFT by a local, relevant operator $\mathcal{V}$ with conformal dimension $\Delta_{\mathcal{V}}$.

$$S = S_{\text{CFT}} + g \int d^d x \mathcal{V}(x)$$

CFT uniquely defined by a set of operators $\mathcal{O}_i$, conformal dimensions $\Delta_i$ and OPE coefficients $f_{i,j,k}$

$$[D, \mathcal{O}_i(0)] = \Delta_i \mathcal{O}_i(0), \quad \langle \mathcal{O}_i(x) \mathcal{O}_j(y) \mathcal{O}_k(z) \rangle \propto f_{\mathcal{O}_i \mathcal{O}_j \mathcal{O}_k}$$

Yurov, A.B. Zamolodchikov, 1990
Lassig, Mussardo, Cardy 1991
Klassen, Melzer 1991
James, Konik, Lecheminant, Robinson, Tsvelik, 2017
Define Hamiltonian on the cylinder via Weyl transformation

\[ H = H_{CFT} + V \]

\[ \langle i | H_{CFT} | j \rangle = L^{-1} \Delta_j \delta_{ij} \]

\[ \langle i | V | j \rangle \propto L^{-1} (g L^{d-\Delta_V}) f_{\mathcal{O}_i \mathcal{O}_j} \]

Cylinder radius \( L \) acts as IR regulator

Truncate \( H_{ij} \) up to \( \Delta_i \leq \Delta_{\text{max}} \) and diagonalize it.

Read off low-energy spectrum and take limit \( E_T = L^{-1} \Delta_{\text{max}} \rightarrow \infty \)
HT in general successfully applied to many 2-dimensional systems in and out of equilibrium. Examples:

- Transverse Ising perturbed by longitudinal field Fonseca, Zamolodchikov, 2003
- Tricritical Ising deformed by energy operator Lässig, Mussardo, Cardy, 1991
- Sine-Gordon model Feverati, Ravanini, Tacaks, 1999
- . . .

TCSA is suited for studying RG flows starting from (strongly)-interacting CFTs, assuming they are known (analytically or numerically via conformal bootstrap).
Convergence

- Convergence w.r.t. $L$ is fast: corrections are exponentially small in $L m_{\text{phys}}$ (in gapped phase)


- What is the convergence w.r.t $E_T$?

- How to improve the convergence rate?
Case study: $\phi^4$ in $d = 2$

$$\mathcal{L}_E = \frac{1}{2} (\partial \phi)^2 + \frac{1}{2} m^2 \phi^2 + g \phi^4, \quad m \equiv 1$$

Hogervorst, Rychkov, Van Rees, 2014, (d = 2.5)
Brandino, Konik, Mussardo, 2014
Bajnok, Lajer, 2015
Elias-Miro, Rychkov, LV, 2017

- Not integrable
- Can tune $g$ from weak to strong coupling
- $\mathbb{Z}_2$ symmetry $\phi \leftrightarrow -\phi$ in perturbative region. Is it preserved at strong coupling? (Phase transition at $g = g_c \approx 3$)
- No UV divergences (absorbed by normal ordering) for $d < 2.66$
Massive Fock space basis

- Define unperturbed Hamiltonian as massive Hamiltonian
  \[ H_0 = \frac{1}{2} \left( \partial \phi \right)^2 + \frac{1}{2} m^2 \phi^2 \]

- Construct basis of eigenstates out of momentum modes, in the zero total momentum sector
  \[ |\psi\rangle = a_{k_1}^\dagger \cdots a_{k_n}^\dagger |0\rangle, \quad \sum_i k_i = 0 \]
  \[ H_0 = \sum_k \omega_k a_k^\dagger a_k, \quad \omega_k = \sqrt{k^2 + m^2} \]

- Impose periodic boundary condition in finite volume \( k_i = \frac{2\pi n_i}{L} \)

- Compute matrix elements of \( V = g \int_0^L dx \phi^4(x) \), truncate \( H = H_0 + V \) to states with energy \( E \leq E_T \) and diagonalize it.

