Some consequences of GUP induced ultraviolet wavevector cutoff in one-dimensional Quantum Mechanics

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A projection method is proposed to treat the one-dimensional Schrödinger equation for a single particle when the Generalized Uncertainty Principle (GUP) generates an ultraviolet (UV) wavevector cutoff. The existence of a unique coordinate representation called the naive one is derived from the one-parameter family of discrete coordinate representations. In this bandlimited Quantum Mechanics a continuous potential is reconstructed from discrete sampled values observed by means of a particle in maximally localized states. It is shown that bandlimitation modifies the speed of the center and the spreading time of a Gaussian wavepacket moving in free space. Indication is found that GUP accompanied by bandlimitation may cause departures of the low-lying energy levels of a particle in a box from those in ordinary Quantum Mechanics much less suppressed than commonly thought when GUP without bandlimitation is in work.

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I. INTRODUCTION

There are several theoretical indications that Quantum Gravity may have consequences in the behaviour of low-energy quantum systems [1–4]. The corresponding effective Quantum Mechanics is believed to be based on the Generalized Uncertainty Principle (GUP) [5–11], various modifications of Heisenberg's Uncertainty Principle (HUP). Recently even a proposal has been put forward to probe experimentally the departure from HUP in a direct manner [12]. Among the various realizations of GUP there is a class when the deformation of the commutator relation for the operators of the coordinate $\hat{x}$ and the canonical momentum $\hat{p}_x$ depends only on the canonical momentum,

$$[\hat{x}, \hat{p}_x] = i\hbar f(\alpha|\hat{p}_x|) \tag{1}$$

with the deformation function $f(|u|)$, where $u = \alpha p_x$ and $\alpha = \mathcal{O}(\ell_P/\hbar)$ with the Planck length $\ell_P \approx 1.616 \times 10^{-35}$ m is a small parameter. In the present paper we shall restrict ourselves to deformation functions for which there exists a minimal wavelength, i.e. a maximal magnitude K of the wavevector but the canonical momentum can take arbitrary large values (as opposed to the cases discussed e.g. in [13]). Then physical states are restricted to those of finite band width, i.e. the wavevector operator $\hat{k}_x$ can only take values in the interval $[-K, K]$.

The mathematical structure of Quantum Mechanics with finite band width is rather delicate [14], even in the one-dimensional case. Namely, while both operators of the wavevector $\hat{k}_x$ and the canonical momentum $\hat{p}_x$ are self-adjoint, the coordinate operator $\hat{x}$ cannot be self-adjoint, but only Hermitian symmetric in order to satisfy the deformed commutator relation (1). It has, however, a one-parameter family of self-adjoint extensions with eigenvalues determining equidistant grids on the coordinate axis, defining a minimal length scale a, while the grids belonging to the various extensions are continuously shifted to each other. This is a sign that positions can only be observed with a maximal precision $\Delta x_{min} \approx a$, while momenta can be measured with arbitrary accuracy [9, 15–21].

Although there exist formal coordinate eigenstates even in that case, but – as opposed to ordinary Quantum Mechanics, – they cannot be approximated now by a sequence of physical states with uncertainty in position decreasing to zero [15]. A so-called naive coordinate representation can be built up representing the operator algebra of $[\hat{x}, \hat{k}_x] = i\hbar$ as $\hat{x} \Rightarrow x$ and $\hat{k}_x \Rightarrow -i\partial_x$ on square-integrable functions of the coordinate $x \in \mathbb{R}$, referred to below as coordinate wavefunctions. Then the canonical momentum satisfying the relation in Eq. (1) can be represented as $\hat{p}_x \Rightarrow \alpha^{-1}F^{-1}(-i\alpha\hbar\partial_x)$ where F^{-1} stands for the inverse of the function $F(u) = \int_0^u \frac{du'}{f(|u'|)}$ and relates the operators of the wavevector and the canonical momentum via $\hat{k}_x = (\alpha\hbar)^{-1}F(\alpha\hat{p}_x)$. Let us note that the commutator in the left-hand side of Eq. (1) is invariant under the reflection $x \to -x$, $p_x \to -p_x$ so that the deformation function should be an even function of p_x which implies that both functions $F(u)$ and its inverse are even, as well. Furthermore, $f(0) = 1$ has to be required in order to recover HUP in the limit $\alpha \to 0$. Here we shall restrict ourselves to particular choices of the deformation function which are monotonically increasing with raising $|u|$ and for which the limits $F(\pm\infty) = \pm\alpha\hbar K$ remain finite. There are known a few explicit cases of such deformation functions, e.g. $f = 1 + \alpha^2 p_x^2$ with $F(u) =$ arc tan u [15, 22], $f = \exp(\alpha^2 p_x^2)$ with $F(u) = (\sqrt{\pi}/2)$ erf u [20], and $f = \exp(\alpha|p_x|)$ with $F(u) = (1 - e^{-|u|})$ sign u used after Taylor expansion in [23, 24] and all implying $\hbar K \approx 1/\alpha$ and $a \approx \alpha\hbar \approx \ell_P$.

In the present paper we shall take the point of view that the minimal length scale is of the order of the Planck length. Nevertheless, one has to be aware of the lack of an unquestionable theoretical proof of such a conjecture

(see e.g. [11]). Therefore, all the formulae derived in the present paper can also be considered from another point of view put forward in a series of papers [26–34], namely, that the scale $\hbar\alpha \approx \Delta x_{min} \approx a$ denoted here by ℓ_P is an unknown parameter for which an upper bound should be laid either by the discrepancies between data on some observables measured with very high accuracy and their best theoretical estimates, or by the error of some very accurately measured observable. In the former case the best theoretical estimate means a one obtained by incorporating all our knowledge on physics affecting the given observable, and the tiny discrepancy between theory and data is ascribed to the GUP effect, while in the latter case the error of the measurement is considered like an upper bound on the GUP effect. Making use of the deformation function $f = 1+\alpha^2 p_x^2$ several upper bounds on Δx_{min} have been obtained [26–34]. The smallest upper bounds are found, for example, from the investigation of the shift of energy levels of an electron in a Penning trap, $\Delta x_{min} \lesssim 2\times 10^{-16}$ m (1 GeV^{-1} in $\hbar = c = 1$ units) [26] and from that of the $1S$ Lamb shift of the Hydrogen atom $\Delta x_{min} \lesssim 3 \times 10^{-17}$ m (1/7 GeV^{-1}) [31, 32]. In that respect it is interesting to note that even a length scale as small as $\Delta x_{min} \sim 2 \times 10^{-19}$ m (1 TeV^{-1}) [35] is not expected to influence the Cosmic Microwave Background in any observable way [27], although there occurs a suppression of the high-frequency modes in black-body radiation.

In bandlimited Quantum Mechanics the coordinate space turns out to exhibit features of discreteness [25] and continuity at the same time like information does [36–42]. The main idea is that space can be thought of a differentiable manifold, but the physical degrees of freedom cannot fill it in arbitrarily dense manner. It has also been conjectured that degrees of freedom corresponding to structures smaller than the resolvable Planck scale turn into internal degrees of freedom [43–46]. Although the coordinate wavefunctions introduced in the manner described above do not have the simple probabilistic meaning, yet provide useful tools to characterize the quantum states of the particle which can then be analyzed e.g. in terms of maximally localized states [16–19]. Below we shall discuss the justification of that naive coordinate representation for one-dimensional bandlimited Quantum Mechanics in more detail.

In the present paper we shall concentrate on the solution of the Schrödinger equation for the coordinate wavefunctions in the case when GUP implies finite band width. It is well-known that GUP directly affects the Hamiltonian through the modification of the canonical momentum and that of the kinetic energy operator $(\hat{p}_x^2/2m) - (\hbar^2\hat{k}_x^2/2m)$ which can be expanded – when low-energy states are considered – in powers of the small parameter α. This pure GUP effect has been treated in the framework of the perturbation expansion using the naive coordinate representation and discussed in detail for various quantum systems (see Refs. [22, 24, 47–59] without the quest of completeness), among others for the particle in a box [23, 24, 52, 53, 56, 60, 61]. Treatments in the Bargmann-Fock representation [62–64], and various path-integral formulations [65–67] have been worked out. Here we shall take the viewpoint that the bandlimited Quantum Mechanics is an effective theory in the framework of which no quantum fluctuations of wavelength smaller than those of the order of the minimal length are possible, i.e. the coordinate wavefunctions should not contain Fourier components with wavevectors outside of the finite band with $k_x \in [-K, K]$. In order to built in this restriction into the Schrödinger equation we propose to use Hamiltonians operating on the subspace of the square-integrable coordinate wavefunctions with finite band width. To ensure this we introduce the projector $\hat{\Pi}$ onto that subspace and restrict the solutions of the Schrödinger equation to the bandlimited subspace $\mathcal{H}$ of the Hilbert space. We shall also show that the above mentioned naive coordinate representation of the bandlimited Hilbert space $\mathcal{H}$ uniquely exists and solutions of the bandlimited Schrödinger equation automatically reflect the symmetry that the formulations of the theory on any of the equidistant spatial grids of spacing a exhibit the same physical content. Moreover, we shall discuss the reconstruction of a unique continuous bandlimited potential from sampled values taken on such grids by means of maximally localized states. The bandlimitation will be shown to broaden the peaks and smear out the sudden jumps of the microscopic potential over a region of the Planck scale. Below we shall apply our projection method to determine the free motion of a Gaussian wavepacket as well as the energy shifts of the low-lying stationary states of a particle in a box. The stationary problem shall be treated in the framework of first-order perturbation theory.

It is appropriate to make the following remarks: *(i)* As to our viewpoint of removing the UV components of the wavefunctions, it is rather a naive approach to estimate the additional effects due to the existence of the finite UV cutoff. Our viewpoint would be exact when the coordinate space were discrete, but it is not although the self-adjoint extensions of the coordinate operator have discrete eigenvalues forming a grid on the coordinate axis. However, there exists a one-parameter family of such extensions and that of the corresponding grids which can be transformed into each other by continuous shifts. This indicates that quantum fluctuations of wavelength smaller than the minimal length scale a cannot be probably excluded completely, but rather should have been treated by more sophisticated methods, like e.g. renomalization group methods. Fortunately, in the one-dimensional case the solutions of the bandlimited Schrödinger equation in the naive coordinate representation used by us reflect inherently the physical equivalence of any of those grids. Therefore, our projection technique can give a reliable order-of-magnitude estimate of the importance of the additional effect of the UV cutoff as compared to the pure GUP effect. *(ii)* As to our choice of the model, the particle in a box, it is rather a toy model. The pure GUP

effect on the low-lying stationary states has already been discussed and noticed that the model with precisely given box size L is ill-defined in the sense that a change of the box size of the order ℓ_P, i.e. that of the maximal accuracy Δx_{min} of the position determination causes an energy shift of the order $\mathcal{O}(\ell_P/L)$ as compared to the pure GUP effect of the order $\mathcal{O}\left((\ell_P/L)^2\right)$ [68]. In our approach the Hamiltonian operates on the subspace of states with finite band width and transforms the originally local potential effectively into a nonlocal one. Projecting out the UV components of the potential results in a kind of smearing out the edges of the box in regions of the size of $\mathcal{O}(\Delta x_{min})$. Our purpose is to determine the additional shift of the low-lying energy levels caused by the existence of the finite UV cutoff. We shall see that this turns out to be of the order $\mathcal{O}(\ell_P/L)$, being much more significant than the pure GUP effect, so that in some sense the result of [68] will be recovered. Nevertheless, our approach may be a hint that this kind of energy shift might be the true effect, when the physically realistic box with smeared out walls is considered and modeled by performing the projection which determines the operation of the Hamiltonian on the bandlimited Hilbert space $\mathcal{H}$.

