Quantum gravity and the Coulomb potential

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We apply a singularity resolution technique utilized in loop quantum gravity to the polymer representation of quantum mechanics on $\mathbb{R}$ with the singular $-1/|x|$ potential. On an equispaced lattice, the resulting eigenvalue problem is identical to a finite difference approximation of the Schrödinger equation. We find numerically that the antisymmetric sector has an energy spectrum that converges to the usual Coulomb spectrum as the lattice spacing is reduced. For the symmetric sector, in contrast, the effect of the lattice spacing is similar to that of a continuum self-adjointness boundary condition at $x = 0$, and its effect on the ground state is significant even if the spacing is much below the Bohr radius. Boundary conditions at the singularity thus have a significant effect on the polymer quantization spectrum even after the singularity has been regularized.

I. INTRODUCTION

It is expected that a viable quantum theory of gravity will have to say something about what happens to the curvature singularities in classical solutions of general relativity. This would involve making concrete intuitive ideas about the role to be played by the Planck length as a fundamental discreteness scale. A possible guide concerning how to do this is the quantum resolution of the Coulomb potential in quantum mechanics, where the basic result is that the expectation value $\langle\widehat{1/r}\rangle$ is finite in all eigenstates of the Hamiltonian. This kinematic result together with dynamical Coulomb scattering may be taken to constitute quantum singularity avoidance associated with the classically singular $-1/r$ potential.

In the Hamiltonian approach to quantum gravity, the problem of quantization from a mathematical point of view is to find a suitable representation of an algebra of functions of position and momentum as operators on a Hilbert space. The Wheeler-DeWitt approach utilizes a functional Schrodinger representation where the basic variables are the Arnowitt-Deser-Misner (ADM) variables [1, 2]. The loop quantum gravity (LQG) approach uses a Poisson algebra of functions of a connection and triad, based on loops and surfaces, to build a quantum theory [3]. The basic variables quantized are the holonomy of the connection along a curve, and the integral of the (densitized) triad over a surface. The latter approach naturally leads to a non-separable kinematical Hilbert space associated with graphs embedded in a spatial manifold [3]. Because of the association of kinematic states with graphs, there is an intrinsic space discreteness built into the quantum theory which is not apriori present in the Schrödinger approach. Field excitations of the basic operators are probed on graphs rather than at points.

An approach similar to that of loop quantum gravity can be employed for the quantum mechanics of a particle moving in a potential in one or more dimensions. Here graphs are replaced by lattices of spatial points (not necessarily equispaced), and the basic observables realized in the quantum theory are the configuration and translation operators. This is of course natural since generators of infinitesimal translations cannot be represented on a spatial lattice. For a given equispaced lattice, the position eigenstates are normalizable, and the Hilbert space is obviously separable. However, the Hilbert space that incorporates all possible lattices (equispaced or not) is non-separable. The quantum theory that utilizes this space has been referred to as polymer quantization [4].

From a mathematical viewpoint, conventional Schrödinger quantization and polymer quantization are inequivalent. In the former, wave functions are square-integrable functions on $\mathbb{R}^3$, with position and momentum operators acting as multiplication and differential operators, respectively. A remarkable fact is that this is quantization is unique up to unitary equivalence provided that the configuration space of the system is topologically $\mathbb{R}^3$ and that the representation of the Weyl-Heisenberg algebra of exponentiated position and momentum operators is weakly continuous [4]. It is

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known, however, that if either of these assumptions is abandoned, there are infinitely many inequivalent representations. A simple example is a system where the configuration space is the torus rather than $\mathbb{R}^3$. Polymer quantization provides another example. Its non-separable Hilbert space may be viewed as the inductive limit of the separable Hilbert spaces associated with quantum mechanics on all possible lattices, including the one-parameter family of equispaced ones.

From a practical viewpoint, since only a countable number of calculations are possible, the full polymer Hilbert space can never be utilized. Rather, only a separable subspace is computationally useful. In this case, however, polymer quantization appears to reduce to the finitely-differenced Schrödinger equation on a lattice. We elaborate on this below by observing that various finite difference schemes for differential equations may be rewritten using configuration and translation operators on a lattice.

In the representation used in LQG, there is a way to write inverse triad operators using certain classical Poisson bracket identities due to Thiemann [5]. These identities are in fact much more general than the context in which they first arose; similar ones may be written for any theory on a lattice. They may be used to write inverse scale factor operators that are bounded on kinematical states in quantum cosmology in both the connection-triad and ADM variables [6, 7], as well as curvature operators for a field theoretic formalism for gravitational collapse [8]. The boundedness property of such operators has been used in discussions of singularity avoidance in quantum gravity at the kinematical level [9, 10].

