The Perfect Laplace Operator for Non-Trivial Boundaries

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The application of Renormalization Group (RG) methods to find perfect discretizations of partial differential equations is a promising but little investigated approach. We calculate the classically perfect fixed-point Laplace operator for boundaries of non-trivial shape analytically and numerically and present a parametrization that can be used for solving the Poisson equation.

1. INTRODUCTION

In Lattice QCD, the perfect action provides a discrete formulation of the theory which is free from lattice artifacts \[1\]. Few attempts have so far been made to examine perfect discretizations also for classical problems like the numerical solution of differential equations \[2–4\]. We present an exploratory study of a perfect differential operator in presence of non-trivial boundary conditions, as they appear in classical field theory applications. This work is in some more detail also presented in \[5\].

Our toy model is the Laplace equation on a two-dimensional region with fixed boundaries which are built from vertical and horizontal lines as shown in Fig. 1.

We construct such a set of operators with the perfect action formalism. In order to check how well this construction works, we examine how the boundary influences the perfect Laplacian. We find that not only the operator itself is local (i.e. its couplings decrease exponentially with distance), but also the effect of the boundary on the operator (so that for example in point \(B\) we don’t have to care about any boundaries).

Figure 1. A two-dimensional bounded region.

Figure 2. The set of Laplace operators \(\rho_i(r_1, r_2)\) near straight boundaries, including couplings with \(r_i \leq 2\) \((i = 1, 2)\).
2. THE PERFECT LAPLACIAN

The perfect Laplace operator in $d$ dimensions can be calculated from the fixed point action of a free real scalar field with the continuum action

$$A^{\text{cont.}}(\phi) = \frac{1}{2} \int d^d x \, \partial_\mu \phi(x) \partial_\mu \phi(x).$$

(1)

The corresponding equation of motion is the Laplace equation. A general discretization of the action (1) contains terms which couple the field at one lattice site to the field at another one:

$$A(\phi) = \frac{1}{2} \sum_{n,r} \rho_n(r) \phi_n + r,$$

(2)

with the couplings $\rho(r)$, $r = (r_1, \ldots, r_d)$. For the standard Laplacian in two dimensions, $\rho(0) = 4$ and $\rho(r) = -1$ ($\forall |r| = 1$). A RG transformation of the form

$$C \cdot e^{-A(\chi)} = \prod_n \int d\phi_n \, e^{-A(\phi)} - \mathcal{T}(\chi, \phi).$$

(3)

relates the actions $A(\phi)$ on a fine and $A'(\chi)$ on a coarse lattice with lattice units $a$ and $2a$, respectively. $C$ is a normalization constant and $\mathcal{T}$ the blocking kernel

$$\mathcal{T}(\chi, \phi) = 2\kappa \sum_{n,B} (\chi_{n,B} - b \cdot \frac{1}{2a} \sum_{n \in B} \phi_n)^2.$$  

(4)

where $\kappa$ is a parameter used for optimizing the fixed point Laplacian in terms of locality. We use the kernel $[4]$ with $\kappa = 2$ in the following, as this gives a very local operator (the couplings decrease exponentially $e^{-\gamma r}$ with a large decay coefficient $\gamma \approx 3.5$) $[4]$. The fixed point of the RG transformation (3) can be calculated analytically $[3]$. In momentum space, the result is

$$\frac{1}{\rho^*(q)} = \sum_{l \in \mathbb{Z}^d} \frac{1}{(q + 2\pi l)^2} \prod_\mu \sin^2 \left( \frac{q_\mu + \pi l_\mu}{2} \right)^2 + \frac{1}{3\kappa}.$$  

The couplings $\rho^*(n)$ of the fixed point Laplacian are found by Fourier transformation. From this result we derive the element $\rho_1$ of the set of operators in Fig. 2.

3. SQUARE-SHAPED BOUNDARIES

Consider a square region with $\phi = 0$ on the boundaries and side length $Na$. In this case, the perfect Laplacian can be calculated analytically. The easiest way to construct it in $d = 2$ is from symmetries: Extend the field $\phi$ onto the whole plane by periodically mirroring it at the boundary with alternating sign

$$\phi(x_1, x_2) = (-1)^{k_1 + k_2} \phi((-1)^{k_1} x + 2lN),$$

(5)

for any $k_i = 0, 1$ and $l_i \in \mathbb{Z}$, $i = 1, 2$. In Fig. 3, the square in the center shows the region we are interested in, the field $\phi$ is mirrored at all straight lines and its sign is given explicitly.

