Singularity resolution by lattice shifts in discretised quantum mechanics

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Abstract

We investigate the robustness of singularity avoidance mechanisms in non-relativistic quantum mechanics on the discretised real line when lattice points are allowed to approach a singularity of the classical potential. We consider the attractive Coulomb potential and the attractive scale invariant potential, on an equispaced parity-noninvariant lattice and on a non-equispaced parity-invariant lattice, and we examine the energy eigenvalues by a combination of analytic and numerical techniques. While the lowest one or two eigenvalues descend to negative infinity in the singular limit, we find that the higher eigenvalues remain finite and form degenerate pairs, close to the eigenvalues of a theory in which a lattice point at the singularity is regularised either by Thiemann’s loop quantum gravity singularity avoidance prescription or by a restriction to the odd parity sector. The approach to degeneracy can be reproduced from a nonsingular discretised half-line quantum theory by tuning a boundary condition parameter. The results show that Thiemann’s singularity avoidance prescription and the discretised half-line boundary condition reproduce quantitatively correct features of the singular limit spectrum apart from the lowest few eigenvalues.
1 Introduction

In nonrelativistic quantum mechanics, a system whose classical evolution is incomplete due to singularities in the potential may yield a quantum theory with unitary time evolution provided the singularities are sufficiently weak [1, 2, 3]. A celebrated example is the attractive Coulomb potential on $\mathbb{R}^3$, proportional to $-1/|x|$, whose quantum theory is unitary if a boundary condition at the origin is specified for the spherically symmetric sector [4]. Another example is the attractive scale invariant potential on $\mathbb{R}_+$, proportional to $-1/x^2$, where the quantum theory is unitary if a boundary condition is specified at the origin [5].

In this paper we address systems with a singular potential within a quantisation framework that introduces a discrete lattice on the classical configuration space. We shall examine the spectrum in the limit in which one or more lattice points approach the singularity.

While this question may be of pragmatic interest when the discrete lattice is adopted as a practical tool for approximating a standard Schrödinger quantisation, our main motivation comes from the context in which the discreteness is fundamental, and specifically from the polymer quantisation framework [6, 7] that has been employed in loop quantum gravity [8]. If a lattice point is taken to coincide with the classical singularity, the discrete quantum theory may be defined by explicitly regularising the potential [10, 11, 12], or by restriction to the odd parity sector [12], or by introducing a singularity boundary condition [13] that mimics the Robin family of boundary conditions in Schrödinger quantisation on the half-line [3, 14]: for the attractive Coulomb potential and the attractive scale invariant potential, all these regularisations yield spectra that approximate the continuum quantum theory in the relevant limit [11, 12, 13]. Were this approximation to the continuum theory however found not to exist when there are lattice points arbitrarily close to the singularity but not at the singularity itself, one would be forced to conclude that the regularisation mechanisms of [10, 11, 12, 13] rely on a fine-tuning. Such fine-tuning would be undesirable in an implementation of fundamental discreteness in quantum theory.

The purpose of this paper is to alleviate these fine-tuning concerns: we provide evidence that the singularity avoidance mechanisms based on a lattice point at the classical singularity [10, 11, 12, 13] are in quantitative agreement with the spectrum that is obtained in the limit of lattice points approaching the singularity. Our results can be understood as indirect support for the Thiemann singularity avoidance prescription in loop quantum gravity [10] and quantum field theory [15, 16, 17, 18].

Concretely, we consider the attractive Coulomb potential and the attractive scale invariant potential on the discretised real line, first on an equispaced lattice whose shift with respect to the origin approaches zero, and then on a lattice that is equispaced except for two lattice points that approach the origin symmetrically from both sides. We evaluate numerically the eigenenergies of the ground state and a selection of low-lying excited states. An analytic variational argument shows that the ground state energy must decrease to negative infinity, and for the non-equispaced lattice the same
holds also for the eigenenergy of the first excited state in the scale invariant potential. However, the first key outcome is that all the higher eigenvalues, within the range that our numerics is able to probe, tend to finite limits, and in this limit the eigenvalues form degenerate pairs. The second key outcome is that all but the lowest few of these pairs approach the eigenvalues of a discrete theory that has a lattice point at the origin but whose singularity is regularised by restriction to the odd parity sector \[12\]. Finally, the approach to degeneracy can be reproduced from the discretised half-line quantum theory of \[13\] by tuning the boundary condition parameter, with a linear relation between the lattice shift and the boundary condition parameter.