In this paper we apply these ideas of singularity avoidance in quantum gravity to polymer representation quantum mechanics on $\mathbb{R}$ with the singular $-1/|x|$ potential. For $x > 0$, and with an appropriate boundary condition at $x = 0$, this may be thought of as the spherically symmetric sector of the Coulomb problem on $\mathbb{R}^3$. We address two main questions. First, we show that in any lattice context, the LQG singularity resolution technique amounts to replacing a (singular) derivative by a (non-singular) finite difference approximation using standard differencing techniques [11]. Second, we show that even after the singularity in the potential has been resolved, the spectra in the symmetric and antisymmetric sectors are significantly different. The latter is close to the usual Coulomb spectrum when the lattice spacing is much below the Bohr radius, but in the former the lattice spacing plays a role similar to a continuum self-adjointness boundary condition at $x = 0$, and the effect on the ground state is significant even when the spacing is much below the Bohr radius. We conclude that boundary conditions at the singularity have a significant effect on the polymer quantization spectrum even after the singularity itself has been regularized.

The rest of the paper is as follows: In section II we recall the basic structure of polymer quantization on $\mathbb{R}$. In section III we specialise to the potential $-1/|x|$, introducing the lattice regularization of the potential and showing that the boundary conditions of the radial Coulomb problem can be implemented by the restriction to the antisymmetric sector. Our numerical results for the spectrum are given in section IV. The symmetric sector is analysed in section V. Section VI summarises the results and discusses their implications and limitations for the problem of singularity resolution in quantum gravity.

II. POLYMER QUANTIZATION ON $\mathbb{R}$

In this section we briefly describe how a mechanical system is quantized in the polymer representation [4]. To keep the notation simple, and because the radial Coulomb problem we discuss later is a one-dimensional system, we will consider a particle on the real line. The generalization to n particles in $\mathbb{R}^3$ is straightforward.

Recall that the Hilbert space for the Schrödinger quantization of a particle on the real line is $L_2(\mathbb{R})$, the space of square-integrable functions on $\mathbb{R}$ in the Lebesgue measure. The operators corresponding to configuration and momentum variables act respectively as multiplication and differentiation operators. The Hilbert space is separable; an example of a countable basis are the harmonic oscillator eigenfunctions.

To introduce polymer quantization on $\mathbb{R}$, we start with the basis states

$$\psi_{x_0}(x) = \begin{cases} 1, & x = x_0 \\ 0, & x \neq x_0 \ . \end{cases} \tag{1}$$

The polymer Hilbert space is the Cauchy completion of the linear span of these basis states in the inner product

$$\langle \psi_x, \psi_{x'} \rangle = \delta_{x,x'}, \tag{2}$$

where the quantity on the right-hand side is the Kronecker (rather than Dirac) delta. This space is clearly nonseparable, and hence inequivalent to $L_2(\mathbb{R})$ [12, 13, 14]. Intuitively, building from the polymer basis states, a single nonzero $L_2(\mathbb{R})$ state would require an uncountable superposition, and thus lead to an unnormalizable state in the polymer Hilbert space. Conversely, any state in the polymer Hilbert space has support on at most countably many points, and will thus represent the zero state in $L_2(\mathbb{R})$.

Next we define the action of the basic quantum operators. The position operator $\hat{x}$ acts by multiplication,

$$\big(\hat{x}\psi\big)(x) = x\psi(x), \tag{3}$$

and its domain contains the linear span of the basis states (1). The translation operators $\hat{U}_\lambda$, $\lambda \in \mathbb{R}$, act by

$$\big(\hat{U}_\lambda\psi\big)(x) = \psi(x+\lambda), \tag{4}$$

and are clearly unitary. Formulas (3) and (4) are identical to those in $L_2(\mathbb{R})$. In $L_2(\mathbb{R})$, the action of $\hat{U}_\lambda$ is weakly continuous in λ, and there exists a densely-defined self-adjoint momentum operator $\hat{p}$ such that $\hat{p} = -i\big[\partial_\lambda \hat{U}_\lambda\big]_{\lambda=0} = -i\partial_x$ and $\hat{U}_\lambda = e^{i\lambda\hat{p}}$. By contrast, in the polymer Hilbert space the action of $\hat{U}_\lambda$ is not weakly continuous in λ, and a basic momentum operator does not exist.

The states in the polymer Hilbert space can be described as points in a certain compact space, the (Harald) Bohr compactification of the real line, and the operators introduced above can be described in terms of a representation of the Weyl algebra associated with the classical position and momentum variables [12, 13, 14]. There exists also a mirror-image quantization in which a a momentum operator and a family of translation operators in the momenta exist, but there is no basic position operator [15]. These mathematical structures will however not be used in the rest of the paper.