Our paper is constructed as follows. In Sect. II the projection method is introduced and the integral kernels for the various projected operators determined. For one-dimensional bandlimited Quantum Mechanics a justification of the naive coordinate representation is given in Sect. III. A method is given in Sect. IV which enables one to reconstruct a bandlimited continuous potential from sampled values obtained by means of a particle in maximally localized state. The free motion of a Gaussian wavepacket is then discussed in Sect. V in the framework of bandlimited Quantum Mechanics. In Sect. VI the determination of the shifts of the low-lying energy levels of a particle in a potential is formulated in the framework of the first-order perturbation theory. The problem of a particle in a box is considered in Sect. VII as the limiting case of a particle in a square-well potential taking the limit of infinite depth. After setting some notations in Subsect. VII A and recovering the well-known result for the pure GUP effect in Subsect. VII B, in Subsect. VII C the additional energy shifts of the low-lying levels caused by the existence of the finite UV cutoff are shown to be dominant. It is also argued that the latter might influence the estimates on the upper bound of the minimal length scale, as well. Finally, the results are summarized in Sect. VIII. Several technical details are given in the Appendix. App. A reminds the reader on some mathematics relevant for the self-adjoint extension of the Hermitian symmetric coordinate operator. In App. B the wavefunctions of the unperturbed system, i.e. those for a particle in the square-well potential in the framework of usual Quantum Mechanics are derived. The operation of the GUP modified kinetic energy operator on exponential functions is determined in App. C. The details of the evaluation of the additional energy shifts of the low-lying energy levels for a particle in a box are presented in Appendices D and E. In App. F maximally localized states of a particle are constructed. Finally, in App. G the bandlimited potential reconstructed from sampled values of a Dirac-delta like potential is presented.

II. PROJECTORS ONTO THE SUBSPACE OF WAVEFUNCTIONS WITH FINITE BAND WIDTH

Let $\psi(x)$, $\tilde{\psi}(p_x)$ and $\tilde{\tilde{\psi}}(k_x)$ be the wavefunctions of the state $|\psi\rangle$ in the naive coordinate, canonical momentum and wavevector representations, respectively. The scalar product of arbitrary states $|\psi\rangle$ and $|\phi\rangle$ can be written as

$$\begin{aligned}\langle\phi|\psi\rangle &= \int_{-\infty}^{\infty} dx\phi^*(x)\psi(x) = \int_{-K}^{K}\frac{dk_x}{2\pi}\tilde{\tilde{\phi}}^*(k_x)\tilde{\tilde{\psi}}(k_x)\\ &= \int_{-\infty}^{\infty}\frac{dp_x}{2\pi\hbar f(\alpha|p_x|)}\tilde{\phi}^*(p_x)\tilde{\psi}(p_x)\end{aligned} \tag{2}$$

and is kept invariant under the transformation

$$\begin{aligned}\psi(x) &= \int_{-K}^{K}\frac{dk_x}{2\pi}e^{ik_xx}\tilde{\tilde{\psi}}(k_x),\\ \tilde{\tilde{\psi}}(k_x) &= \int_{-\infty}^{\infty}dxe^{-ik_xx}\psi(x).\end{aligned} \tag{3}$$

An arbitrary square integrable function $\psi(x) \in L^2(-\infty,\infty)$ contains ultraviolet (UV) Fourier components with $|k_x| > K$, as well. In order to ensure that the solutions of quantum mechanical eigenvalue equations, as well as that of the Schrödinger equation belong to the subspace $L^2_K(-\infty,\infty)$ of wavefunctions with finite band width, any operator $\hat{O}$ of an observable should be projected onto that subspace by an appropriate projector $\hat{\Pi}$, $\hat{O} \Rightarrow \hat{\Pi}\hat{O}\hat{\Pi}$. The projector should cut off the UV components of any square integrable function $f(x) \in L^2(-\infty,\infty)$, i.e. for its kernel $\Pi(x,y)$ the relation

$$\begin{aligned}(\Pi f)(x) &= \int_{-\infty}^{\infty}dy\Pi(x,y)f(y)\\ &= \int_{K}^{K}\frac{dk_x}{2\pi}e^{ik_xx}\tilde{\tilde{f}}(k_x) \in L^2_K(-\infty,\infty)\end{aligned} \tag{4}$$

should hold that implies

$$\Pi(x,y) = \int_{-K}^{K}\frac{dk_x}{2\pi}e^{ik_x(x-y)} = \frac{\sin[K(x-y)]}{\pi(x-y)}. \tag{5}$$

It is straightforward to show that $\hat{\Pi}$ is a projector satisfying $\hat{\Pi}^2 = \hat{\Pi}$. When $K \to \infty$ the operation of any Hermitian symmetric operator $\hat{O}$ on any state $|\psi\rangle$ can be represented as

$$\int_{-\infty}^{\infty}dyO(x,y)\psi(y) = \int_{-\infty}^{\infty}\frac{dk_x}{2\pi}\tilde{\tilde{\psi}}(k_x)\tilde{\tilde{O}}_{k_x}e^{ik_xx} \tag{6}$$

where the kernel $O(x,y)$ and the formal differential operators O_x and $\tilde{\tilde{O}}_{k_x}$ are related as

$$O(x,y) = O_x\delta(x-y) = \int_{-\infty}^{\infty}\frac{dk_x}{2\pi}e^{-ik_xy}\tilde{\tilde{O}}_{k_x}e^{ik_xx}. \quad (7)$$

Hermitian symmetry implies $O(x,y) = [O(y,x)]^*$ and $\tilde{\tilde{O}}_{k_x} = [\tilde{\tilde{O}}_{-k_x}]^*$. A few examples are summarized in the table:

O_x	$\tilde{\tilde{O}}_{k_x}$
$x^n\ (n\in\mathbb{N})$	$\frac{1}{2}[(-i\partial_{k_x}^{\rightarrow})^n + (i\partial_{k_x}^{\leftarrow})^n]$
$(-i\partial_x)^n\ (n\in\mathbb{N})$	k_x^n
$\lvert -i\partial_x\rvert = \sqrt{(i\partial_x)^2}$	$\lvert k_x\rvert$

It is straightforward to show that the symmetrized form of $\tilde{\tilde{O}}_{k_x}$ for $O_x = x^n$ with partial derivatives $\partial_{k_x}^{\rightarrow}$ and $\partial_{k_x}^{\leftarrow}$ acting to the right and left, respectively, is in agreement with Heisenberg's commutation relation $[\hat{x},\hat{k}_x] = i$.

In Quantum Mechanics with finite band width K the kernel $O(x,y)$ should be projected as

$$\begin{aligned}(\Pi O\Pi)(x,y) &= \int_{-\infty}^{\infty}dz\int_{-\infty}^{\infty}du\Pi(x,z)O(z,u)\Pi(u,y)\\ &= \int_{-K}^{K}\frac{dk_x}{2\pi}e^{-ik_xy}\tilde{\tilde{O}}_{k_x}e^{ik_xx} \quad (8)\end{aligned}$$

while Hermitian symmetry is preserved, $[(\Pi O\Pi)(y,x)]^* = (\Pi O\Pi)(x,y)$. Now, one easily finds the kernel of $\hat{\Pi}\hat{k}_x^n\hat{\Pi}$,

$$\begin{aligned}(\Pi k_x^n\Pi)(x,y) &= \int_{-K}^{K}\frac{dk_x}{2\pi}e^{ik_x(x-y)}k_x^n\\ &= (-i\partial_x)^n\Pi(x,y), \quad (9)\end{aligned}$$

and that of $\hat{\Pi}\hat{x}^n\hat{\Pi}$,

$$\begin{aligned}&(\Pi x^n\Pi)(x,y)\\ &= \int_{-K}^{K}\frac{dk_x}{2\pi}e^{-ik_xy}\frac{1}{2}[(-i\partial_{k_x}^{\rightarrow})^n + (i\partial_{k_x}^{\leftarrow})^n]e^{ik_xx}\\ &= \frac{1}{2}(x^n+y^n)\Pi(x,y) \quad (10)\end{aligned}$$

which imply for the kernels of the functions $f(\hat{k}_x)$ and $V(\hat{x})$ of operators $\hat{k}_x$ and $\hat{x}$, respectively,

$$\begin{aligned}(\Pi f(k_x)\Pi)(x,y) &= f(-i\partial_x)\Pi(x,y),\\ (\Pi V(x)\Pi)(x,y) &= \frac{1}{2}[V(x)+V(y)]\Pi(x,y). \quad (11)\end{aligned}$$

Making use of the projector $\hat{\Pi}$ introduced above, the time-dependent and the stationary Schrödinger equations can be written as

$$i\hbar\partial_t|\psi\rangle = \hat{\Pi}\hat{H}\hat{\Pi}|\psi\rangle, \quad (12)$$

$$\hat{\Pi}\hat{H}\hat{\Pi}|\psi\rangle = E|\psi\rangle, \quad (13)$$

respectively, in terms of the projected Hamiltonian $\hat{\Pi}\hat{H}\hat{\Pi}$ when Quantum Mechanics with finite band width is considered. The initial condition for the time-dependent Schrödinger equation (12) should be a physical state, i.e. also bandlimited. The usage of the projected Hamiltonian obviously ensures that the state will not contain the UV Fourier components. The rules in Eq. (11) for projecting functions of operators enable one to make both the kinetice energy and the potential energy piece of the projected Hamiltonian explicit in the naive coordinate representation.

III. COORDINATE REPRESENTATIONS

In this section we show that the naive coordinate representation for one-dimensional bandlimited Quantum Mechanics formulated by means of the projection technique proposed in Sect. II is equivalent with any of the discrete coordinate representations based on the complete orthonormal sets of eigenvectors of the various self-adjoint extensions of the coordinate operator. Moreover, the time-dependent Schrödinger equation (12) and the stationary one, Eq. (13) in the naive coordinate representation as well as their solutions reflect inherently the $U(1)$ symmetry which reveals itself in the unique physical content of the formulations of the theory in terms of the various discrete coordinate representations. Therefore, the so-called naive coordinate representation is correct for one-dimensional bandlimited Quantum Mechanics, although the coordinate wavefunction looses its direct probability meaning as opposed to ordinary Quantum Mechanics.