Within our potentials and lattices, there is hence quantitative agreement between the limit in which one or two lattice points approach the singularity and the regularised quantum theories in which a lattice point resides at the singularity. A qualitative discrepancy occurs only with the one or two lowest-lying eigenenergies that descend to negative infinity in the singular limit.

We begin in Section 2 by recalling relevant features of quantisation on the discretised real line, for both of our lattices. The spectra for the Coulomb potential and the scale invariant potential are presented respectively in Sections 3 and 4, and these spectra are compared with the discrete half-line theory in Section 5. Section 6 gives a summary and concluding remarks.

We use dimensionless units, with $\hbar = 1$. Complex conjugation is denoted by an overline.

### 2 Quantum mechanics on the discretised real line

In this section we outline our quantisation formalism on the discretised real line with our two lattices. For the equispaced lattice, a summary in the language of polymer quantum mechanics \[6\] is given in \[13\]. We start by assuming that the potential is nonsingular and address the case of a singular potential in subsection 2.4.

#### 2.1 Real line: continuum

We consider a system whose classical phase space is $\mathbb{R}^2 = \{(x, p)\}$ with the Poisson bracket $\{x, p\} = 1$ and the Hamiltonian

$$H = p^2 + V(x),$$

where the potential $V$ is real-valued and sufficiently well behaved.

In standard Schrödinger quantisation, the classical Hamiltonian is promoted into the operator

$$\hat{H}_S = -\partial_x^2 + \hat{V},$$

densely defined in the Hilbert space $L_2(\mathbb{R}, dx)$, such that $(\partial_x^2 \psi)(x) = \psi''(x)$ and $(\hat{V} \psi)(x) = V(x) \psi(x)$. If $\hat{H}_S$ can be defined as a self-adjoint operator by a suitable
choice of the domain, $\hat{H}_S$ generates unitarity evolution in $L_2(\mathbb{R}, dx)$ by Schrödinger’s equation, $i\partial_t \psi = \hat{H}_S \psi$.

### 2.2 Equispaced lattice

Our first lattice consists of the points $x_m = (m - \rho)\bar{\mu}$, where $m \in \mathbb{Z}$ indexes the lattice points, the positive parameter $\bar{\mu}$ is the lattice spacing, and the real-valued parameter $\rho$ is such that the lattice point $x_0$ has been shifted left from the origin by $\rho\bar{\mu}$. We may assume $\rho \in [0, 1)$ without loss of generality.

The Hilbert space is the space of two-sided sequences, $c := (c_m)_{m=-\infty}^{\infty}$, square summable in the inner product $(d, c) = \sum_m \overline{d_m} c_m$. We define the Hamiltonian $\hat{H}_{eq}$ by

$$
(\hat{H}_{eq} c)_m = \frac{2c_m - c_{m+1} - c_{m-1}}{\bar{\mu}^2} + V(x_m) c_m ,
$$

where the kinetic term is the standard three-point equispaced discretisation of $-\partial_x^2$.

$\hat{H}_{eq}$ is symmetric, and a study of the deficiency indices [1] shows that $\hat{H}_{eq}$ has at least one self-adjoint extension. If the set $\{ V(x_m) \mid m \in \mathbb{Z} \}$ is bounded, the Kato-Rellich theorem [1] can be applied as in [12] to show that $\hat{H}_{eq}$ is essentially self-adjoint.

The special cases $\rho = 0$ and $\rho = \frac{1}{2}$ give lattices that are invariant under the reflection $x \mapsto -x$, the former with a lattice point at the origin, the latter with the origin half-way between two lattice points. When $V$ is even, we may choose $\rho \in [0, \frac{1}{2}]$ without loss of generality, and the special cases $\rho = 0$ and $\rho = \frac{1}{2}$ then make $\hat{H}_{eq}$ parity invariant, so that the spectrum decomposes into the sector of even eigenfunctions and the sector of odd eigenfunctions. For $\rho \in (0, \frac{1}{2})$, $\hat{H}_{eq}$ does not have a similar parity invariance for generic even $V$, and the spectrum does not need to decompose into the even and odd sectors.