- \( H \) is sparse, so there are efficient diagonalization routines for low-energy spectrum (e.g. Lanczos)
Spectrum dependence on cutoff

- HT converges for $E_T \to \infty$. In this plot up to $\sim 10^7$ states included.
Composition of ground state

\[
w(E) \equiv \sum_{E_i \in [E, E+1]} |\langle \psi_i \mid \psi_{\text{vac}} \rangle|^2
\]

- No real separation between low energy and high energy d.o.f.s.
- However, high energy states decouple. How to exploit that?
Renormalization

- Divide the Hilbert space in low-energy and high-energy sectors:
  \[ \mathcal{H} = \mathcal{H}_l \oplus \mathcal{H}_h \]

\[
\begin{pmatrix}
H_{ll} & V_{lh} \\
V_{hl} & H_{hh}
\end{pmatrix}
\begin{pmatrix}
cl \\
ch
\end{pmatrix}
= \mathcal{E}
\begin{pmatrix}
cl \\
ch
\end{pmatrix}, \quad H_{ll} \equiv P_l H P_l
\]

\[
|\psi\rangle = \sum_{i=1}^{\dim \mathcal{H}_l} (c_l)_i |i\rangle + \sum_{j=1}^{\infty} (c_h)_j |j\rangle
\]

- Integrate out \( c_h \)

\[ c_h = (\mathcal{E} - H_{hh})^{-1} V_{hl} c_l \]

- Write down exact effective equation for low energy degrees of freedom

\[
(H_{ll} + \Delta H(\mathcal{E})) \cdot c_l = \mathcal{E} c_l
\]

\[
\Delta H(\mathcal{E}) = V_{lh} \cdot (\mathcal{E} - H_{hh})^{-1} \cdot V_{hl}
\]

Hogervorst, Rychkov, Van Rees, 2014

\( \Delta H(\mathcal{E}) \) measures the convergence error of the method

Approximate \( \Delta H(\mathcal{E}) \) by fixing \( \mathcal{E} \sim \mathcal{E}_* \) and expanding in powers of the perturbation

\[
\Delta H(\mathcal{E}) = V_{lh} \cdot \frac{1}{\mathcal{E} - H_{0hh} - V_{hh}} \cdot V_{hl} \simeq \Delta H_2 + \Delta H_3 + \ldots
\]

\[
\Delta H_2 = V_{lh} \cdot \frac{1}{\mathcal{E}_* - H_{0hh}} \cdot V_{hl}
\]

\[
\Delta H_3 = V_{lh} \cdot \frac{1}{\mathcal{E}_* - H_{0hh}} \cdot V_{hh} \cdot \frac{1}{\mathcal{E}_* - H_{0hh}} \cdot V_{hl}
\]

Truncation error comes from mixing between low and high energy states.
Local approximation

- $\Delta H_2$ is a non-local operator. Approximate by local expansion
  \[ \Delta H_2 \simeq \Delta H_2^{\text{loc}} = \sum_i \kappa_i(E_T) \int \mathcal{O}_i \]

- The leading term is the vacuum renormalization, $\mathcal{O}_0 = 1$
  \[ \kappa_0(E_T) \propto g^2 E_T^{2\Delta_V - d} \]

- For $\Delta_V < d/2$ renormalization is finite and HT converges. For $\Delta_V \geq d/2$ there are UV divergences to be subtracted (not yet treated in detail the literature)
Renormalization: local approximation

- Local approximation can be taken seriously to reduce convergence error ("local LO" procedure)
  \[
  (H_{ll} + \Delta H_{2}^{\text{loc}}).c_l = \mathcal{E}_{\text{loc}}.c_l
  \]

- Local approximation of $\Delta H_2$ works well for states well below the cutoff. States just below the cutoff are unimportant empirically.

- It has been applied to many examples. Here we will see the application to the $\phi^4$ model in 2d.
Plot of subtracted spectrum $\mathcal{E}_I - \mathcal{E}_0$ vs. quartic coupling

- $\mathbb{Z}_2$ symmetry breaking at $g > g_c$.
- Exponential finite volume corrections for $g \neq g_c$. 