One might accept the usage of the naive coordinate representation with some reservation because the coordinate operator $\hat{x}$ is not self-adjoint (see App. A). Therefore, no coordinate eigenstates exist in the physical domain and the introduction of the coordinate representation becomes questionable. There exists, however, a one-parameter family of the self-adjoint extensions $\hat{x}_\theta$ of the coordinate operator, labeled by the parameter $\theta\in[0,a)$. Any of these extensions for fixed θ exhibits an orthonormal complete set of eigenvectors $|x_n^\theta\rangle$ in the bandlimited Hilbert space $\mathcal{H}$. In the wavevector representation the corresponding eigenfunctions $\langle k_x|x_n^\theta\rangle = \tilde{\tilde{\psi}}_{x_n}^\theta(k_x)$ with $k_x\in[-K,K]$ are given by Eq. (A10) in App. A, whereas the corresponding discrete nondegenerate eigenvalues $x_n^\theta = an+\theta$ form a grid with spacing a in the one-dimensional space. Therefore, any vector $|\psi\rangle\in\mathcal{H}$ can be represented as a linear superposition of the base vectors $|x_n^\theta\rangle\in\mathcal{H}$ for any given θ, $|\psi\rangle = \sqrt{a}\sum_{n=-\infty}^{\infty}\langle x_n^\theta|\psi\rangle|x_n^\theta\rangle$, so that discrete coordinate representations $\mathcal{R}_\theta$ of the normalized vectors $|\psi\rangle\in\mathcal{H}$ via the vectors $\{\psi_n^\theta = \langle x_n^\theta|\psi\rangle\}\in\ell^2$ arise (the normalization implies $a\sum_{n=-\infty}^{\infty}|\psi_n^\theta|^2 = 1$). Then the operators $\hat{O}$ over the bandlimited Hilbert space $\mathcal{H}$ should be represented by the countably infinite dimensional matrices $O_{nn'}^\theta = \langle x_n^\theta|\hat{O}|x_{n'}^\theta\rangle$. Thus a one-

parameter family of discrete coordinate representations $\mathcal{R}_\theta$ is available.

Using the wavevector representation, one realizes immediately that the transformation from a discrete coordinate representation $\mathcal{R}_\theta$ to another one $\mathcal{R}_{\theta'}$ belongs to the $U(1)$ group because $\tilde{\tilde{\psi}}^{\theta'}_{x_n}(k_x) = e^{ik_x(\theta'-\theta)}\tilde{\tilde{\psi}}^{\theta}_{x_n}(k_x)$. Such a transformation means a shift of the spatial grid from $\{x^\theta_n = na+\theta\}$ to $\{x^{\theta'}_n = na+\theta'\}$ on which one describes one-dimensional bandlimited Quantum Mechanics. Nevertheless, there should be a distinction of Quantum Mechanics discretized on a grid and the case discussed here. In the latter case space reveals discrete and continuous features at the same time, similarly as information does [36–46]. Namely, the physical content of any of the discrete coordinate representations $\mathcal{R}_\theta$ should be identical, i.e. the $U(1)$ group of the transformations among them should be a symmetry. Thus, physics contained in the scalar products

$$\langle\phi|\psi\rangle = a\sum_{n=-\infty}^{\infty}\phi^{\theta *}_n\psi^\theta_n \tag{14}$$

of arbitrary vectors $|\psi\rangle,\ |\phi\rangle \in \mathcal{H}$ should be independent of the particular choice of the representation $\mathcal{R}_\theta$. In that respect it is important to underline that the Schrödinger equations obtained by using the projection method are given in their abstract forms in Eqs. (12) and (13) without referring to any representation, and their solutions $|\psi\rangle$ are authomatically in the bandlimited Hilbert space, $|\psi\rangle \in \mathcal{H}$.

Now we show that to each vector $|\psi\rangle \in \mathcal{H}$, i.e. to each vector $\{\psi^\theta_n = \langle x^\theta_n|\psi\rangle\}$ of the representation $\mathcal{R}_\theta$ one can associate a single coordinate wavefunction $\psi(x)$, and the latter is independent of the choice of the representation $\mathcal{R}_\theta$ used for its construction.

1. To any position $x \in \mathbb{R}$ belongs exactly a single eigenvalue $x^{\theta'}_{n'} = an' + \theta' = x$ of a particular self-adjoint extension $\hat{x}^{\theta'}$ of the coordinate operator (see the discussion at the end of App. A). This enables one to construct a wavefunction of continuous variable,

$$\psi(x) = \langle x^{\theta'}_{n'} = x|\psi\rangle = \sum_{n=-\infty}^{\infty}\langle x^{\theta'}_{n'} = x|x^\theta_n\rangle\psi^\theta_n \tag{15}$$

in a reliable manner, where $\psi(x^\theta_n) = \psi^\theta_n$ are sampled values of the coordinate wavefunction on the arbitrarily chosen grid $\{x^\theta_n\}$. Here figures the matrix element $\langle x^{\theta'}_{n'} = x|x^\theta_n\rangle = a\Pi(x, x^\theta_n)$ of the unitary transformation from the discrete coordinate representation characterized by θ to the one characterized by θ', which is directly related to the projector $\hat{\Pi}$ onto the bandlimited Hilbert space. Thus Eq. (15) recasted into the form

$$\psi(x) = a\Pi(x, x_n)\psi^\theta_n \tag{16}$$

can be interpreted as the particular case of the sampling theorem in the bandlimited Hilbert space [38], a generalization of Shannon's sampling theorem [69]. With a similar logic identifying $x = x^{\theta'}_{n'}$ and $y = x^{\theta''}_{n''}$ as the n'-th and n''-th eigenvalues of the appropriate self-adjoint extensions $\hat{x}_{\theta'}$ and $\hat{x}_{\theta''}$, respectively, one is enabled to reexpress any matrix element $(\Pi O\Pi)(x, y) = \langle x|\hat{\Pi}\hat{O}\hat{\Pi}|y\rangle$ of an arbitrary operator $\hat{O}$ in terms of the matrix $O^\theta_{nm} = \langle x^\theta_n|\hat{\Pi}\hat{O}\hat{\Pi}|x^\theta_m\rangle = \langle x^\theta_n|\hat{O}|x^\theta_m\rangle$ as

$$O(x, y) = a^2\sum_{n,m=-\infty}^{\infty}\Pi(x, x^\theta_n)O^\theta_{nm}\Pi(x^\theta_m, y) \tag{17}$$

implying $O(x^\theta_n, x^\theta_m) = O^\theta_{nm}$. Therefore, to any vector of the bandlimited Hilbert space represented by the vector $\{\psi^\theta_n\} \in \ell^2$ in the discrete coordinate representation $\mathcal{R}_\theta$ there corresponds a continuous coordinate wavefunction $\psi(x)$, and to any operator $\hat{\Pi}\hat{O}\hat{\Pi}$ mapping the bandlimited Hilbert space into itself, i.e. to any matrix of the discrete coordinate representation $\mathcal{R}_\theta$ corresponds the kernel $O(x, y)$ of the continuous coordinate representation.

2. Being aware of the construction of the coordinate wavefunction $\psi(x) = \sum_{n=-\infty}^{\infty}\langle x = x^{\theta'}_n|\hat{\mathbb{1}}|\psi\rangle$ via Eq. (15), one can insert any of the decompositions of the unit operator $\hat{\mathbb{1}} = \sum_{n=-\infty}^{\infty}|x^\theta_n\rangle\langle x^\theta_n|$ over $\mathcal{H}$ associated with any of the representations $\mathcal{R}_\theta$. This means, on the one hand, that the resulting wavefunction $\psi(x)$ associated in the naive coordinate representation to the bandlimited vector $|\psi\rangle \in \mathcal{H}$ is unique, independent of the representation $\mathcal{R}_\theta$ used to its construction. On the other hand it also means that taking sampled values on various spatially shifted grids $\{x^\theta_n\}$ and inserting those into Eq. (16) one obtains finally the same wavefunction of the continuous variable x. Similar arguments lead to the unique kernel $O(x, y)$ associated to the operator $\hat{O}$ mapping $\mathcal{H}$ into itself.

Thus one can conclude that the solutions of the bandlimited Schrödinger equations for one spatial dimension, being bandlimited themselves, satisfy the generalized sampling theorem expressed in Eq. (16) authomatically and therefore reflect inherently the $U(1)$ symmetry under the continuous shifts of the spatial grid determined by the discrete eigenvalues of the various self-adjoint extensions of the coordinate operator.

IV. BANDLIMITED POTENTIALS

Let us here illustrate the manner one could observe the formally local potential $V(x)$ in the framework of Quantum Mechanics with finite band width. The best one can do to construct maximally localized states $\varphi_{\bar{x}}(x)$ centered

at arbitrary positions $\bar{x}$ [16–19] and detect the potential exerted on it. One should however be aware of the fact that there exist only a countable set of physically distiguishable positions x_n^θ, those of the eigenvalues of an arbitrarily chosen self-adjoint extension $\hat{x}^\theta$ of the coordinate operator, which form a grid of spacing $a = \pi/K$. Thus we can sample the potential only at the grid points. Let $\{|\varphi_n^\theta\rangle\}$ be the sequence of the maximally localized states centered on the grid points. Thus, potential values

$$\bar{V}_n^\theta = \langle\varphi_n^\theta|\hat{\Pi}\hat{V}\hat{\Pi}|\varphi_n^\theta\rangle \tag{18}$$

can only be observed at a discrete set of points of a grid with spacing a. The maximally localized states $|\varphi_n^\theta\rangle$ belong to the subspace of bandlimited wavefunctions, $\hat{\Pi}|\varphi_n^\theta\rangle = |\varphi_n^\theta\rangle$, so that Eq. (18) reduces to

$$\bar{V}_n^\theta = \langle\varphi_n^\theta|\hat{V}|\varphi_n^\theta\rangle. \tag{19}$$

According to Shannon's basic sampling theorem on bandlimited real functions [69], a continuous potential $\bar{V}(\bar{x})$ with finite bandwidth K ($k_x \in [-K, K]$) can perfectly be reconstructed from its values $\bar{V}_n^\theta = \bar{V}(x_n^\theta)$ taken on the set of equidistant points $\{x_n^\theta\}$ spaced $\frac{2\pi}{2K} = a$ apart:

$$\bar{V}(\bar{x}) = a\sum_{n=-\infty}^{\infty} \bar{V}_n^\theta \Pi(\bar{x} - x_n^\theta). \tag{20}$$

Now one has to show that the reconstructed potential $\bar{V}(\bar{x})$ is bandlimited and does not depend on the particular choice of the grid, i.e. that of the self-adjoint extension of the coordinate operator. One can choose the sampled values $\bar{V}_n^\theta$ on the grid $\{x_n^\theta = na + \theta\}$ shifted by any constant $\theta \in [0, a)$. Let $\mathcal{V}(\bar{x})$ be the function which takes the values $\mathcal{V}(x_n^\theta) = \bar{V}_n^\theta$ for any $n \in \mathbb{Z}$ and $\theta \in [0, a)$. It is generally not bandlimited, implying

$$\mathcal{V}(x) = \int_{-\infty}^{\infty} \frac{dl}{2\pi} e^{ilx}\tilde{\mathcal{V}}(l). \tag{21}$$