As there is no basic momentum operator, any phase space function containing the classical momentum p, most importantly the Hamiltonian, has to be quantized in an indirect way. Following [4], we fix a length scale $\lambda > 0$ and define

$$\hat{p} = \frac{1}{2i\lambda}(\hat{U}_\lambda - \hat{U}_\lambda^{-1}), \tag{5a}$$

$$\widehat{p^2} = \frac{1}{\lambda^2}(2 - \hat{U}_\lambda - \hat{U}_\lambda^\dagger). \tag{5b}$$

The Hamiltonian operator that corresponds to the classical Hamiltonian $H = \frac{1}{2}p^2 + V(x)$ is then

$$\hat{H} = \frac{1}{2\lambda^2}(2 - \hat{U}_\lambda - \hat{U}_\lambda^\dagger) + \hat{V}, \tag{6}$$

where V is assumed so regular that $\hat{V}$ can be defined by pointwise multiplication, $\big(\hat{V}\psi\big)(x) = V(x)\psi(x)$. In $L_2(\mathbb{R})$, the $\lambda \to 0$ limit in (5) would give the usual momentum and momentum-squared operators $-i\partial_x$ and $-\partial_x^2$, and the kinetic term in (6) would reduce to $-\frac{1}{2}\partial_x^2$. In the polymer Hilbert space the $\lambda \to 0$ limit does not exist, and λ is regarded as a fundamental length scale. For $\lambda \ll 1$, one expects the polymer dynamics to be well approximated by the Schrödinger dynamics, and certain results to this effect are known [4, 16, 17].

Although the polymer Hilbert space is nonseparable, the dynamics generated by $\hat{H}$ (6) breaks into separable superselection sectors. To discuss this, it is convenient to introduce a Dirac bra-ket notation in which the basis state ψ_μ (1) is denoted by $|\mu\rangle$. From (2), (3) and (4) we then have

$$\langle\mu|\mu'\rangle = \delta_{\mu,\mu'}, \tag{7}$$

$$\hat{x}\,|\mu\rangle = \mu|\mu\rangle, \tag{8}$$

$$\hat{U}_\lambda|\mu\rangle = |\mu - \lambda\rangle. \tag{9}$$

The action of $\hat{H}$ on $|\mu\rangle$ gives a state with support at μ, $\mu - \lambda$ and $\mu + \lambda$. The time evolution of $|\mu\rangle$ thus has support only on the regular λ-spaced lattice $\big\{\mu + n\lambda \mid n \in \mathbb{Z}\big\}$. This means that the time evolution breaks into superselection sectors, where each sector has support on a regular λ-spaced lattice and is hence separable, and the sectors can be labelled by the lattice point $\mu \in [0, \lambda)$. The time evolution of any given initial state will consequently have support only on a countable union of λ-spaced lattices. The upshot is that the time evolution of any separable subspace is restricted to a separable subspace. Thus, even though the polymer Hilbert space is nonseparable, the fundamental length scale λ and the choice of an initial state or an initial separable subspace will result in quantum dynamics that takes place in a separable Hilbert space.

We note that on a fixed λ-spaced lattice, the Hamiltonian (6) agrees with a conventional discretisation of Schrödinger's equation by the replacement

$$\psi''(x_n) \to \frac{1}{\lambda^2}\left(\psi_{n+1} - 2\psi_n + \psi_{n-1}\right). \tag{10}$$

This suggests investigating versions of (6) in which the kinetic term is replaced by an operator that, in the finite difference approximation context, is higher-order accurate in λ. The discussion of superselection sectors would extend to such versions with only minor changes. As the main interest in the present paper concerns singular potentials rather than higher order accurate discretizations of the second derivative, we shall work with (6).

In summary, the restriction of the polymer dynamics into any of its superselection sectors is mathematically equivalent to a conventional discrete approximation to the continuum Schrödinger equation on the corresponding equispaced lattice. The conceptual difference is, however, that in the polymer theory the lattice spacing is regarded as a new fundamental scale.

III. THE RADIAL COULOMB PROBLEM ON A LATTICE

Reduction of Schrödinger's equation with the Coulomb potential to the spherically symmetric ($l = 0$) sector yields the radial Hamiltonian operator

$$\hat{H}_{\rm rad} = -\frac{d^2}{dr^2} - \frac{1}{r}, \tag{11}$$

acting in the Hilbert space of square integrable functions on $(0, \infty)$ in the measure dr [18]. (For numerical convenience, the radial coordinate r has been chosen as twice the Rydberg radial coordinate.) $\hat{H}_{\rm rad}$ has a one-parameter family of self-adjoint extensions, each characterised by a boundary condition at $r \to 0$ [19]. The conventional choice for the self-adjoint extension is to assume the three-dimensional eigenfunctions in $L_2(\mathbb{R}^3, d^3\mathbf{x})$ to be bounded at the origin: in terms of the rescaled wave functions on which $\hat{H}_{\rm rad}$ acts, this means that the wave function vanishes at $r \to 0$ [18]. The spectrum then consists of the positive continuum and the negative discrete eigenvalues

$$\epsilon_n = -\frac{1}{4n^2}, \quad n = 1, 2, \dots \ . \tag{12}$$

We shall return to the other possible choices of the self-adjointness boundary condition in section V.