### 2.3 Non-equispaced lattice

Our second lattice consists of the points

$$
y_m = \begin{cases} (m - 1 + \rho)\bar{\mu}, & \text{for } m > 0, \\ (m - \rho)\bar{\mu}, & \text{for } m \leq 0, \end{cases}
$$

where $m \in \mathbb{Z}$ indexes the lattice points, the positive parameter $\bar{\mu}$ is the spacing between adjacent lattice points except $y_0$ and $y_1$, and the positive parameter $\rho$ is such that the spacing between $y_0$ and $y_1$ is $2\rho\bar{\mu}$. Note that $y_m = x_m$ for $m \leq 0$, and the lattice is invariant under the reflection $x \mapsto -x$.

The Hilbert space is again the space of two-sided sequences, $c := (c_m)_{m=-\infty}^{\infty}$, now square summable in the inner product $(d, c) = \frac{1}{2}(1 + 2\rho)(\overline{d_0} c_0 + \overline{d_1} c_1) + \sum_{m \neq 0,1} \overline{d_m} c_m$,.
and the Hamiltonian $\hat{H}_{\text{eq}}$ is defined by

$$
(\hat{H}_{\text{eq}})_{m} = \begin{cases} 
2c_m - \frac{c_{m+1} - c_{m-1}}{\mu^2} + V(y_m)c_m, & \text{for } m > 1 \text{ and } m < 0, \\
\frac{(1 + 2\rho)c_1 - 2\rho c_2 - c_0}{\rho(1 + 2\rho)\bar{\mu}^2} + V(y_1)c_1, & \text{for } m = 1, \\
\frac{(1 + 2\rho)c_0 - 2\rho c_{-1} - c_1}{\rho(1 + 2\rho)\bar{\mu}^2} + V(y_0)c_0, & \text{for } m = 0.
\end{cases}
$$

(2.5)

The kinetic term in (2.5) is the unique three-point discretisation of $-\partial_x^2$ that is exact for quadratic polynomials, and the weights of the $m = 0$ and $m = 1$ terms in the inner product have been chosen so that $\hat{H}_{\text{eq}}$ is symmetric. It can be shown as above that $\hat{H}_{\text{eq}}$ has at least one self-adjoint extension, and that $\hat{H}_{\text{eq}}$ is essentially self-adjoint if the set $\{V(y_m) | m \in \mathbb{Z}\}$ is bounded.

As noted above, the lattice is invariant under the reflection $x \mapsto -x$. When $V$ is even, $\hat{H}_{\text{eq}}$ is hence parity invariant, and the spectrum decomposes into the even and odd sectors. In the special case $\rho = \frac{1}{2}$, the lattice coincides with the equispaced lattice with $\rho = \frac{1}{2}$. In the limit $\rho \to 0$, both $y_0$ and $y_1$ approach the origin.

### 2.4 Singular potential on a lattice

We have assumed above that the potential $V$ has domain $\mathbb{R}$. We now turn to the case in which $V$ has a singularity at $x = 0$ but is defined elsewhere. The equispaced lattice theory of subsection 2.2 remains well defined provided $\rho \in (0, 1)$, and the non-equispaced lattice theory of subsection 2.3 remains well defined as it stands since there $\rho$ is by construction positive. Note that on both lattices the distance from the origin to the closest lattice point(s) equals $\rho\bar{\mu}$.

Suppose hence that $\rho$ is positive. We consider the attractive Coulomb potential, $V(x) = -1/|x|$, and the attractive scale invariant potential, $V(x) = -\lambda/x^2$, where $\lambda$ is a positive constant. We may assume $0 < \rho \leq \frac{1}{2}$. It follows as in [12] that $\hat{H}_{\text{eq}}$ and $\hat{H}_{\text{neq}}$ are essentially self-adjoint and bounded below, for the Coulomb potential by $-1/(\rho\bar{\mu})$ and for the scale invariant potential by $-\lambda/(\rho^2\bar{\mu}^2)$.