$R = 2(- -), 2.5(- -), 3(- -)$
In this paper we investigated the two dimensional theory in the broken phase by the massive generalization of the truncated conformal space approach. We called this method the truncated Hilbert space approach and we developed a code based on the diagonalization of large sparse matrices to diagonalize the truncated dimensionless Hamiltonian. We determined the spectrum numerically for various volumes and quartic couplings and both for periodic and antiperiodic boundary conditions. In the periodic case we found it useful to adapt the mini superspace approach. We compared the results with semiclassical calculations and also with finite size corrections. These finite size corrections are expressed in terms of the infinite volume masses and scattering matrices, for which we proposed parametrizations from the unitarity relations. We summarized the infinite volume mass spectrum and scattering parameter as functions of the coupling on Figure 24.

![Graph showing mass spectrum vs coupling]

- Kink mass can be computed also from splitting of degenerate vacua in periodic sector, \((E_1 - E_0) \sim e^{-M_{\text{kink}}L}\). Agreement with semiclassical result.
$\mathbb{Z}_2$-broken phase

- In this model there is an interesting duality relating theories with opposite sign of squared mass [Chang, 1976]

$$\frac{1}{2}(\partial\phi)^2 + \frac{1}{2}m^2\phi^2 + g\phi^4 \leftrightarrow \frac{1}{2}(\partial\phi)^2 - \frac{1}{2}M^2\phi^2 + g\phi^4$$

- It allows us to study the theory in the very strongly coupled region $g \gg g_c$ as a theory with negative $m^2$ and small coupling.

- We modify the Fock space massive basis to deal with this case. Solve for the QM of the zero mode first, then it becomes weakly coupled with the other modes.

\[
H' = \tilde{H}_0 + \hat{H} + W,
\]

\[
\hat{H} \equiv \frac{\pi^2}{2L} - \frac{1}{4}L M^2: \phi_0^2: + L g : \phi_0^4 : ,
\]

\[
W \equiv \left[ 6g: \phi_0^2: - \frac{3}{4}M^2 \right] \bar{V}_2 + 4g\phi_0 \bar{V}_3 + g \bar{V}_4
\]
Convergence greatly improved over Hamiltonian without renormalization ("raw")

- There are non-smooth fluctuations due to hard cutoff in $E_T$, which make it hard to perform a controlled extrapolation.
Improve renormalization?

- It is hard to go beyond $\sim 10^7$ states, corresponding to $E_T \sim 35$. Problem made worse in higher dimensions and for more relevant operators

$$D = \dim(\mathcal{H}_l) \sim e^{\#(LET)^{1-1/d}}$$

- Expansion $\Delta H = \Delta H_2 + \Delta H_3 + \ldots$ is not convergent for all entries of $\Delta H$. Including $\Delta H_3$ makes convergence worse

Elias-Miro, Montull, Riembau, 2015

- Need a renormalization procedure which is better both numerically and conceptually

- Basic idea: add a carefully constructed set of states to the variational Ansatz.
Renormalization via tails

Let us go back to the key equation

\[ c_h = (\mathcal{E} - H_{hh})^{-1} V_{hl} c_l \]

Define a finite subspace \( \mathcal{H}_{RR} = \mathcal{H}_l \oplus \mathcal{H}_t \) where \( \mathcal{H}_t \) is spanned by optimal “tail” states

\[ |\Psi_i\rangle = (\mathcal{E} - H_0 - V_{hh})^{-1} V_{hl} |i\rangle \]

Diagonalizing \( H \) in this subspace would reproduce the exact wavefunctions.

\[ |\psi\rangle = \sum_{i=1}^{D} (c_l)_i |i\rangle + \sum_{j=1}^{D} (c_t)_j |\Psi_j\rangle \]