To introduce a polymer counterpart of $\hat{H}_{\rm rad}$ along the lines of (6), we need to address the positivity of r, the boundary condition at $r = 0$, and the singularity of the potential at $r \to 0$. Suppressing the singularity issue for the moment, the first two issues can be solved by extending r to negative values: denoting this extended coordinate by $x \in \mathbb{R}$, and assuming that the discretized potential is symmetric under the reflection $x \mapsto -x$, we require the states to be antisymmetric under $x \mapsto -x$. In the two superselection sectors in which the lattice points are at respectively $x_n = n\lambda$ and $x_n = (n + \frac{1}{2})\lambda$, $n \in \mathbb{Z}$, this antisymmetry condition just chooses the antisymmetric states. The remaining superselection sectors are pairwise coupled by the antisymmetry condition. However, since the potential is by assumption symmetric under $x \mapsto -x$, the energy eigenvalues can be found within each sector without using an antisymmetry condition, and the antisymmetric eigenstates are then obtained by just taking appropriate linear combinations.

Let us return now to the singularity of the potential at $x = 0$. Although this issue only arises in the single superselection sector that has a lattice point at $x = 0$, we wish to give a prescription that handles all the superselection sectors in a unified manner. Let x_n denote the lattice points. Since

$$\frac{\mathrm{sgn}(x)}{\sqrt{|x|}} = 2\frac{d(\sqrt{|x|})}{dx}, \tag{13}$$

we can represent $\big(\mathrm{sgn}(x)\big)/\big(\sqrt{|x|}\big)$ by a finite-difference version of the derivative,

$$\frac{\mathrm{sgn}(x_n)}{\sqrt{|x_n|}} \to \frac{1}{\lambda}\left(\sqrt{|x_{n+1}|} - \sqrt{|x_{n-1}|}\right). \tag{14}$$

Taking the square, this leads to the lattice potential

$$-\frac{1}{|x_n|} \to -\frac{1}{\lambda^2}\left(\sqrt{|x_{n+1}|} - \sqrt{|x_{n-1}|}\right)^2, \tag{15}$$

which is well defined even for $x_n = 0$. The resulting Hamiltonian operator can be written in terms of the fundamental translation and multiplication operators as

$$\begin{aligned}\hat{H} &= \frac{1}{\lambda^2}\left(2 - \hat{U}_\lambda - \hat{U}_\lambda^\dagger\right) - \frac{1}{\lambda^2}\left(\hat{U}_\lambda\sqrt{|x|}\,\hat{U}_\lambda^\dagger - \hat{U}_\lambda^\dagger\sqrt{|x|}\,\hat{U}_\lambda\right)^2 \\ &= \frac{1}{\lambda^2}\left(2 - \hat{U}_\lambda - \hat{U}_\lambda^\dagger\right) - \frac{1}{\lambda^2}\left(\hat{U}_\lambda^\dagger\left[\hat{U}_\lambda, \sqrt{|x|}\,\right] - \hat{U}_\lambda\left[\hat{U}_\lambda^\dagger, \sqrt{|x|}\,\right]\right)^2,\end{aligned} \tag{16}$$

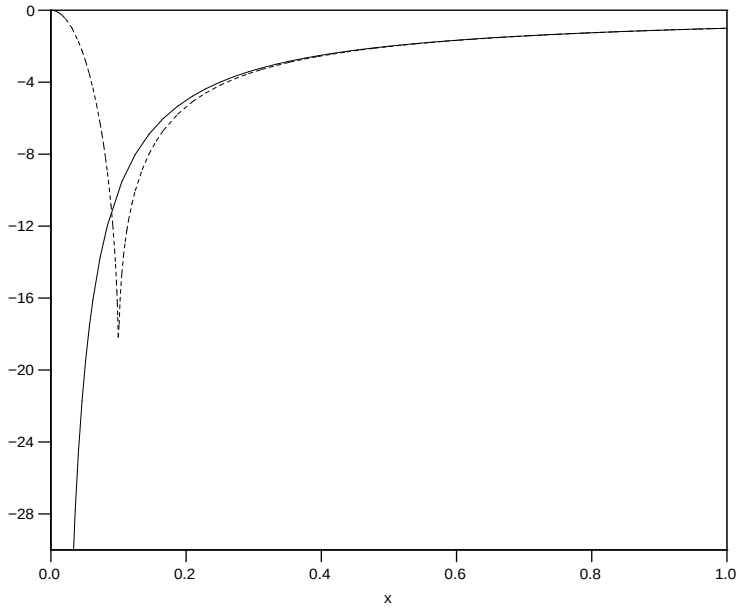

FIG. 1: The solid line is the Coulomb potential and the dashed line is the lattice regularized potential (17) for $\lambda = 0.1$