Let us now reconstruct a potential $\bar{V}(\bar{x})$ from the sampled values $\bar{V}_n^\theta$ for given θ and ask how far the resulted function depends on the particular choice of θ, i.e. that of the particular choice of the self-adjoint extension of the coordinate operator $\hat{x}$. According to the reconstruction formula in Eq (20) we get

$$\bar{V}(\bar{x}) = a\sum_{n=-\infty}^{\infty} \mathcal{V}(x_n^\theta)\Pi(\bar{x} - x_n^\theta) \tag{22}$$

which implies

$$\begin{aligned}
&\bar{V}(\bar{x} + \theta) \\
&= a\sum_{n=-\infty}^{\infty} \mathcal{V}(na + \theta)\Pi(\bar{x} - na) \\
&= a\int_{-\infty}^{\infty} \frac{dl}{2\pi}\tilde{\mathcal{V}}(l)\int_{-K}^{K} \frac{dq}{2\pi} e^{il\theta + iq\bar{x}} \sum_{n=-\infty}^{\infty} e^{i(l-q)na}.
\end{aligned} \tag{23}$$

Making use of the sum (G2), one obtains

$$\bar{V}(\bar{x} + \theta) = \int_{-K}^{K} \frac{dl}{2\pi}\tilde{\mathcal{V}}(l)e^{il(\bar{x}+\theta)} = \mathcal{V}_K(\bar{x} + \theta) \tag{24}$$

i.e. the reconstructed function $\bar{V}(\bar{x}) = \mathcal{V}_K(\bar{x})$ which is independent of the choice of the particular self-adjoint representation of $\hat{x}$ and is bandlimited, $\mathcal{V}_K(\bar{x}) = (\hat{\Pi}\mathcal{V})(\bar{x})$. One cannot, of course, reconstruct the function $\mathcal{V}(\bar{x})$ which contains modes outside of the band $[-K, K]$. Below we shall take the sampled potential values on the grid $x_n = na$ (for $\theta = 0$) and, for the sake of simplicity, suppress the upper indices θ.

In App. F we have determined the maximally localized state $\tilde{\tilde{\varphi}}_{\bar{x}}(k_x)$ in the wavevector representation by making use of the method of Detournay, Gabriel, and Spindel [18], see Eq. (F7). Rewriting it into the coordinate representation, one finds

$$\begin{aligned}
\varphi_{\bar{x}}(x) &= \int_{-K}^{K} \frac{dk_x}{2\pi} e^{ik_x x}\tilde{\tilde{\varphi}}_{\bar{x}}(k_x) \\
&= \sqrt{\frac{a}{2}}[\Pi(x - \bar{x} + \frac{1}{2}a) + \Pi(x - \bar{x} - \frac{1}{2}a)],
\end{aligned} \tag{25}$$

implying a position inaccuracy of $\langle\varphi_{\bar{x}}|\hat{x}^2 - \bar{x}^2|\varphi_{\bar{x}}\rangle = a^2/4$. The wavefunction (25) is real, has a maximum at $x = \bar{x}$, varies slightly in the small interval $x \in \mathcal{I}_{\bar{x}} \equiv [\bar{x} - \frac{1}{2}a, \bar{x} + \frac{1}{2}a]$ centered at the point $\bar{x}$ and falls off rapidly in an oscillatory manner outside of the interval $\mathcal{I}_{\bar{x}}$. Obviously such a state enables one to detect a bandlimited potential $\bar{V}(\bar{x})$ smeared out as compared to $V(x)$. For example, the Dirac-delta like potential, $V(x) = V_0 a\delta(x)$ is observed as a broadened one with finite height V_0 and finite width,

$$\bar{V}_n = V_0 a|\varphi_{x_n}(0)|^2 = \frac{V_0 a^2}{2}[\Pi(x_n - \frac{1}{2}a) + \Pi(x_n + \frac{1}{2}a)]^2. \tag{26}$$

The reconstructed bandlimited continuous potential is then given by Eq. (G6) in App. G and is shown in Fig. 1.

It is peaked taking values of the order V_0 in the interval $\bar{x} \in [-\frac{1}{2}a, \frac{1}{2}a]$ and falls off rapidly in an oscillatory manner outside of that interval. The characteristic wavelength of the oscillations is $2a$.

Another example is that the finite jump at $x = 0$ of the potential step $V(x) = V_0\Theta(-x)$ becomes smeared out. The sampled values taken at $x_n = na$ are

$$\bar{V}_n = V_0\int_{-\infty}^{0} dx|\varphi_{na}(x)|^2. \tag{27}$$

The values $\bar{V}_n$ are monotonically decreasing with increasing n. Moreover, the relation $|\varphi_{na}(x)|^2 = |\varphi_0(x - na)|^2$ holds for the integrand, implying

$$\bar{V}_n = V_0\int_{-\infty}^{-na} dx|\varphi_0(x)|^2. \tag{28}$$

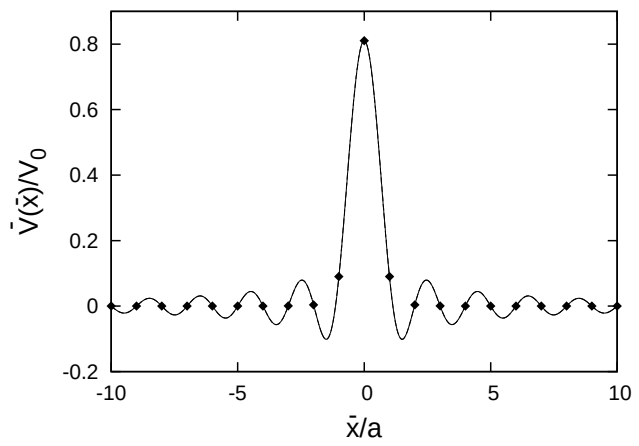

FIG. 1. Sampled values (boxes) and the reconstructed bandlimited continuous potential (solid line) for $V(x) = V_0 a\delta(x)$. The numerical result obtained by terminating the sum in Eq. (20) at $n = \pm 50$ and the analytic one given by Eq. (G4) cannot be distinguished on the figure.

Because $\varphi_0(x)$ is even and normalized to 1, one gets $\bar{V}_0 = \frac{1}{2}V_0$, and $\bar{V}_{\pm n} = V_0(\frac{1}{2} \pm r_n)$ with $r_n = \int_0^{na} dx|\varphi_0(x)|^2$ for $n > 0$, where trivially r_n increases strictly monotonically from $r_0 = 0$ to 1 with n going to infinity so that $\bar{V}_n$ takes the value V_0 for large negative index n and decreases strictly monotonically through the value $\bar{V}_0 = \frac{1}{2}V_0$ at $n = 0$ to zero when n increases to infinitely large integer values. So long the localized state $\varphi_{na}(x)$ almost entirely extends over a region where the potential is V_0 or zero, it detects its original value, but when it 'feels' the sudden jump of the potential step it detects monotonically decreasing values when the increasing sequence x_n runs through $x = 0$. The sampled values already smear out the sudden jump over a region of width a. Reconstruction of the bandlimited potential $\bar{V}(\bar{x})$ from the sample shall make the fall of the potential around $x = 0$ oscillatory. Instead of evaluating analytically the reconstructed potential itself we shall illustrate the oscillations introduced by the reconstruction on a more simple example. For that purpose let us choose the sample $\mathcal{V}_n = \mathcal{V}(x_n = an)$ taken of the simple step function $\mathcal{V}(x) = V_0\Theta(-x)$ for which the well-known integral representation

$$\mathcal{V}(x) = \frac{V_0}{2\pi i}\int_{-\infty}^{\infty} dl \frac{e^{-ilx}}{l - i\epsilon} \tag{29}$$

holds. The bandlimited potential reconstructed from this sample $\mathcal{V}_n$ is then given as

$$\bar{\mathcal{V}}(x) = \frac{V_0}{2\pi i}\int_{-K}^{K} dl \frac{e^{-ilx}}{l - i\epsilon}. \tag{30}$$

Let us evaluate this integral by closing the straightline section $[-K, K]$ on the real axis via a half circle $\mathcal{C}_-$ of radius K on the lower half of the complex l plane, along which one has $l = Ke^{-i\alpha}$ with α running from zero to π,

$$\bar{\mathcal{V}}(x) = \frac{V_0}{2\pi i}\int_{\mathcal{C}_-} dl \frac{e^{-ilx}}{l}$$

$$= \frac{V_0}{2\pi}\int_0^{\pi} d\alpha e^{-iKx\cos\alpha - Kx\sin\alpha}. \tag{31}$$

Changing the integration variable from α to $\beta = \alpha - \frac{1}{2}\pi$, one can recast the integral in the form

$$\bar{\mathcal{V}}(x) = \frac{V_0}{\pi}\int_0^{\pi/2} d\beta \cos(Kx\sin\beta)e^{-Kx\cos\beta}$$
$$= V_0\left(\frac{1}{2} - \frac{\mathrm{Si}\ (Kx)}{\pi}\right). \tag{32}$$

The reconstructed potential tends to V_0 for $x \to -\infty$, zero for $x \to +\infty$ taking the value $\frac{1}{2}V_0$ at $x = 0$ and it falls in an oscillatory manner from the value V_0 to zero. The reconstructed potential and its analytic approximation in Eq. (32) are demonstrated in Fig. 2.

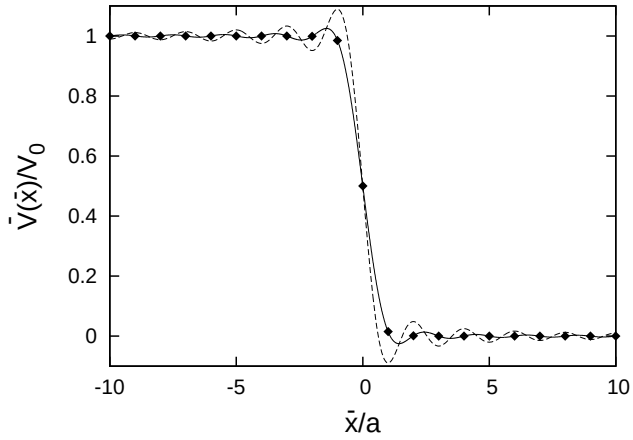

FIG. 2. Sampled values (boxes), the reconstructed bandlimited continuous potential (solid line) and its analytic approximation (dashed line) for the potential step $V(x) = V_0\Theta(-x)$. The numerical result (solid line) has been obtained by terminating the sum in Eq. (20) at $n = \pm 50$.