If the system has a ground state, the ground state energy can be bounded from above by a variational ansatz. For $\hat{H}_{\text{eq}}$, the ansatz $c_m = \delta_{m,0}$ gives the upper bound $2/(\bar{\mu}^2) - 1/(\rho\bar{\mu})$ for the Coulomb potential and the upper bound $2/(\bar{\mu}^2) - \lambda/(\rho^2\bar{\mu}^2)$ for the scale invariant potential. For $\hat{H}_{\text{neq}}$, the ansatz $c_m = \delta_{m,0} + \delta_{m,1}$ gives similarly the upper bounds $2/[(1 + 2\rho)\bar{\mu}^2] - 1/(\rho\bar{\mu})$ and $2/[(1 + 2\rho)\bar{\mu}^2] - \lambda/(\rho^2\bar{\mu}^2)$. It follows, for both $\hat{H}_{\text{eq}}$ and $\hat{H}_{\text{neq}}$, that the ground state energy decreases to negative infinity as $\rho \to 0$.

For $\hat{H}_{\text{neq}}$, if the odd sector has a lowest-energy state, we can obtain an upper bound for this eigenenergy by the variational ansatz $c_m = \delta_{m,0} - \delta_{m,1}$. For the scale invariant potential, the upper bound is $2(1 + \rho)/[(\rho + 1)\bar{\mu}^2] - \lambda/(\rho^2\bar{\mu}^2)$, showing that the lowest eigenenergy decreases to negative infinity as $\rho \to 0$. For the Coulomb potential, the
upper bound is $2(1 + \rho)/[\rho(1 + 2\rho)\bar{\mu}^2] - 1/(\rho\bar{\mu})$. This shows that the lowest eigenenergy decreases to negative infinity as $\rho \to 0$ when $\bar{\mu} > 2$, but does not guarantee such decrease when $\bar{\mu} \leq 2$.

We shall see these phenomena in the numerical evaluation of the low energy eigenvalues in Sections 3 and 4 below.

We note in passing that the singularity in both the attractive Coulomb potential and the attractive scale invariant potential is so strong that in the continuum quantum theory the positive half-line and the negative half-line are decoupled from each other [4, 5]. In a lattice quantum theory that incorporates points from both halves of the real axis, this suggests that a comparison to the continuum theory should only use parity-invariant observables. If this suggestion is adopted, the even and odd sectors on a parity-invariant lattice become superselected, in the sense that all observables map even states to even states and odd states to odd states [19]. The even and odd sectors on our on-equispaced lattice can hence be viewed as superselection sectors. For a regular lattice with one point at the singularity, this superselection terminology was adopted in [11].

3 Coulomb potential

In this section we consider the attractive Coulomb potential. We first recall relevant facts about the continuum quantum theory and then analyse the discrete quantum theory on our two lattices.

3.1 Continuum

We write the attractive Coulomb potential as $V(x) = -1/|x|$. This is the theory of the spherically symmetric sector of the hydrogen atom in Rydberg units, with $|x|$ being twice the Rydberg radial coordinate [20].

The singularity at $x = 0$ is so strong that the positive and negative halves of the real axis decouple, and we may take the Hilbert space to be $L^2(\mathbb{R}_+, dx)$. The self-adjoint extensions of $\hat{H}_S$ (2.2) then form a U(1) family, specified by a boundary condition at the origin [4]. The spectrum of each extension consists of the positive continuum and a countable set of negative eigenvalues. In the particular extension whose boundary condition is $\psi(0) = 0$, the eigenvalues are $E = -1/(4s^2)$ with $s = 1, 2, 3, \ldots$: this is the textbook quantisation of the spherically symmetric sector of the hydrogen atom [20].

A detailed technical analysis can be found in [4].

3.2 Equispaced lattice

We consider first the equispaced lattice. We look for the negative energy eigenvalues by solving the eigenvalue equation $\hat{H}_{eq}\psi = E\psi$ numerically.