and its action on the basis state $|\mu\rangle$ is

$$\hat{H}|\mu\rangle = \frac{1}{\lambda^2}\big(2|\mu\rangle - |\mu-\lambda\rangle - |\mu+\lambda\rangle\big) - \frac{1}{\lambda^2}\left(\sqrt{|\mu+\lambda|} - \sqrt{|\mu-\lambda|}\right)^2 |\mu\rangle. \tag{17}$$

The potential term in the last form of (16) could have been arrived at by considering a phase space version of the identity (13), namely

$$\frac{\mathrm{sgn}(x)}{\sqrt{|x|}} = \frac{2}{i\lambda} e^{-i\lambda p}\left\{\sqrt{|x|}, e^{i\lambda p}\right\}, \tag{18}$$

where x and p are canonically conjugate variables. This would be similar to the route that led to Thiemann's regularisation of inverse triad operators in LQG [5]. In the present context, we have arrived at (16) simply by representing a derivative by a finite difference on a lattice. A comparison of the Coulomb potential and its lattice regulated version is given in Fig. 1 for $\lambda = 0.1$. This shows a striking repulsive modification near $x = 0$, a result which in its quantum gravity incarnation leads to a bounded curvature at the Planck scale [8].

IV. SPECTRUM

Let us focus now on the superselection sector with the lattice points $x_n = n\lambda$, $\lambda \in \mathbb{Z}$. As this is the sector in which resolving the singularity at $x = 0$ is necessary, we expect it will provide the most interesting test of the resolution proposal (15).

We look for energy eigenstates in the form $\sum_n c_n|n\lambda\rangle$, where the coefficients c_n are subject to the normalizability condition $\sum_n |c_n|^2 < \infty$ and the antisymmetry condition $c_n = -c_{-n}$. The energy eigenvalue equation with eigenvalue ϵ reads

$$\hat{H}\sum_n c_n|n\lambda\rangle = \epsilon\sum_n c_n|n\lambda\rangle. \tag{19}$$

It reduces to the recursion relation

$$c_n\left(2-\lambda f_n-\lambda^2\epsilon\right)=c_{n+1}+c_{n-1}, \tag{20}$$

where

$$f_n=\left(\sqrt{|n-1|}-\sqrt{|n+1|}\right)^2. \tag{21}$$

Suppose from now on that $\epsilon<0$. The asymptotic form of the recursion relation (20) as $n\to\infty$ is

$$c_n(2-\lambda^2\epsilon)=c_{n+1}+c_{n-1}. \tag{22}$$

It has the linearly independent solutions

$$c_n=\left[1-\tfrac{1}{2}\lambda^2\epsilon+\sqrt{\left(1-\tfrac{1}{2}\lambda^2\epsilon\right)^2-1}\right]^{\pm n}. \tag{23}$$

It follows [20] that the exact recursion relation (20) has only one linearly independent solution that does not grow exponentially as $n\to\infty$, and this solution has the asymptotic form (23) with the lower sign, and is hence exponentially decreasing in n. We use this observation to set up a shooting method for a numerical computation of the eigenenergies. We start at an initial $n_0\gg 1/(-\epsilon\lambda)$, in which regime the asymptotic recursion relation (22) holds, compute c_{n_0-1} using (23), and then compute c_0 using the exact recurrence relation (20). Because of the antisymmetry condition $c_n=-c_{-n}$, the eigenenergies are those for which $c_0=0$. The accuracy of the method is monitored by increasing the value of n_0 until the results no longer change to the desired accuracy.

When $\lambda=0.1$, we find that the lowest 14 eigenvalues are such that the quantity $k=1/\sqrt{-4\epsilon}$ is a few per cent below the lowest 14 positive integers, being thus a good approximation to the continuum spectrum (12). For the higher eigenvalues the numerics becomes slow, and we do not have an estimate of when k starts to differ significantly from integers.