V. MOTION OF A WAVEPACKET IN FREE SPACE

The Schrödinger equation for the free motion of a particle in one-dimensional space, say the x axis is

$$i\hbar\partial_t\psi(x,t) = \int_{-\infty}^{\infty} dy(\Pi H^{free}\Pi)(x,y)\psi(y,t) \tag{33}$$

with the Hamiltonian

$$H^{free}(x,y) = \frac{1}{2m\alpha^2}[F^{-1}(-i\alpha\hbar\partial_x)]^2\delta(x-y). \tag{34}$$

The Hamiltonian $\hat{H}^{free}$, the operators of the wavevector $\hat{k}_x$ and the canonical momentum $\hat{p}_x = F^{-1}(\alpha\hbar\hat{k}_x)/\alpha$ are

pairwise commuting, and their common set of eigenfunctions are the plane waves $e^{ik_x x}$. The projector acts on plane waves as

$$\int_{-\infty}^{\infty} dy \Pi(x,y) e^{ik_x y} = \Theta(K - |k_x|) e^{ik_x x} \tag{35}$$

so that the subset of plane waves with wavevector $k_x \in [-K, K]$, canonical momentum $p_x(k_x) = F^{-1}(\alpha\hbar k_x)/\alpha \in (-\infty, \infty)$ and energy $E_{k_x} = [F^{-1}(\alpha\hbar k_x)]^2/(2m\alpha^2) \in [0, \infty)$ eigenvalues, respectively, form the set of common eigenfunctions of the operators $\hat{\Pi}\hat{H}^{free}\hat{\Pi}$, $\hat{\Pi}\hat{k}_x\hat{\Pi}$ and $\hat{\Pi}\hat{p}_x\hat{\Pi}$ in bandlimited Quantum Mechanics. For canonical momenta much less than the Planck momentum, i.e. for $|p_x| \ll (1/\alpha)$, one can expand the deformation function in powers of the magnitude of $u = \alpha p_x$ as $f(u) = 1 + f_1|u| + f_2 u^2 + \ldots$ which implies the expansions $F(u) = u - \frac{1}{2} f_1 u|u| + \frac{1}{3}(f_1^2 - f_2)u^3 + \ldots$, $F^{-1}(v) = v + \frac{1}{2} f_1 v|v| + \frac{1}{6}(f_1^2 + 2f_2)v^3 + \ldots$ with $v = \alpha\hbar k_x$ and the well-known modification of the energy eigenvalue due to the GUP

$$E_{k_x} \approx \frac{\hbar^2 k_x^2}{2m}\left(1 + f_1\alpha\hbar|k_x| + \frac{1}{12}(7f_1^2 + 8f_2)\alpha^2\hbar^2 k_x^2 + \ldots\right) \tag{36}$$

for $|k_x| \ll K$. As to the plane waves the only effect due to the finite band width is the lack of plane waves with wavevectors from the UV region.

Now let us seek the solution of the time-dependent Schrödinger equation (33) in the form of a wavepacket, i.e. that of a superposition from plane waves belonging to the finite band of wavevectors,

$$\psi(x,t) = \int_{-K}^{K} \frac{dk_x}{2\pi} a(k_x, t) e^{ik_x x}, \tag{37}$$

$$i\hbar\partial_t a(k_x, t) = \frac{[p_x(k_x)]^2}{2m} a(k_x, t). \tag{38}$$

In order to choose an initial condition $a_0(k_x) = a(k_x, t = 0)$ consistent with the generalized uncertainty relation implied by Eq. (1), one has to be rather cautious. In the wavevector representation the coordinate operator $\hat{x}$ is represented by the formal differential operator $i\partial_{k_x}$ defined in the dense domain $\mathcal{D}_x \subset L^2[-K, K]$ of square integrable wavefunctions $\tilde{\tilde{\psi}}(k_x)$, consisting of absolutely continuous functions whose derivatives also belong to $L^2[-K, K]$. The physical domain $\mathcal{D}_{phys}$ consisting of the wavefunctions satisfying the generalized uncertainty relation should be a subset of the domain $\mathcal{D}_x$, $\mathcal{D}_{phys} \subseteq \mathcal{D}_x$. We should choose the initial condition from that physical domain, $a_0(k_x) \in \mathcal{D}_{phys}$. For $\hat{x}$ being a symmetric operator, only two types of boundary conditions are allowed [71]. In the set of functions satisfying $\tilde{\tilde{\psi}}(K) = C\tilde{\tilde{\psi}}(-K)$ with $|C| = 1$ the coordinate operator is self-adjoint, but in our case this should be excluded because in that case the coordinate operator were diagonal in the coordinate representation and the GUP in Eq. (1) could not be satisfied. Thus the wavefunctions $\tilde{\tilde{\psi}}(k_x) \in \mathcal{D}_{phys}$ should satisfy the other type of boundary conditions, namely Dirichlet's boundary conditions $\tilde{\tilde{\psi}}(-K) = \tilde{\tilde{\psi}}(K) = 0$ for which $\hat{x}$ is not self-adjoint. Therefore we choose an initial condition $a_0(k_x)$ satisfying the boundary conditions $a_0(\pm K) = 0$,

$$a_0(k_x) = \mathcal{N}\exp\left(-\frac{[p_x(k_x) - \bar{p}]^2}{4\sigma_p^2}\right), \tag{39}$$

corresponding to a Gaussian wavepacket with the mean wavevector $\bar{k}$, the mean canonical momentum $\bar{p} = p_x(\bar{k})$, the variance σ_p, and the normalization factor $\mathcal{N}$. Without loss of generality one can assume $\bar{k} > 0$ (i.e. $\bar{p} > 0$) and $\sigma_p \ll K\hbar$. The solution of Eq. (38) with the initial condition (39) is

$$a(k_x, t) = a_0(k_x)\exp\left(-\frac{i}{\hbar}\frac{[p_x(k_x)]^2}{2m}t\right) \tag{40}$$

and the evolution of the wavepacket is given by the time-dependent wavefunction

$$\psi(x,t) = \int_{-K}^{K} \frac{dk_x}{2\pi} a_0(k_x)\exp\left(-\frac{i}{\hbar}\frac{[p_x(k_x)]^2}{2m}t + ik_x x\right). \tag{41}$$

For the sake of simplicity let us assume that the deformation function $f(u)$ is analytic at $u = 0$. For sufficiently sharp distribution, $\sigma_p \ll K\hbar$ one can expand the exponent at the mean $\bar{k}$ as

$$\text{Exp.} = -\frac{i}{\hbar}\frac{\bar{p}^2}{2m}t + i\bar{k}x - A(t)s^2 + iB(x,t)s \tag{42}$$

where

$$A(t) = \frac{\hbar^2\bar{f}^2}{4\sigma_p^2} + \frac{i\beta_2 t}{2m\hbar}, \quad B(x,t) = x - \frac{\beta_1 t}{2m\hbar},$$
$$\beta_1 = 2\hbar\bar{p}\bar{f}, \quad \beta_2 = \hbar^2\bar{f}(\bar{f} + 2\alpha^2\bar{p}^2\bar{f}'), \tag{43}$$

with $s = k_x - \bar{k}$, $\bar{p} = p_x(\bar{k})$, $\bar{f} = f(\alpha^2\bar{p}^2) > 1$, $\bar{f}' = f'(\alpha^2\bar{p}^2)$, $f'(u) = df(u)/du$. The time-dependent wavefunction (41) can then be rewritten as

$$\psi(x,t) = \mathcal{N}\exp\left(-\frac{i}{\hbar}\frac{\bar{p}^2}{2m}t + i\bar{k}x\right) \times \int_{-K+\bar{k}}^{K+\bar{k}} \frac{ds}{2\pi} e^{-A(t)s^2 + iB(x,t)s}. \tag{44}$$

Let us now make use of $\sigma_k \ll K$ and consider the limiting cases (i) $\bar{k} = 0$ and (ii) $\bar{k} = K$. As a good approximation we can replace the definite integrals by improper ones for case (i) $\int_{-K}^{K} dk_x \Rightarrow \int_{-\infty}^{\infty} dk_x$ and for case (ii) $\int_{-2K}^{0} dk_x \Rightarrow \int_{-\infty}^{0} dk_x$. Because of the inequality $\text{Re}\, A(t) > 0$, the integral remains convergent and one ends up with

$$\psi(x,t) \propto A^{-\frac{1}{2}}(t)\exp\left(-\frac{i}{\hbar}\frac{\bar{p}^2}{2m}t + i\bar{k}x - \frac{B^2(x,t)}{4A(t)}\right) \tag{45}$$

implying the Gaussian spatial distribution

$$|\psi(x,t)|^2 \propto A^{-1}(t)\exp\left(-\frac{(x - \bar{v}t)^2}{2\sigma_x^2(t)}\right), \tag{46}$$

centered at the position $\bar{x} = \bar{v}t$ at time t and moving with the speed $\bar{v} = \bar{f}\bar{p}/m > \bar{p}/m$. Therefore, the center of the wavepacket moves with a larger speed in the bandlimited case than in ordinary Quantum Mechanics. The variance of the position distribution is given by

$$\sigma_x^2(t) = \frac{|A(t)|^2}{\text{Re } A(t)} = \frac{\hbar^2 \bar{f}^2}{4\sigma_p^2}\left[1 + \frac{t^2}{\tau^2}\right], \tag{47}$$

where the characteristic time for the spreading of the wavepacket is given as

$$\tau = \tau_0 \frac{\bar{f}}{\bar{f} + 2\alpha^2 \bar{p}^2 \bar{f}'} < \tau_0 \tag{48}$$

in terms of the characteristic spreading time $\tau_0 = m\hbar/(2\sigma_p^2)$ in ordinary Quantum Mechanics. We see that the finite band width can cause a much faster spread of the wavepacket when its mean wavevector approaches the limiting value K.

VI. STATIONARY STATES OF A PARTICLE IN A POTENTIAL

Let us discuss now the problem of stationary states of a particle in a potential $V(x)$. Even if GUP does not imply a finite wavevector cutoff, it results in the modified kinetic energy operator $\hat{H}^{free}$, introduced in the previous section, so that the Hamiltonian can be written as $\hat{H} = \hat{H}^{free} + \hat{V}$. In order to determine the low-energy states the non-degenerate stationary perturbation expansion has been widely applied with an expansion in powers of the small parameter α (see e.g. [22–24, 47–61]). When additionally even a finite band width is enforced by GUP, the projected Hamiltonian $\hat{\Pi}(\hat{H}^{free} + \hat{V})\hat{\Pi}$ figures in the stationary Schrödinger equation (13). Now we shall use the perturbation expansion for the low-energy states in another manner, without expanding in the small parameter α. Namely, we shall simply say that the whole GUP effect, including the effect of projection to states with finite band width, is a perturbation and account it for in the first order. Therefore we split the projected Hamiltonian as

$$\hat{\Pi}\hat{H}\hat{\Pi} = \hat{H}_0 + \hat{H}', \tag{49}$$

where $\hat{H}_0 = \hat{T}_0 + \hat{V}$ is the Hamiltonian in ordinary Quantum Mechanics with the usual kinetic energy operator $\hat{T}_0 = \hbar^2 \hat{k}_x^2/(2m)$ and

$$\hat{H}' = \hat{h} + \hat{v} + \hat{t} \tag{50}$$

represents the perturbation caused by GUP and the restriction to finite band width. The latter consists of the pure GUP effect $\hat{h} = \hat{H} - \hat{H}_0 = \hat{H}^{free} - \hat{T}_0$ discussed widely in the literature and the pieces $\hat{v} = \hat{\Pi}\hat{V}\hat{\Pi} - \hat{V}$ and $\hat{t} = \hat{\Pi}\hat{H}^{free}\hat{\Pi} - \hat{T}_0$ responsible for the additional modification of the potential and the kinetic energy operator due to the restriction of the states to those with finite band width. Obviously, the projection alters the local potential and kinetic energy into nonlocal quantities.