Figure 3. The field is periodically mirrored on the walls of squares.

In the perfect Laplace equation for the whole plane (with the perfect Laplacian $\rho^*(n)$), the sum over all lattice points splits up into sums over $N$-squares

$$\sum_r \rho^* r(\phi_{n+r}) = \sum_{l_i \in \mathbb{Z}} \sum_{k_i=0}^{N-1} \sum_{s_i=0}^{N-1} \rho^*(r-n) \phi_r = 0,$$  

(6)

where the variable $r$ running over the lattice points is given by $r_i = (-1)^i k_i - k_i + 2l_i N$ for $i = 1, 2$. Using the symmetry $\rho^*(r_1, r_2) = \rho^* (r_1, r_2)$ and the relation (3), the perfect Laplacian for square boundaries is given by the infinite sum of couplings

$$\rho^*(n, r) = \sum_{l_i \in \mathbb{Z}} (-1)^{k_1 + k_2} \rho^*(r + 2kn + k + 2lN),$$

with both $n$ and $n + r$ lying inside the boundary. The sum converges very fast because of the
locality of \( \rho^*(r) \). From this result we derive the operators \( \rho^2 - \rho_6 \).

The perfect Laplace operator for square boundaries can also be received by performing the RG transformation analytically in Fourier space, using basis functions \( \Psi_Q \) which enforce the condition \( \phi = 0 \) on the boundary. The result is

\[
\frac{1}{\rho^*(Q)} = \sum_{i=-\infty}^{\infty} \frac{1}{(Q + 2\pi i)^2} \prod_{i=1}^{2} \frac{\sin^2 \left( \frac{Q_i}{2} \right)}{\frac{Q_i}{2} + \pi i^2} + \frac{1}{3\kappa}.
\]

The couplings of the perfect Laplacian are found by reverse Fourier transformation

\[
\rho^*(n,n') = \frac{1}{N^2} \sum_Q \Psi_Q(n)\Psi_Q(n') \cdot \rho^*(Q) \quad \text{with} \quad \Psi_Q(n) = \xi_Q (n_1) \cdot \xi_Q (n_2)
\]

\[
\xi_Q (n_i) = \begin{cases} \sqrt{2} \sin (Q_i(n_i + \frac{1}{2})) & , Q_i \neq \pi, \\ \sin (Q_i(n_i + \frac{1}{2})) & , Q_i = \pi. \end{cases}
\]

\((Q_i = k_i \pi/N, \ k_i = 1, \ldots, N.) \) A comparison of the results for the two different constructions shows that they provide the same couplings. They are also in agreement with \( \rho^2 - \rho_6 \).

4. CONCAVE CORNERS

In the case where the boundaries form a concave corner (as in \( \rho^2 - \rho_6 \)), the perfect operator can’t be calculated analytically. Therefore we perform a numerical RG transformation iteratively on a \( N = 32 \) lattice with L-shaped boundaries as shown in Fig. 5:

For quadratic actions and blocking kernels, the RG transformation can be written as a minimizing condition for the fine field \( \phi \): \( A'(\chi) = \min_{\phi} [A(\phi) + T(\chi, \phi)] + \text{const.} \) (8)

To get close to a fixed point, we have to iterate this RGT step. The results of the previous step – which are the couplings of the resulting coarse action – are then used as an input for the next step, that is as a new starting guess for the fine action \( A(\phi) \). After \( O(20) \) iterations, we find a very close approximation to the couplings of the fixed point action.