The eigenvalue equation is a difference equation with a three-term recurrence relation, and for negative $E$ the boundary condition is that the solutions must decrease
at both infinities sufficiently rapidly to be normalisable. Our numerical scheme is adapted from that in [11]. Given an $E < 0$ and a (large) positive integer cut-off $m_0$, we first use the method of [11] to find a solution $\{c_{m}^{(+)} \mid m = 0, 1, \ldots, m_0\}$ that is exponentially suppressed at large positive $m$, and we then similarly find a solution $\{c_{m}^{(-)} \mid m = -m_0, -m_0 + 1, \ldots, 0, 1\}$ that is exponentially suppressed at large negative $m$. The eigenvalues are those $E$ for which these two solutions coincide at $c_0$ and $c_1$ up to normalisation. The condition that determines the eigenvalues is hence $c_{0}^{(-)}c_{1}^{(+)} - c_{0}^{(-)}c_{0}^{(+)} = 0$, which we solve by the shooting method. Numerical accuracy is monitored by increasing $m_0$ until the results stabilise.

Motivated by the eigenvalues of the continuum theory, we parametrise the lattice eigenvalues as $E = -1/(4s^2)$ where $s > 0$. Figure 1 shows the lowest seven eigenvalues as a function of $\rho$ for $0.004 \leq \rho \leq 0.01$. Probing arbitrarily small values of $\rho$ is not numerically possible, but the plot presents strong evidence for the asymptotic behaviour as $\rho \to 0$. The eigenvalues split into two alternating sets, which we call the A set and the B set, such that the A set includes the ground state. In the A set, the eigenvalues approach their asymptotic limits from above, and for the ground state this limit appears to be at negative infinity, in agreement with the bound given in subsection 2.4. In the B set, the eigenvalues approach their asymptotic limits from below. In the limit, the excited state eigenvalues appear to form degenerate pairs, to the numerical accuracy that we have been able to probe, stabilising at values that are slightly above those of the continuum theory with the textbook boundary condition.

For $\bar{\mu} = 0.1$, the behaviour of the eigenvalues is qualitatively similar, and the $\rho \to 0$ limits of the excited eigenvalues are slightly further above the continuum textbook eigenvalues. This could have been expected on the grounds that if we choose $\rho = 0$ at the start and regularise the singularity at the origin by restriction to the odd parity sector, the $\bar{\mu} \to 0$ limit appears to converge to the continuum textbook theory [12]. At $\bar{\mu} < 0.01$ the numerics becomes significantly slower and we have not examined this regime.

### 3.3 Non-equispaced lattice

On the non-equispaced lattice, the Hamiltonian $\hat{H}_{\text{neq}}$ is parity invariant, and the spectrum hence decomposes into the even and odd sectors for all values of $\rho$. In the numerical solution of the eigenvalue equation $\hat{H}_{\text{neq}} \psi = E \psi$, we may therefore proceed as with the equispaced lattice to compute first the solution $\{c_{m}^{(+)} \mid m = 0, 1, \ldots, m_0\}$ for fixed $E$ and $m_0$, and then find the eigenvalues as those $E$ for which $c_0 = \pm c_1$, where the upper (lower) sign gives the even (odd) sector.

A plot of the lowest seven eigenvalues with $\bar{\mu} = 0.01$ is shown in Figure 1. For $\rho = \frac{1}{2}$, the equispaced and non-equispaced lattices coincide, and we find that the $A$ and $B$ eigenvalue sets found above coincide respectively with the even and odd sectors. As $\rho$ decreases, the coincidence is no longer precise, but it continues to hold to a good approximation: the even sector eigenvalues lie closely below the set A eigenvalues, while
Figure 1: Eigenvalues for the Coulomb potential with $\tilde{\mu} = 0.01$. The quantity plotted is $s = 1/\sqrt{-4E}$. The equispaced lattice is on the left, showing the lowest seven eigenvalues as a function of $\rho$. The plot on the right reproduces the data from the left as solid (red) lines and superposes the corresponding data for the non-equispaced lattice as dashed (blue) lines.
the odd sector eigenvalues lie closely above the set B eigenvalues. In particular, the ground state eigenvalue again descends to the negative infinity as $\rho \to 0$, in agreement with the bound given in subsection 2.4, and the excited state eigenvalues are sandwiched between the equispaced lattice set A and set B eigenvalues, forming degenerate pairs as $\rho \to 0$.