Let $\{\varphi_n\}$ be the complete set of eigenstates of the unperturbed Hamiltonian $\hat{H}_0$,

$$\hat{H}_0|\varphi_n\rangle = \epsilon_n|\varphi_n\rangle, \tag{51}$$

then the energy levels $E_n = \epsilon_n + \Delta\epsilon_n$ of the perturbed system are shifted by

$$\Delta\epsilon_n = \langle\varphi_n|\hat{H}'|\varphi_n\rangle = h_{nn} + v_{nn} + t_{nn}, \tag{52}$$

where $h_{nn} = \langle\varphi_n|\hat{h}|\varphi_n\rangle$, $v_{nn} = \langle\varphi_n|\hat{v}|\varphi_n\rangle$, and $t_{nn} = \langle\varphi_n|\hat{t}|\varphi_n\rangle$ represent the energy shifts caused by pure GUP effect and by the projection of the potential and that of the kinetic energy, respectively.

VII. TOY MODEL: PARTICLE IN A BOX

A. Energy shifts of stationary states

We shall apply the method described in the previous section to a toy model, a particle bounded in a square-well potential

$$V(x) = V_0[\Theta(-x) + \Theta(x - L)] \tag{53}$$

of width L and let go finally the depth of the potential well V_0 to infinity. Although a sudden jump of the potential is unrealistic in bandlimited Quantum Mechanics as emphasized in [68], but in our treatment that problem shall be cured by projection that makes potential edges effectively smeared out over a range of the order a, as argued in Sect. IV previously.

When GUP effects (including finite band width) are neglected, the solutions $\varphi_n(x)$ corresponding to the unperturbed bound states with energy $\epsilon_n < V_0$ in the square well potential are given in App. B. The expressions for asymptotically large depth V_0 of the potential, i.e. for states with $\epsilon_n/V_0 \ll 1$ are also given. The matrix elements h_{nn}, v_{nn} and t_{nn} contributing additively to the energy shift can be expressed in terms of the various pieces $\varphi_i(x)$ $(i = I,\ II,\ III)$ of the wavefunction defined in the intervals I_i, respectively (c.f. App B). Since the operator $\hat{h}$ is local, while the operators $\hat{v}$ and $\hat{t}$ are nonlocal due to the projection operator, we can write their matrix elements in the form:

$$\begin{aligned}
h_{nn} &= \sum_{i=I}^{III} h_i, \quad h_i = \int_{I_i} dx \varphi_i^*(x) h_x \varphi_i(x), \\
v_{nn} &= \sum_{i,j=I}^{III} v_{i,j}, \quad v_{i,j} = \int_{I_i} dx \int_{I_j} dy \varphi_i^*(x) v(x,y) \varphi_j(y), \\
t_{nn} &= \sum_{i,j=I}^{III} t_{i,j}, \quad t_{i,j} = \int_{I_i} dx \int_{I_j} dy \varphi_i^*(x) t(x,y) \varphi_j(y),
\end{aligned} \tag{54}$$

where

$$h_x = \frac{1}{2m}\left(\frac{1}{\alpha^2}[F^{-1}(-i\alpha\hbar\partial_x)]^2 - (-\hbar^2\partial_x^2)\right),$$
$$v(x,y) = \frac{1}{2}[V(x)+V(y)][\Pi(x,y)-\delta(x-y)],$$
$$t(x,y) = \frac{1}{2m\alpha^2}[F^{-1}(-i\alpha\hbar\partial_x)]^2[\Pi(x,y)-\delta(x-y)] \quad (55)$$

are the appropriate kernels. Hermitian symmetry of the operators $\hat{h}$, $\hat{v}$, and $\hat{t}$, reflection symmetry of the potential to $x = L/2$ and being the operator $[F^{-1}(\alpha\hbar\hat{k}_x)]^2$ even lead to the symmetry relations

$$h_I = h_{III},$$
$$v_{j,i} = (v_{i,j})^*, \quad v_{III,III} = v_{I,I}, \quad v_{III,II} = \pm v_{I,II},$$
$$t_{j,i} = (t_{i,j})^*, \quad t_{III,III} = t_{I,I}, \quad t_{III,II} = \pm t_{I,II}. \quad (56)$$

Here the $\pm$ signs correspond to eigenstates characterized by the wavevectors $k_\pm$. Furthermore, $v_{II,II} = 0$ trivially because $V(x) = 0$ for $x \in I_{II}$.

B. Shift due to pure GUP effect

We call pure GUP effect the energy shift h_{nn} of stationary states because of the modification of the canonical momentum and that of the kinetic energy from $\hbar\hat{k}_x$ and $(\hbar\hat{k}_x)^2/(2m)$ in ordinary Quantum Mechanics to $\alpha^{-1}F^{-1}(\alpha\hbar\hat{k}_x)$ and $(2m\alpha^2)^{-1}[F^{-1}(\alpha\hbar\hat{k}_x)]^2$ when GUP is in work. Making use of the results of App. C one finds that the functions $\varphi_i(x)$ ($i = I,\ ,II,\ III$) are eigenfunctions of the kinetic energy operator. Then one gets

$$h_{II} = \frac{1}{2m}\left(\frac{1}{\alpha^2}[F^{-1}(\alpha\hbar k_\pm)]^2 - \hbar^2 k_\pm^2\right)\int_{I_{II}} dx|\varphi_{II}(x)|^2,$$
$$h_I = \frac{1}{2m}\left(\frac{1}{\alpha^2}[F^{-1}(-i\alpha\hbar\kappa)]^2 + (\hbar\kappa_\pm)^2\right)\int_{I_I} dx|\varphi_I(x)|^2$$
$$= h_{III} \quad (57)$$

and the energy shift due to pure GUP effect

$$h_{nn} = \left[(1+\frac{\sin k_\pm L}{k_\pm L})\left([F^{-1}(\alpha\hbar k_\pm)]^2 - (\alpha\hbar k_\pm)^2\right)\right.$$
$$\left.+\frac{|\rho_\pm|^2}{2\kappa_\pm L}\left([F^{-1}(-i\alpha\hbar\kappa_\pm)]^2 + (\alpha\hbar\kappa_\pm)^2\right)\right]$$
$$\times\left[2m\alpha^2\left(1+\frac{\sin k_\pm L}{k_\pm L}+\frac{|\rho_\pm|^2}{2\kappa_\pm L}\right)\right]^{-1}. \quad (58)$$

Let us consider now the limit $\kappa_\pm \to \infty$, the case of a particle in a box. In that limit $|\rho_\pm|^2 \sim k_\pm^2/\kappa_\pm^2$ and, consequently, one obtains finite energy shift if and only if the limit $\lim_{\kappa\to\infty}[F^{-1}(-i\alpha\hbar\kappa)]^2\kappa^{-3} = C_\infty$ remains finite. We shall assume that only such deformation functions are physically reasonable for which $C_\infty = 0$, which means that the tails of the wavefunction in the outer regions I_I and I_{III} of the square-well potential give vanishing contributions to the kinetic energy when the depth of the potential becomes infinite. The deformation function $f = 1+\alpha^2 p_x^2$ with $F^{-1}(u) = \tan u$ satisfies that condition because the limit $\lim_{u\to\pm\infty}\tanh u = \pm 1$ is finite. Finally, we end up with the pure GUP energy shift $h_{nn} = R_h\epsilon_n$ with

$$R_h = \left(\frac{F^{-1}(\alpha\hbar k_\pm)}{\alpha\hbar k_\pm}\right)^2 - 1 \quad (59)$$

for any deformation function being reasonable in the above discussed sense. For highly excited states characterized by wavevectors $k_\pm \approx K$ close to the UV cutoff the ratio R_h explodes which signals simply that the perturbation expansion seases to work. For low-lying states for which our approach is applicable, the expansion in the small parameter $\alpha\hbar k_\pm = n\alpha\hbar\pi/L$ yields

$$R_h \approx \frac{\alpha\hbar\pi}{L}\left[f_1 n + \frac{1}{12}\left(7f_1^2+8f_2\right)\frac{\alpha\hbar\pi}{L}n^2+\ldots\right]. \quad (60)$$

For $h\alpha = \ell_P$ and $f = 1+\alpha^2 p_x^2$ one gets $f_1 = 0$ and $f_2 = 1$ and the ratio

$$R_h \approx \frac{2}{3}\left(\frac{\ell_P}{2L}\right)^2 n^2 + \mathcal{O}\left((n\ell_P/L)^2\right) \quad (61)$$

raising quadratically with increasing n and being independent of the mass of the particle in the box. Thus we recovered the result obtained in Refs. [70] and [61] (given after Eq. (14) for $j = 1$). An order-of-magnitude estimate gives $(\ell_P/L)^2 \approx 10^{-40}$, 10^{-50}, and 10^{-58} for boxes of the size $L = 10^{-15}$ m (size of a nucleon), 10^{-10} m (size of a H-atom), and 10^{-6} m (the wavelength of infrared radiation), respectively. So even for the first few thousands of energy levels the pure GUP correction remains a tiny correction.

C. Shift due to finite band width

Finite band width, i.e. the existence of the finite UV wavevector cutoff K results in the absence of quantum fluctuations with UV wavevectors $|k_x| > K$, that is expressed in our approach by the projection of the operators of potential and kinetic energies. The energy shift v_{nn} of the n-th energy level caused by the replacement of the potential by its projected counterpart can be expressed in terms of the independent integrals $v_{I,I}$, $v_{I,II}$ and $v_{I,III}$ when the symmetry relations discussed above are accounted for. Here $v_{I,I}$ and $v_{I,III}$ are real because $\varphi_I(x)$ and $\varphi_{III}(x)$ are real functions. As discussed in App. D the leading order contribution comes from the integral $v_{I,II}$ in the limit of infinite potential depth, while the other independent integrals $v_{i,j}$ are suppressed like powers of $1/\kappa_\pm$ as compared to it. One finds (c.f. Eq. (D12)) that v_{nn} vanishes for the energy levels n even and

for the energy levels n odd it is given as (c.f. Eqs. (D10), (D11), and (D12))

$$v_{nn} \approx \frac{\hbar^2 k}{2mL}\Bigg(\frac{2k}{K\pi}[4\sin^2(\nu\pi) + (n\pi)^2\cos(2\nu\pi) + \mathcal{O}\left(n^4\right)] + \mathcal{O}\left((k/K)^2\right)\Bigg). \tag{62}$$

The vanishing of v_{nn} for even n is a consequence of the particular form of the wavefunction in a square-well potential, namely the alternating sign of the tail of the wavefunction in the region III with the alteration of even and odd n values in the numeration of the stationary states with increasing energy. The ratio of the energy shift v_{nn} for odd n to the unperturbed energy ϵ_n of the stationary state n,

$$R_v = \frac{v_{nn}}{\epsilon_n} \approx \frac{2}{KL\pi}[4\sin^2(\nu\pi) + (n\pi)^2\cos(2\nu\pi) + \mathcal{O}\left(n^4\right)] + \mathcal{O}\left((\ell_P/L)^2\right) \tag{63}$$

turns out to take values of the order (ℓ_P/L).