For practical purposes we consider \textit{approximate} tail states

\[ |\Psi_i\rangle \simeq (\mathcal{E}_* - H_0)^{-1} V_{hl} |i\rangle \]
The truncated eigenvalue equation becomes
\[
\begin{pmatrix}
  H_{ll} & H_{lt} \\
  H_{tl} & H_{tt}
\end{pmatrix}
\begin{pmatrix}
  c_l \\
  c_t
\end{pmatrix}
= E_{RR}
\begin{pmatrix}
  1 & 0 \\
  0 & G_{tt}
\end{pmatrix}
\begin{pmatrix}
  c_l \\
  c_t
\end{pmatrix}
\]

\[(G_{tt})_{ij} = \langle \Psi_i | \Psi_j \rangle\]
\[(H_{lt})_{ij} = \langle i | H | \Psi_j \rangle = \Delta H_2(\mathcal{E}_*)_{ij}\]
\[(H_{tt})_{ij} = \langle \Psi_i | H | \Psi_j \rangle = [-\Delta H_2(\mathcal{E}_*) + \Delta H_3(\mathcal{E}_*) + \mathcal{E}_* G_{tt}(\mathcal{E}_*)]_{ij}\]

Due to variational nature of approximation \(\mathcal{E}_{raw} \vartriangleleft \mathcal{E}_{RR} \vartriangleleft \mathcal{E}\).
We are doing better than “raw” procedure, but by how much? To understand that let us integrate out $c_t$. We end up with effective Hamiltonian $H_{ll} + \Delta \tilde{H}$,

$$
\Delta \tilde{H} \simeq \Delta H_2(\mathcal{E}_*) \frac{1}{\Delta H_2(\mathcal{E}_*) - \Delta H_3(\mathcal{E}_*)} \Delta H_2(\mathcal{E}_*) \simeq \Delta H_2 + \Delta H_3 + \ldots
$$

$$
\Delta H_2 = V_{lh} \cdot \frac{1}{\mathcal{E}_* - H_{0hh}} \cdot V_{hl}
$$

$$
\Delta H_3 = V_{lh} \cdot \frac{1}{\mathcal{E}_* - H_{0hh}} \cdot V_{hh} \cdot \frac{1}{\mathcal{E}_* - H_{0hh}} \cdot V_{hl}
$$

$\Delta \tilde{H}$ is a controlled approximation to exact effective operator $\Delta H$. 
Need only $\sim 10^4$ states instead of $\sim 10^7$ to achieve same or better accuracy
Improved convergence and smoother dependence on $E_T$. Extrapolate to $E_T = \infty$. 

- NLO, L = 6
- NLO, L = 8
- NLO, L = 10

- local LO, L = 6
- local LO, L = 8
- local LO, L = 10
\( L = \infty \) mass extracted by parametrizing the S-matrix

\[
\Delta_F m = -m \int_\infty^\infty \frac{d\theta}{2\pi} \cosh(\theta) \left( S(i\pi/2 + \theta) - 1 \right) e^{-mL \cosh(\theta)}
\]
\[
\begin{array}{|c|c|c|}
\hline
 g  & m_{\text{ph}} & \Lambda \\
\hline
 0.2 & 0.979733(5) & -0.0018166(5) \\
 1 & 0.7494(2) & -0.03941(2) \\
 2 & 0.345(2) & -0.1581(1) \\
\hline
\end{array}
\]

<table>
<thead>
<tr>
<th>Year, ref.</th>
<th>( g_c )</th>
<th>Method</th>
</tr>
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<tbody>
<tr>
<td>This work</td>
<td>2.76(3)</td>
<td>NLO-HT</td>
</tr>
<tr>
<td>2015</td>
<td>2.97(14)</td>
<td>LO renormalized HT</td>
</tr>
<tr>
<td>2016</td>
<td>2.78(6)</td>
<td>raw HT (broken phase)</td>
</tr>
<tr>
<td>2009</td>
<td>2.70^{+0.025}_{-0.013}</td>
<td>Lattice Monte Carlo</td>
</tr>
<tr>
<td>2013</td>
<td>2.766(5)</td>
<td>Uniform matrix product states</td>
</tr>
<tr>
<td>2015</td>
<td>2.788(15)(8)</td>
<td>Lattice Monte Carlo</td>
</tr>
<tr>
<td>2015</td>
<td>2.75(1)</td>
<td>Resummed perturbation theory</td>
</tr>
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</table>
The diagram shows the behavior of the energy difference $\mathcal{E}_I - \mathcal{E}_0$ as a function of $L$, the size of the system. The energy difference is approximately given by $\mathcal{E}_I - \mathcal{E}_0 \sim \frac{2\pi}{L} \Delta_I$. The graph includes two curves, one for $k=-1$ (red) and one for $k=1$ (blue), indicating different behaviors at different values of $L$. The y-axis represents the ratio $(\mathcal{E}_I - \mathcal{E}_0) L / (2\pi)$, and the x-axis represents $L$. The scale of the y-axis is from 0.0 to 2.5, and the x-axis from 6 to 10.
Computational cost