For smaller λ the numerics becomes slower but indicates convergence towards the continuum eigenvalues from below as $\lambda\to 0$. Figures 2 and 3 show plots of c_0 as a function of k for $\lambda=0.01$: within the resolution of the plots, the three lowest roots are indistinguishable from $k=1$, $k=2$ and $k=3$. Figures 4 and 5 show the lowest two eigenenergies as functions of λ for $0.005\le\lambda\le 0.3$.

V. SYMMETRIC BOUNDARY CONDITION

The results in section IV show that the singularity resolution method (16) gives good agreement with the continuum results for the antisymmetric boundary condition. While this is the boundary condition that arises from the conventional treatment of the three-dimensional Coulomb problem [19], we now wish to consider the resolution method for the $-1/|x|$ potential on the *full* real line in its own right. We must then find also the energy eigenstates that are symmetric under $x\to -x$.

Staying in the superselection sector in which the lattice points are $x_n=n\lambda$, $\lambda\in\mathbb{Z}$, the numerical algorithm of section IV can be adapted to the symmetric boundary condition by starting again at $n_0\gg 1/(-\epsilon\lambda)$ but computing now c_1 and c_{-1}. The eigenenergies are those for which $c_1=c_{-1}$.

The numerics is now considerably slower than for the antisymmetric boundary condition. When $\lambda=0.1$, we find that there is a ground state at $\epsilon\approx -4.94$, well below the continuum hydrogen ground state, and the first 12 excited states are such that the quantity $k=1/\sqrt{-4\epsilon}$ is approximately 0.2 above the lowest 12 positive integers. When λ decreases to 10^{-5}, the lowest eigenvalue decreases and shows no evidence of converging to a limiting value as $\lambda\to 0$, whereas the higher eigenvalues appear slowly to converge from above to $-1/(4n^2)$, $n=1,2,\ldots$. Eigenenergies of the ground state and the first excited state for selected values of λ are shown in Table I.

The behaviour of the ground state in the limit $\lambda\to 0$ has a counterpart in the continuum theory. In the continuum theory, the solutions to the eigenvalue differential equation $\hat{H}_{\rm rad}\psi=\epsilon\psi$ that do not vanish as $r\to 0_+$ have a logarithmic singularity there, and it is not possible to single out a boundary condition at $r\to 0_+$ by a 'symmetric' extension to negative r. Instead, the self-adjointness boundary conditions at $r\to 0_+$ can be parametrised by a length scale $L\in\mathbb{R}\cup\{\infty\}$, such that the eigenenergies are the solutions to the transcendental equation

$$\frac{1}{L}=G\left(\frac{-1}{\sqrt{-4\epsilon}}\right), \tag{24}$$

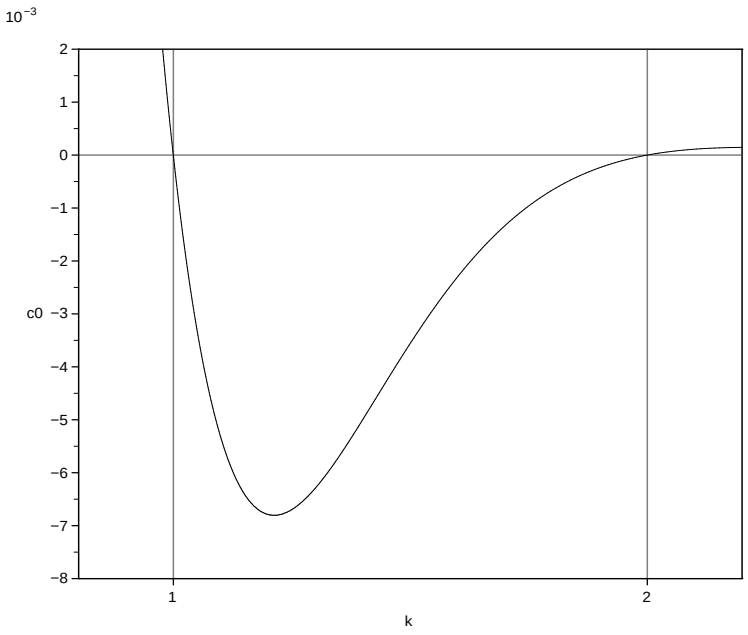

FIG. 2: The coefficient c_0 as a function of $k = 1/\sqrt{-4\epsilon}$ for $0.98 \leq k \leq 2.2$, with $\lambda = 0.01$. The zeroes are near $k = 1$ and $k = 2$.