4 Scale invariant potential

In this section we consider the attractive scale invariant potential. We again first recall relevant facts about the continuum quantum theory and then analyse the discrete quantum theory on our two lattices.

4.1 Continuum

We write the attractive scale invariant potential as $V(x) = -\lambda/x^2$, where $\lambda$ is a positive constant. The positive and negative halves of the real axis again decouple, and we may take the Hilbert space to be $L_2(\mathbb{R}_+, dx)$. The self-adjoint extensions of $\hat{H}_S$ (2.2) are classified in [5]: early analyses were given in [21, 22] and a review with further references can be found in [12]. In the regime $\lambda > \frac{1}{4}$, which we shall consider in the lattice theories below, the spectrum consists of the positive continuum and a countable set of negative eigenvalues, given by

$$E_n = E_0 \exp\left(-\frac{2\pi n}{\sqrt{\lambda - (1/4)}}\right), \quad (4.1)$$

where $n \in \mathbb{Z}$ and the negative constant $E_0$ is determined by the boundary condition.

4.2 Equispaced lattice

On the equispaced lattice we solve the eigenvalue equation $\hat{H}_{eq}\psi = E\psi$ numerically by the same method as for the Coulomb potential. Because the discretisation preserves the scale invariance of the continuum theory, the lattice spacing $\bar{\mu}$ enters the eigenvalues only as the overall multiplicative factor $1/\bar{\mu}^2$. Motivated by the continuum theory eigenvalues (4.1), we parametrise the lattice eigenvalues by $\bar{\mu}^2 E = -\exp(-s)$ where $s \in \mathbb{R}$.

Figure 2 shows the lowest five eigenvalues as a function of $\rho$ for $0.01 \leq \rho \leq \frac{1}{2}$, with $\lambda = 1.25$, $\lambda = 4$ and $\lambda = 8$. In the $\rho \to 0$ limit, the behaviour is qualitatively similar to that with the Coulomb potential. The eigenvalues split into alternating A and B sets, tending to their limits respectively from above and from below. The only eigenvalue that does not tend to a finite limit is the ground state, which descends to negative infinity, in agreement with the bound given in subsection 2.4, and the higher eigenvalues form pairs that become degenerate, to the accuracy that we have been able to probe.
Figure 2: Eigenvalues for the scale invariant potential with $\lambda = 1.25$ (dot-dashed, gold), $\lambda = 4$ (solid, red) and $\lambda = 8$ (dashed, blue). The quantity plotted is $s = -\ln(-\bar{\mu}^2 E)$. The equispaced lattice is on the left, showing the lowest five eigenvalues for each $\lambda$ as a function of $\rho$. The non-equispaced lattice is on the right, showing the lowest six eigenvalues for $\lambda = 1.25$ and the lowest ten eigenvalues for $\lambda = 4$ and $\lambda = 8$. In the plot on the right, the resolution does not suffice to show the descent of the lowest-lying pair towards negative infinity as $\rho \to 0$, and the resolution separates for $\lambda = 4$ only the lowest-lying pair of eigenvalues and for $\lambda = 8$ none of the pairs of eigenvalues.
4.3 Non-equispaced lattice

On the non-equispaced lattice, the eigenvalues break into the even and odd sectors, and they can be investigated by the same numerical methods as with the Coulomb potential.

As $\rho \to 0$, the lowest eigenvalue in each of the two sectors descends towards negative infinity, in agreement with the bounds given in subsection 2.4. Our numerical evidence is inconclusive as to how close to each other the two eigenvalues will remain in the final stages of this descent.

For $\rho \leq 10^{-8}$, the higher eigenvalues in the two sectors coincide to at least 14 decimal places in their $s$-values, and they further coincide with the corresponding set $A$ eigenvalues of the equispaced lattice within our numerical accuracy. In particular, all these eigenvalues tend to finite limits as $\rho \to 0$.

A plot of the low eigenvalues for $\lambda = 1.25$, $\lambda = 4$ and $\lambda = 8$ is shown in Figure 2.