Thus, the potential energy shift due to the UV cutoff seems to be many orders of magnitude larger – at least for the lowest energy levels – as compared to the energy shift caused by pure GUP, because it holds $R_h/R_v \approx \mathcal{O}\left(\ell_P/L\right)$. It is remarkable that R_v oscillates strongly with the fine-tuning of the length of the box L confining the particle. The variation of ν in the interval $[0,1]$ corresponds to the tiny change of the box size L in a range of $\mathcal{O}\left(\ell_P\right) = \mathcal{O}\left(a\right)$, the size of the grid constant, as well as that of the maximal accuracy $\Delta x_{\min}$ of position determination. Therefore, an averaging over ν might be more reliable when one wants to incorporate the indefiniteness of the size of the box, a direct consequence of the impossibility to determine positions more precisely than the distance Δx_{min}. This yields then

$$\int_0^1 d\nu R_v \approx \frac{4}{KL\pi}[1 + \mathcal{O}\left(n^4\right)] + \mathcal{O}\left((KL)^{-2}\right). \tag{64}$$

An order-of-magnitude estimate gives $(KL)^{-1} \sim (\ell_P/L) \approx 10^{-20}$, 10^{-25}, and 10^{-29} for boxes of the size $L = 10^{-15}$ m (size of a nucleon), 10^{-10} m (size of a H-atom), and 10^{-6} m (the wavelength of infrared radiation), respectively. These are still small effects but 20 to 30 orders of magnitude larger than the energy shift due to pure GUP without wavevector cutoff.

Another contribution t_{nn} arises due to finite band width, which represent the difference of the expectation values of the projected and unprojected kinetic energy operators. According to the symmetry relations, the only independent integrals contributing to the kinetic energy shift t_{nn} are $t_{I,I}$, $t_{II,I}$, $t_{III,I}$, $t_{II,II}$ as given in Eqs. (E1) in App. E. Among them $t_{II,II}$ is the only one surviving the limit $\kappa \to \infty$, that of taking the square-well potential with infinite depth. According to Eqs. (E10) and the estimate in Eq. (E12) one obtains

$$t_{II,II} \approx R_t(1 + R_h)\epsilon_n \approx R_t\epsilon_n \tag{65}$$

with

$$R_t(\nu) \approx \frac{t_{II,II}}{\epsilon_n} \approx \mathcal{I}_K(L/2) - 1. \tag{66}$$

Here $R_t(\nu)$ is the ratio defined as the additional shift of the expectation value of the kinetic energy due to the finite band width divided by the unperturbed energy of the stationary state n. While the additional energy shift v_{nn} appeared to be vanishing for states with even n, the shift t_{nn} is nonvanishing for all n. As seen in Eq. (E12) this ratio oscillates with the fine tuning of the length L of the potential box again. Referring to the impossibility of determining positions and distances more precisely than Δx_{min} in bandlimited Quantum Mechanics, one can perform averaging over $\nu \in [0,1]$, similarly to the case for the shift of the expectation value of the potential operator due to the finite band width. The averaging over the interval $\nu \in [0,1]$ results in

$$\int_0^1 d\nu R_t(\nu) \approx \frac{4}{KL\pi} + \mathcal{O}\left((KL)^{-2}\right), \tag{67}$$

being the same as the relative contribution of the shift of the potential energy in Eq. (64).

It is worthwhile to come back now to the viewpoint of considering the length scale Δx_{min} (ℓ_P) as an unknown parameter and looking for its experimental upper bound [26–34] as mentioned in the introduction. The additional effect of the existence of the UV wavevector cutoff $K \sim 1/\ell_P$, taken into account by us by means of the projection method, may have influence on the estimates of such upper bounds. This can be illustrated – although in a rather crude manner – by the following argument. Let us consider, for example, the 1S Lamb shift Δf_L of the Hydrogen atom and ascribe the tiny discrepancy of the best available experimental and theoretical values $\delta f = \Delta f_L^{exp} - \Delta f_L^{th} \approx 1.06 \times 10^5$ s^{-1} to the GUP effect like the authors did in [31, 32]. The lesson learned from our treatment of the particle in a one-dimensional box is that the additional effect of the existence of the UV wavevector cutoff being of the order (ℓ_P/L) is much larger than the direct GUP effect caused by the modification of the free particle's Hamiltonian of the order $(\ell_P/L)^2$. An energy shift of the same order $(\ell_P/L)^2$ has also been found in [31, 32] for the energy shift of the ground state of the Hydrogen atom because the modification of the Hamiltonian due to the direct GUP effect is of that order of magnitude. Let us assume that the indirect effect of GUP via the existence of the UV wavevector cutoff is of the order ℓ_P/R for the Hydrogen-atom ground state, where the Bohr radius $R = 5.29 \times 10^{-11}$ m stands as the box size. Then we expect the relative energy shift of the ground state to be of the order $\delta f/f_{1S} \sim \ell_P/R$, where $f_{1S} \approx 2.447 \times 10^{14}$ s^{-1} is related to the energy $E = -hf_{1S} = -13.6$ eV of the ground state. This would yield an upper bound $\ell_P \lesssim R\delta f/f_{1S} \approx 2.3 \times 10^{-20}$ m $(1.2 \times 10^{-4}$ GeV$^{-1})$ being considerably smaller than the one obtained in [31, 32]. Without taking it word-for-word, we believe that our very crude estimate should

rather be taken as a motivation for the redetermination of the possible bounds on the characteristic length scale with taking the additional effect due to the existence of the UV cutoff into account.

VIII. SUMMARY

The free motion of a wavepacket and the energy levels of a particle in a box have been discussed in one-dimensional Quantum Mechanics when the existence of a finite band width, i.e. that of an UV wavevector cutoff K is present as the consequence of the GUP. The latter is implemented by generalizing Heisenberg's commutation relations for quantization with the particular choice of the deformation function $f(|u|)$ ($u = \alpha p_x$) occuring in the commutator relation for the coordinate $\hat{x}$ and the canonical momentum $\hat{p}_x$. Deformation functions $f(|u|)$ being strictly monotonically increasing with $|u|$, for which $F(u) = \int_0^u \frac{du'}{f(|u'|)}$ remains finite in the limits $u \to \infty$, provide such UV cutoff, $F(\pm\infty) = \pm\alpha\hbar K$. We took the point of view that the existence of the UV wavenumber cutoff, corresponding to infinite canonical momentum eigenvalue, excludes the UV components of the wavefunction. In order to enforce this in the naive coordinate representation, the Hamiltonian and all operators of observables should be sandwiched by a projector restricting wavefunctions to the subspace of bandlimited wavefunctions. Such a projector $\hat{\Pi}$ has been constructed and the rules for the operators acting on the band-limited subspace have been established. It has also been shown that the proposed projection method justifies the usage of the naive coordinate representation through a generalization of Shannon's basic sampling theorem taken from information theory to one-dimensional bandlimited Quantum Mechanics. It has been discussed the relation of the naive coordinate representation using coordinate wavefunctions of continuous variable to discrete coordinate representations based on the self-adjoint extensions of the coordinate operator.

A method is proposed to observe potential values exerted on a particle by means of preparing it in a state of maximal localization. Although any self-adjoint extension of the coordinate operator enables one to take such sampled values at the discrete points of equidistant spacing $a = \pi/K$, the reconstruction of a bandlimited continuous potential is possible according to Shannon's basic sampling theorem on bandlimited real functions. Applying that reconstruction procedure the broadening the Dirac-delta like potential and the smearing out the potential step over a region of the order of the spacing a have been shown, both accompanied with oscillations of wavelength of ca. $2a$, as well.

It has been shown that the free motion of the wavepacket is modified as the consequence of the finite band width. The center of a Gaussian wavepacket with mean canonical momentum $\bar{p}$ moves with a speed $\bar{V}$ larger than $\bar{v} = \bar{p}/m$ (c.f. Eq. (46)) and the spreading time τ of the wavepacket gets smaller than the corresponding characteristic time τ_0 in usual Quantum Mechanics (c.f. Eq. (48)). The ratios $\bar{V}/\bar{v}$ and τ/τ_0 are strictly monotonically increasing and decreasing functions of the mean momentum $\bar{p}$, respectively.

The shifts of the low-lying energy levels of a particle in a box have been determined considering the effect of GUP and the additional effect caused by the UV cutoff in first-order perturbation theory. For the pure GUP effect the well-known result has been recovered being of the order $(\ell_P/L)^2$ for the box size L (in terms of the Planck length ℓ_P) and the deformation function $f = 1 + \alpha p_x^2$. The additional effect caused by the UV cutoff, i.e. by the projection to the subspace of states with finite band width, has occurred as the shift of the expectation values of both the potential and kinetic energy operators and turned out to be of the order ℓ_P/L. This result indicates that the effect of GUP on low-energy Quantum Mechanics may be much more significant indirectly, through the existence of the finite UV cutoff than directly by providing small correction terms to the Hamiltonian. It is also remarkable that the additional effect caused by the UV cutoff appeared to have an oscillatory dependence on the variation of the box size L in a range of the minimal accuracy of position determination. We have suggested that any observation of the box size should average over such a range principally, therefore the true correction should be averaged over that range, as well. We also argued that the existence of the UV wavevector cutoff might affect the determination of the upper bounds on the length scale ℓ_P when it is not taken a priori for the Planck length but instead constrained either by comparison of high-accuracy experimental data with theoretical calculations or by ascribing the tiny error of experimental data entirely to the GUP effect.