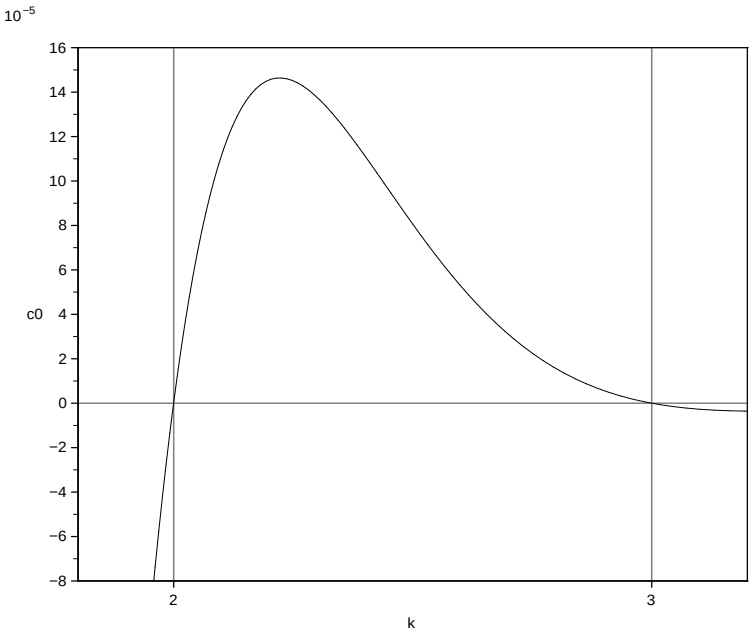

FIG. 3: The coefficient c_0 as a function of $k = 1/\sqrt{-4\epsilon}$ for $1.98 \leq k \leq 3.2$, with $\lambda = 0.01$. The zeroes are near $k = 2$ and $k = 3$.

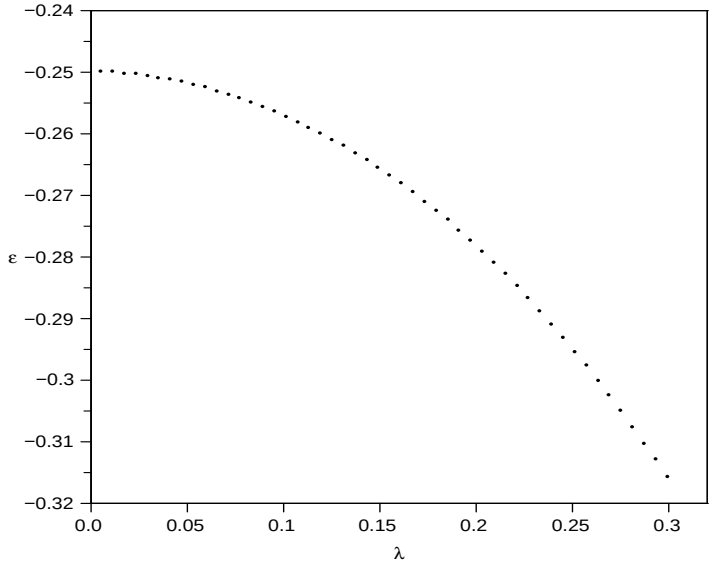

FIG. 4: The lowest eigenenergy as a function of λ for $0.005 \leq \lambda \leq 0.3$. The vertical error bar of each point is 10^{-4}. Convergence to $\epsilon = -0.25$ is apparent as $\lambda \to 0$.

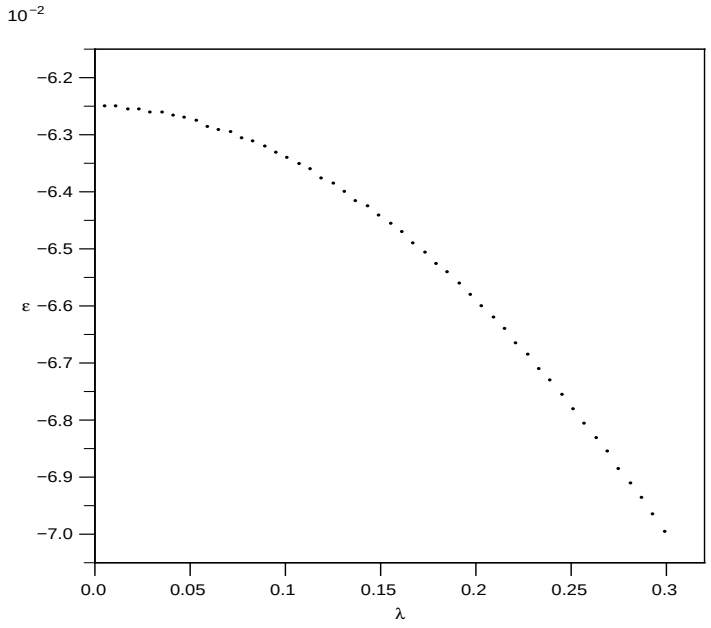

FIG. 5: The second-lowest eigenenergy as a function of λ for $0.005 \leq \lambda \leq 0.3$. The vertical error bar of each point is 5×10^{-5}. Convergence to $\epsilon = -0.0625$ is apparent as $\lambda \to 0$.