We look for the couplings of the coarse field inside the large dashed box. Outside the small dashed box, we use in every RGT step the operators \( \rho^2 - \rho_6 \) for the fine action. For the couplings inside the small dashed box, we use the standard Laplacian in the first iteration, and afterwards the result of the previous iteration. As a result we get the operators \( \rho^2 - \rho_13 \), completing our set.
5. RESULTS

The effect of the boundaries on the fixed-point Laplacian is indeed highly local. This can be seen from the symmetry construction described above: In the even simpler case of a single wall along the second axis the actual operator $\rho^*(n, r)$ in terms of the translation invariant operator $\rho^*(r)$ (i.e. the operator in absence of boundaries) is given by

$$\rho^*(n, r) = \rho^*(r) - \rho^*(r_1 + 2n_1 + 1, r_2),$$  

where $n_1 + 1/2$ denotes the distance from the wall in lattice units ($n_1 = 0, 1, \ldots$). From the argument of the last term we see that the effect of the wall decreases twice as fast with distance as the couplings of $\rho^*(r)$. The size of this difference term in dependence of the distance from the wall is shown in Fig. 6. For $n_1 > 3$ it is below machine precision.

$$\Delta \rho^* = \log |(\rho^*(n, r) - \rho^*(r))/\rho^*(r)|$$

Figure 6. The relative difference $\Delta \rho^* = \log |(\rho^*(n, r) - \rho^*(r))/\rho^*(r)|$ between the couplings near a wall and the respective couplings of the perfect Laplacian on an infinite lattice.

When truncating the operators to nearest- and next-to-nearest neighbour couplings, one has to impose some conditions on the remaining couplings in order to ensure basic properties of the operator. These conditions are the correct dispersion relation $E(k) = |p|$ and the limit for small momenta $\lim_{q \to 0} \rho(q) = q^2$, leading to the sum rules $\sum_{r_1, r_2} \rho(r_1, r_2) = 0$ and $\sum_{r_1, r_2} (r_1^2 + r_2^2) \cdot \rho(r_1, r_2) = -4$.

To check the quality of our parametrization of the perfect Laplace operator, we numerically solved the lattice Poisson equation $A\phi = f$ for square boundaries with the standard $(4, -1, -1, -1)$-Laplacian and with our parametrized Laplace operator made up from $\rho_1 - \rho_6$. For the resulting field configuration, we determined the potential energy $E = f \sum_n \delta_n^{(\text{std})}$ for the field configuration $\delta_n^{(\text{std})}$ computed with the standard Laplacian and $E = f \sum_n \delta_n^{(\text{pp})} + F^2/3\kappa V$ for the configuration $\delta_n^{(\text{pp})}$ computed with the parametrized perfect Laplacian. The additional term $F^2/3\kappa V$ in the potential energy comes from the constant $C$ in the RG transformation (3) for non-zero source [5].

Fig. 7 shows a plot of the relative error $\Delta E = (E - E^{(\text{cont.})})/E^{(\text{cont.})}$ as a function of the inverse lattice volume $1/V = 1/N^2$. The error for our parametrization is proportional to $1/N^2$ and is for any lattice size smaller by a factor of about 180 than the error of the standard Laplacian. This factor can probably still be increased by tuning the normalization procedure of the truncated couplings.

Figure 7. Relative error for the numerical solution of our test problem.
6. THE POISSON EQUATION

So far, we have worked with a constant source term. But the above construction of a parametrized perfect Laplace operator also holds for the general Poisson equation with a non-constant source term \( J(x) \). Consider a RG transformation of the action:

\[
S_f[\phi] = \frac{1}{2} \int d^d x \left[ \partial_{\mu} \phi(x) \partial_{\mu} \phi(x) + J(x) \phi(x) \right]. \tag{10}
\]

Blocking out of continuum with the kernel

\[
T_\kappa[\Phi, \phi] = \kappa \sum_n \left( \Phi_n - \int d^d x \omega(x-n) \phi(x) \right)^2, \tag{11}
\]

where \( \omega(x) \) is an arbitrary blocking function gives the fixed point action, from which we read the equation of motion

\[
\sum_{n'} \rho^*(n-n') \Phi_{n'} = -J_{FP}, \tag{12}
\]

where the fixed point source is given by

\[
\tilde{J}_{FP}(k) = \tilde{\rho}^*(k) \frac{\tilde{\omega}(k)}{k^2} \tilde{J}(k). \tag{13}
\]

In the perfect Poisson equation (12) appears again the perfect Laplacian \( \rho^*(r) \) which is described by our parametrization.

7. CONCLUSION

The very basic examinations presented here show that the fixed-point approach is also applicable to classical field theory problems. We show that the fixed point Laplace operator does not care about boundaries which are a few lattice spacings away, and therefore it is possible to give a simple parametrization which works well in applications. Whether this approach is also fruitful for more complicated problems remains to be investigated.

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