- Computational effort is mostly spent in the evaluation of $\Delta H_2, \Delta H_3$

\[
\begin{align*}
0 & \quad E_T & \quad E_L & \quad E \\
\end{align*}
\]

\[
\Delta H_2(E_*) = \Delta H_2^{\leq} + \Delta H_2^{\geq},
\]

\[
(\Delta H_2^{\leq})_{i,j} = \sum_{k : E_T < E_k \leq E_L} V_{ik} \frac{1}{E_* - E_k} V_{k,j},
\]

\[
(\Delta H_2^{\geq})_{i,j} = \sum_{k : E_k > E_L} (\text{same}).
\]

- $\Delta H_2^{\geq}$ is evaluated with local approximation, while $\Delta H_2^{\leq}$ is evaluated exactly (because no gap between low and high energy states)

- It should be possible to find more efficient prescriptions (e.g. reducing the number of tail states in variational Ansatz)
Summary and future directions

- We studied in detail an incarnation of variational methods for QFTs in the continuum

- Experiment with alternative implementations of the renormalization program, and extend the “NLO” approach to general CFT.

- Apply to the study of QFTs in higher dimensions

- Study analytic dependence of spectrum on complexified coupling

- Explore alternative quantization schemes where dynamics simplifies (Light cone)
Thank you
Evaluation of $\Delta H_2$, $\Delta H_3$

$$\Delta H_2(\mathcal{E}_*) = \Delta H_2^\leq + \Delta H_2^\geq,$$

$$(\Delta H_2^\leq)_{i,j} = \sum_{k : E_T < E_k \leq E_L} V_{ik} \frac{1}{\mathcal{E}_* - E_k} V_{kj},$$

$$(\Delta H_2^\geq)_{i,j} = \sum_{k : E_k > E_L} \text{(same)}.$$

$$(\Delta H_2^\geq)_{i,j} \approx \sum_{N = 0, 2, 4} \kappa_N (E_L)(V_N)_{i,j}, \quad V_N = \int_0^L dx : \phi(x)^N :.$$
\[ \Delta H_3(\mathcal{E}_*) = \Delta H_3^{<<} + \Delta H_3^{>>} + (\Delta H_3^{<<} + \text{h.c.}), \]

\[
(\Delta H_3^{<<})_{ij} = \sum_{k,k' : E_T < E_{k,k'} \leq E_L'} V_{ik} \frac{1}{\mathcal{E}_* - E_k} V_{kk'} \frac{1}{\mathcal{E}_* - E_{k'}} V_{k' j},
\]

\[
(\Delta H_3^{>>})_{ij} = \sum_{k,k' : E_{k,k'} > E_L'} \text{(same)},
\]

\[
(\Delta H_3^{<<})_{ij} = \sum_{k : E_T < E_k \leq E_L'} (\text{same}),
\]

\[
(\Delta H_3^{>>})_{ij} = \sum_{k' : E_{k'} > E_L'} (\text{same}),
\]
Polynomial finite-size corrections

Bethe-Yang equation

\[ e^{im_1 L} \sinh \theta S(2\theta) = 1 \]

\[ S(\theta) = S(\theta, i\zeta) \exp \left\{ \int_{\theta_t}^{\infty} \frac{d\theta'}{2\pi i} \rho(\theta') \log S(\theta', \theta) \right\} \]
Exponential finite-size corrections

\[ E_0(L) = -m \int_\infty^\infty \frac{d\theta}{2\pi} \cosh(\theta) e^{-mL \cosh(\theta)} \]

\[ \Delta_F m = -m \int_\infty^\infty \frac{d\theta}{2\pi} \cosh(\theta) \left( S(i\pi/2 + \theta) - 1 \right) e^{-mL \cosh(\theta)} \]