TABLE I: The energy eigenvalue as a function of λ for the ground state (ϵ_0) and the first excited state (ϵ_1) with the symmetric boundary condition.

λ	$-\epsilon_0$	$-\epsilon_1$
10^{-1}	4.94	0.153
10^{-2}	14.8	0.181
10^{-3}	32.3	0.196
10^{-4}	58.5	0.207
10^{-5}	93.9	–

where

$$G(z) := \Psi(1+z) - \ln|z| - 1/(2z) \tag{25}$$

and Ψ is the digamma function [19]. The usual boundary condition is obtained with $L = 0$. For all the other values of L, the eigenenergies are shifted downwards: in the limit $L \to 0_+$, the lowest eigenenergy tends to $-\infty$ as $-1/L^2$, while the higher eigenenergies tend to the $L = 0$ values from above, with corrections that are proportional to L [19]. Our symmetric boundary condition on the lattice produces thus eigenenergies that appear at $\lambda \to 0$ to be in qualitative agreement with the continuum eigenenergies at $L \to 0$, although the rate of convergence on the lattice is significantly slower.

The singularity resolution method appears therefore to be in qualitative agreement with the continuum theory also for the symmetric sector. The contrast between the symmetric sector and the antisymmetric sector shows, however, that boundary conditions on the quantum states at the singularity have a significant effect on the spectrum even after the singularity has been regularized.

VI. DISCUSSION

In this paper we have discussed polymer quantization in the $-1/|x|$ potential on the real line. We resolved the singularity of the potential at $x = 0$ by representing a derivative by its finitely-differenced lattice version, in a way that mimicks the regularization of the inverse triad operator in LQG [5]. Focusing on an equispaced lattice with a lattice point at $x = 0$, our numerical simulations indicated that the energy eigenvalues in the antisymmetric sector converge rapidly to those of the conventional continuum Coulomb problem as the lattice scale λ goes to zero. This is not unexpected, since antisymmetry on the full real line corresponds to the conventional boundary condition at the origin in the spherically symmetric three-dimensional Coulomb problem. In contrast, for the symmetric sector we found that the ground state eigenvalue appears to decrease without bound as λ approaches zero, while the eigenvalues of the excited states appear to approach the eigenvalues of the conventional Coulomb problem from above. The singularity resolution method in the symmetric sector thus yields dynamics that is qualitatively similar to that in the Coulomb problem with an *un*conventional choice of the self-adjointness boundary condition at the origin, with λ corresponding to the length scale associated with this boundary condition.

We view these results as evidence that the singularity resolution method yields physically reasonable results for the $-1/|x|$ potential on the real axis, whether one regards the finite difference equation simply as a discrete approximation to the Schrödinger dynamics in $L_2(\mathbb{R})$ or whether one regards the lattice scale λ as a fundamental length within polymer quantization. We emphasise that the symmetric and antisymmetric sectors were found to have qualitatively different spectra, where the antisymmetric sector produces the conventional continuum eigenvalues in the limit of small λ. This shows that even after the singularity in the potential has been regularized, boundary conditions that one may wish to impose at the locus of the singularity can have a significant effect on the spectrum.

Our results may be viewed as supporting Thiemann's regularization of the inverse triad operator in LQG [5]. Furthermore, they suggest that a boundary condition at the classical singularity may have a significant role also in the loop quantum gravity context, both when evolving through a spacelike singularity [6, 21, 22] and when setting boundary conditions at a timelike singularity [23].

There are however at least three subtleties in this respect. (i) We focused the numerical simulations on a regular lattice that has a lattice point at the origin. Will the situation remain similar also on irregular lattices, and is there a systematic control on the singularity effects when the lattice is refined [16, 17, 24]? In particular, would a significant symmetry-antisymmetry distinction emerge also on irregular lattices? (ii) We introduced the polymer quantization after first reducing the continuum Coulomb problem to the spherically symmetric sector. If one wanted to discuss polymer quantization corrections to the Coulomb energy levels from a phenomenological viewpoint, the polymer Hilbert space should presumably be introduced already at the level of three independent spatial dimensions. (iii) The

polymer Hilbert space utilized was the genuine physical Hilbert space of the system, and the energy eigenstates were simply the normalizable solutions to the eigenvalue difference equation in the polymer inner product. In LQG, the polymer Hilbert space is only the kinematical Hilbert space, and further issues may emerge when the physical Hilbert space for solutions of the Hamiltonian constraint is introduced [3, 25, 26].

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