5 Comparison with discrete half-line

In all the cases analysed above, we have seen that in the limit $\rho \to 0$ the spectrum breaks into two subsets, each of which has a strong qualitative resemblance with the eigenvalues obtained by regularising the singularity of the potential, whether by explicitly modifying the functional form of the potential [11, 12], by a parity argument [12], or by formulating the lattice theory on a half-line with a Robin-type boundary condition at the singularity [13]. The only exceptions in this qualitative resemblance occur in the one or two states of lowest energy.

We shall now investigate the resemblance quantitatively.

Among the regularised theories, we consider the theory defined on the discrete half-line [13]. The lattice is semi-infinite, the lattice points are at $z_m = m\bar{\mu}$ with $m = 1, 2, 3, \ldots$, and the inner product reads $(d, c) = \sum_{m=1}^{\infty} d_m c_m$. The Hamiltonian $\hat{H}_\alpha$ is given by

$$
(\hat{H}_\alpha d)_m = \begin{cases} 
\frac{2c_m - c_{m+1} - c_{m-1}}{\bar{\mu}^2} + V(m\bar{\mu})c_m, & \text{for } m > 1, \\
\frac{(2 - \alpha)c_1 - c_2}{\bar{\mu}^2} + V(\bar{\mu})c_1, & \text{for } m = 1.
\end{cases}
$$

(5.1)

where $\alpha$ is a real-valued parameter. Note that as $z_0 = 0$ is not part of the lattice, the value of the potential at the singularity does not enter the Hamiltonian.

The parameter $\alpha$ may be thought of as specifying a Robin-like boundary condition at the fictitious lattice point $m = 0$, with the special case $\alpha = 0$ corresponding to the Dirichlet-like condition $c_0 = 0$. The theory with $\alpha = 0$ is equivalent to a theory that is defined on an equispaced lattice over the full real line, with one lattice point at the singularity, but regularised by restriction to the odd parity sector [12]. This observation will be significant below.
\[ \mu = 0.1 \]  
\[ \mu = 0.01 \]

Table 1: Coulomb potential on the equispaced lattice. The table shows the coefficient \( K \) in the asymptotic small \( \rho \) relation \( \alpha = K \rho \) for the set A and set B eigenvalues, with \( \bar{\mu} = 0.1 \) and with \( \bar{\mu} = 0.01 \).

We pose the following questions. For the equispaced lattice, can the set A (respectively set B) eigenvalues be reproduced from the discrete half-line theory with some choice of \( \alpha \) as a function of \( \rho \) in the limit \( \rho \to 0 \)? For the non-equispaced lattice, can the eigenvalues in the even (respectively odd) sector be reproduced from the discrete half-line theory with some choice of \( \alpha \) as a function of \( \rho \) in the limit \( \rho \to 0 \)?

We consider the Coulomb potential and the scale invariant potential in turn.

### 5.1 Coulomb potential

For the Coulomb potential, we have carried out a numerical analysis on the equispaced lattice with \( \bar{\mu} = 0.01 \) and \( \bar{\mu} = 0.1 \).

We find that the answer is affirmative: the eigenvalues in set A and set B can be reproduced from the discrete half-line theory in the limit \( \rho \to 0 \), and for each of the sets the dependence of \( \alpha \) on \( \rho \) fits the linear relation \( \alpha = K \rho \) to a good approximation when \( \rho \leq 10^{-5} \). The values of the coefficient \( K \) for each set and each value of \( \bar{\mu} \) are shown in Table 1. The only eigenvalue that does not fit the pattern is the ground state.

Note that \( \alpha \to 0 \) as \( \rho \to 0 \). This means that in the \( \rho \to 0 \) limit, the eigenvalue pairs approach the eigenvalues in the equispaced lattice theory in which one lattice point is at the singularity but the theory is regularised by restriction to the odd parity sector [12].

We have not carried out a similar computation on the non-equispaced lattice. However, the sandwiching of the nonequispaced lattice eigenvalues between the equispaced lattice eigenvalues, shown in Figure 1, strongly suggests that a similar correspondence holds, so that the even sector and the odd sector can be matched to the discrete half-line theory in the \( \rho \to 0 \) limit, each with a linear relation between \( \rho \) and \( \alpha \). The sandwiching gives bounds on the coefficients in these linear relations, in terms of the coefficients shown in Table 1. In particular, the sandwiching shows that in the \( \rho \to 0 \) limit the eigenvalue pairs again approach the eigenvalues in the equispaced lattice theory with a lattice point at the singularity but regularised by restriction to the odd parity sector.

### 5.2 Scale invariant potential

Consider the scale invariant potential with the equispaced lattice. For \( \rho \leq 10^{-4} \), we find that both the set A eigenvalues and the set B eigenvalues can be reproduced from the discrete half-line theory with the linear relation \( \alpha = K \rho \), provided we exclude the three lowest eigenvalues from the A set and the two lowest eigenvalues from the B set. The
values of the coefficient $K$ are shown in Table 2 for each set, with $\lambda = 4$ and $\lambda = 8$. The coefficients for the two sets differ only in the overall sign, within our numerical accuracy: we have not investigated analytically whether this difference by only the sign might be exact.

On the non-equispaced lattice, we saw above that in each sector all eigenvalues except the lowest one coincide with those of the equispace lattice as $\rho \to 0$, to high precision. We hence have again a correspondence to the half-line theory, with the linear relation $\alpha = K\rho$, and the values of the coefficient $K$ are given by column A in Table 2.

Note again that $\alpha \to 0$ as $\rho \to 0$. Hence, with the exception of the lowest few eigenvalues, the eigenvalue pairs approach the eigenvalues in the equispaced lattice theory with a lattice point at the singularity but regularised by restriction to the odd parity sector [12].

6 Conclusions

In this paper we have investigated nonrelativistic quantum mechanics on the discretised real line in two classically singular potentials, the attractive Coulomb potential and the attractive scale invariant potential. We considered an equispaced lattice and a lattice that is equispaced except for one shorter interval that ensconces the classical singularity, and we analysed the spectrum in the limit in which one or two lattice points approach the singularity, by numerical evaluation of the bound state eigenvalues. We found that while one or two of the lowest energy eigenstates descend to negative infinity in this limit, the remaining eigenvalues tend to finite limits that form degenerate pairs and are close to the eigenvalues of the continuum theory, and also close to the eigenvalues of discrete theories in which the singularity has been regularised by the Thiemann mechanism introduced in loop quantum gravity [10], by a parity argument [12], or by a discrete version of the continuum Robin boundary condition [13]. We in particular established that the approach to degeneracy can be quantitatively reproduced from the discrete half-line theory by tuning the boundary condition parameter therein to be a linear function of the distance from the singularity to the closest lattice point(s).

These results bear witness to unanimity amongst the mechanisms by which a classically singular continuum theory becomes nonsingular on quantisation, whether the quantisation is built on a continuous configuration space or on a discrete configuration.
space. If the discreteness is thought of as a pragmatic tool, as an approximation to a ‘true’ quantisation with a continuous configuration space, the results are evidence that the various discrete treatments of the classical singularity yield compatible results and efficient approximations. If the discreteness is thought of as fundamental, the results are evidence that the core properties of the discrete theory do not rely on fine-tuning in the way in which the discreteness implements singularity avoidance. From this viewpoint, our results provide indirect support for the Thiemann singularity avoidance prescription in loop quantum gravity [10] and quantum field theory [15, 16, 17, 18].

For the Coulomb potential, the cases of one or two lattice points approaching the singularity were qualitatively very similar, even in the lowest eigenvalues. For the scale invariant potential, by contrast, approaching the singularity with two lattice points affected the lowest eigenvalues significantly more strongly than with just one lattice point. This could perhaps have been expected on the grounds that the singularity in the scale invariant potential is stronger than in the Coulomb potential. There would be scope for a systematic study of this phenomenon within a wider range of singular potentials, power-law and beyond, and within a wider variety of lattices.

Finally, in this paper we have considered only the bound state part of the spectrum. It would be equally interesting to study the behaviour of travelling wave packets [23] in the limit where one or more lattice points approach the singularity: does the unbounded descent of the lowest one or two eigenvalues leave a footprint in the reflection and transmission of waves? If yes, can the footprint be reproduced from a manifestly nonsingular theory, or could it possibly contain evidence of pathology, detectable by low energy observations?

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