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Appendix A: Self-adjoint extensions of the coordinate operator

Here we give a short summary of some mathematical results [71] relevant for the self-adjoint extension of the coordinate operator (c.f. also [14, 36–42]). In the wavevector representation the states are represented by the wavevector wavefunctions $\tilde{\tilde{\psi}}(k_x)$, the coordinate operator by the formal differential operator $i\partial_{k_x}$ (it is called formal because the definition of an operator should include the boundary conditions set on the functions on which it operates, as well). The coordinate operator $\hat{x}$ is defined in the dense domain $\mathcal{D}(\hat{x}) \subset L^2[-K,K]$ of those square integrable functions, which are absolutely continuous (implying infinite differentiability) inside the interval $[-K,K]$, and whose derivatives also belong to $L^2[-K,K]$. The physical domain $\mathcal{D}_{phys}$ consisting of the wavefunctions satisfying the generalized uncertainty relation implied by GUP in Eq. (1) should be a subset of the domain $\mathcal{D}(\hat{x})$, $\mathcal{D}_{phys} \subseteq \mathcal{D}(\hat{x})$. In order to have real expectation values, the coordinate operator $\hat{x}$ should be symmetric. Therefore, only two types of boundary conditions are allowed to be set at $k_x = \pm K$ for the wavefunctions $\tilde{\tilde{\psi}}(k_x)$. It is well-known that the operator $i\partial_{k_x}$ is self-adjoint for the boundary conditions $\tilde{\tilde{\psi}}(K) = C\tilde{\tilde{\psi}}(-K)$ with $|C| = 1$, i.e. $C = e^{i\alpha}$ with $\alpha \in [0, 2\pi)$, and it is not self-adjoint although Hermitian symmetric operating on functions satisfying Dirichlet's boundary conditions $\tilde{\tilde{\psi}}(-K) = \tilde{\tilde{\psi}}(K) = 0$. If $\hat{x}$ were self-adjoint in the physical domain $\mathcal{D}_{phys}$, its eigenstates $e^{-ik_x x}$ would belong to that domain. This cannot, however, be the case because the formal eigenfunctions of the operator $i\partial_{k_x}$ cannot satisfy the boundary condition $e^{-iKx} = e^{i\alpha+iKx}$ for arbitrary eigenvalue x. One can also argue, that would $\hat{x}$ be self-adjoint in the physical domain, the coordinate eigenstates with zero position uncertainty were physical states and that would contradict GUP implying a wavevector cutoff, i.e. a nonvanishing minimal position uncertainty. Therefore, it remains the only possibility of $\hat{x}$ being symmetric on functions with Dirichlet's boundary condition.

In this case the adjoint operator $\hat{x}^\dagger$ represented formally also by $i\partial_{k_x}$ has the domain $\mathcal{D}(\hat{x}^\dagger)$ consisting of all differentiable functions of $L^2[-K,K]$ whose derivatives also belong to $L^2[-K,K]$ and which are not restricted by any kind of boundary conditions. Thus clearly one has $\mathcal{D}(\hat{x}) \subset \mathcal{D}(\hat{x}^\dagger)$. Symmetric operators can be characterized by their deficiency indices $\nu_\pm$, the dimensions of the nullspaces of the operators $\hat{x}^\dagger - (\pm i)\xi$, respectively, where $\xi \in \mathbb{R}$. The solutions of the equations

$$0 = (i\partial_{k_x} \mp i\xi)\tilde{\tilde{\varphi}}_\pm, \quad \xi \in \mathbb{R} \tag{A1}$$

are the square-integrable functions $\tilde{\tilde{\varphi}}_\pm(x) = e^{\pm\xi k_x}$, which span one-dimensional null-spaces, so that the deficiency indices of $\hat{x}$ are equal, $\nu_+ = \nu_- \equiv \nu = 1$. Then there exist self-adjoint extensions $\hat{x}_e = \hat{x}_e^\dagger$ of $\hat{x}$. According to the general theory, these can be constructed by means of the boundary conditions prescribed for the functions of the domain $\mathcal{D}(\hat{x}_e)$. In the case with $\nu = 1$ a single boundary condition is needed to specify the domains $\mathcal{D}(\hat{x}_e)$ of the self-adjoint extension $\hat{x}_e$ and that can be done in terms of a single function $f_1(k_x) \in \mathcal{D}(\hat{x}^\dagger)$ being linearly independent relative to $\mathcal{D}(\hat{x})$ (because $\hat{x}$ is a closed operator):

$$\mathcal{D}(\hat{x}_e) = \{f | f \in \mathcal{D}(\hat{x}^\dagger), [f(k_x)f_1^*(k_x)]_{-K}^K = 0, \\ [f_1(k_x)f_1^*(k_x)]_{-K}^K = 0, f_1 \in \mathcal{D}(\hat{x}^\dagger)\} \tag{A2}$$

with $[fg^*]_a^b = f(b)g^*(b) - f(a)g^*(a)$. The function f_1 linearly independent relative to $\mathcal{D}(\hat{x})$ can be constructed as the linear combination $f_1(k_x) = \beta h_1(k_x) + \gamma h_{-1}(k_x)$

($\beta, \gamma \in \mathbb{C}$) of a number of $2\nu = 2$ functions, $h_s(k_x)$ ($s = 1, -1$) which are linearly independent relative to $\mathcal{D}(\hat{x})$, i.e. for which the relations

$$[h_r h_s]_{-K}^{K} = r(2K)^2 \delta_{rs}, \quad r, s = 1, -1 \tag{A3}$$

hold. These are the functions $h_1 = K + k_x$ and $h_2 = K - k_x$. Then one finds $f_1(k_x) = \beta(K + k_x) + \gamma(K - k_x)$ and

$$\begin{aligned} 0 = [f_1 f_1]_{-K}^{K} &= \beta\beta^* h_1^2(K) - \gamma\gamma^* h_{-1}^2(-K) \\ &= (2K)^2(\beta\beta^* - \gamma\gamma^*) \end{aligned} \tag{A4}$$

implying

$$\begin{aligned} \beta/\gamma &= \frac{1}{(\beta/\gamma)^*}, \quad \Rightarrow \quad |\beta/\gamma|^2 = 1, \\ \beta/\gamma &= e^{i\alpha + 2\pi n i}, \quad \alpha \in [0, 2\pi), \ n \in \mathbb{Z} \end{aligned} \tag{A5}$$

and

$$[f f_1]_{-K}^{K} = f(K) f_1^*(K) - f(-K) f_1^*(-K) = 0, \tag{A6}$$

restricting the domain of the self-adjoint extension to the functions with boundary conditions

$$f(K) = f(-K) \frac{f_1^*(-K)}{f_1^*(K)} = f(-K) e^{-i\alpha}, \tag{A7}$$

given through a particular choice of the parameter $\alpha \in [0, 2\pi)$ (when $f(\pm K) \neq 0$) and to those with Dirichlet's boundary conditions. This means, that the various self-adjoint extensions $\hat{x}_e$ of the operator $\hat{x}$ are obtained when the domain of the formal differential operator $i\partial_{k_x}$ is defined as

$$\begin{aligned} \mathcal{D}(\hat{x}_e) = \mathcal{D}(\hat{x}) \cup \{ f | f \in \mathcal{D}(\hat{x}^\dagger), \quad f(K) = f(-K) e^{-i\alpha}, \\ \alpha \in [0, 2\pi) \}. \end{aligned} \tag{A8}$$

Thus the various self-adjoint extensions are identical on the domain $\mathcal{D}(\hat{x})$ and can be parametrized by the real number $\alpha \in [0, 2\pi)$ so that we can write for them $\hat{x}_e = \hat{x}_\alpha$. The eigenfunctions $e^{-ik_x x} \in \mathcal{D}(\hat{x}_\alpha)$ (but $\notin \mathcal{D}(\hat{x})$) of the particular self-adjoint extension $\hat{x}_\alpha$ are those satisfying the boundary conditions in Eq. (A7)

$$e^{-iKx} = e^{iKx - i\alpha} \tag{A9}$$

belonging to the eigenvalues $x = x_n^\theta = na + \theta$ with $a = \pi/K$ and $\theta = \alpha/2K \in [0, a)$. These eigenvalues determine a grid of equidistant points on the coordinate axis with spacing a. We can change the notation of the particular self-adjoint extensions from $\hat{x}_\alpha$ to $\hat{x}_\theta$. Since the eigenfunctions

$$\tilde{\psi}_{x_n}^{\theta}(k_x) = \sqrt{a} e^{ik_x x_n^\theta}, \quad k_x \in [-K, K] \tag{A10}$$

of any particular self-adjoint extension $\hat{x}_\theta$ form a complete orthonormal set, satisfying the orthonormality conditions (the upper index θ of the eigenvalues are suppressed)

$$\begin{aligned} \delta_{nn'} &= \int_{-K}^{K} \frac{dk_x}{2\pi} \tilde{\psi}_{x_n}^{\theta\,*}(k_x) \tilde{\psi}_{x_n'}^{\theta}(k_x) \\ &= \int_{-\infty}^{\infty} \frac{dp_x}{2\pi f(\alpha|p_x|)} \tilde{\psi}_{x_n}^{\theta *}(p_x) \tilde{\psi}_{x_n'}^{\theta}(p_x), \end{aligned} \tag{A11}$$

There exists a one-parameter family of such orthonormal bases in the Hilbert space $\mathcal{H}$ of bandlimited wavefunctions. Moreover, the one-parameter family of all eigenvalues, i.e. the union $\cup_{\theta \in [0,a)} \{x_n^\theta\}$ of all sets of eigenvalues of the various self-adjoint extensions can be mapped trivially in a one-to-one way on the real line $\mathbb{R}$. Namely, each real number $x \in \mathbb{R}$ occurs as a single eigenvalue of a single self-adjoint extension $\hat{x}_\theta$.

Appendix B: Bound states in a square-well potential

The solution $\varphi_n(x)$ with energy $\epsilon_n < V_0$ of the stationary Schrödinger equation (51) for the square-well potential in Eq. (53) should be sewed from the functions $\varphi_i(x)$ ($i = I,\ II,\ III$) defined in the intervals $I_I : x \in (-\infty, 0]$, $I_{II} : x \in [0, L]$, and $I_{III} : x \in [L, \infty)$, respectively, satisfying the equations

$$\begin{aligned} -\frac{\hbar^2}{2m} \varphi_{II}''(x) &= \epsilon \varphi_{II}(x), \\ -\frac{\hbar^2}{2m} \varphi_i''(x) &= -(V_0 - \epsilon)\varphi_i(x), \quad i = I,\ III \end{aligned} \tag{B1}$$

(We shall suppress the index n numerating the energy levels.) The boundary conditions ensure continuous differentiability of the solution at the boundaries $x = 0$ and $x = L$ of the various intervals, as well as exponential fall-off at infinities $|x| \to \infty$ for square integrability. Looking for the solutions of Eqs. (B1) in the form

$$\begin{aligned} \varphi_{II}(x) &= B e^{ikx} + C e^{-ikx}, \\ \varphi_I(x) &= A e^{\kappa x}, \quad \varphi_{III} = D e^{-\kappa x}, \end{aligned} \tag{B2}$$

with the real parameters $k = \sqrt{2m\epsilon}/\hbar$ and $\kappa = \sqrt{2m(V_0 - \epsilon)}\hbar$, the boundary conditions at $|x| \to \infty$ are automatically satisfied. The boundary conditions at $x = 0$ and $x = L$ result in the set of homogenoeus linear equations,

$$A = B + C, \tag{B3}$$

$$A\kappa = ik(B - C), \tag{B4}$$

$$B e^{ikL} + C e^{-ikL} = D e^{-\kappa L}, \tag{B5}$$

$$ik(B e^{ikL} - C e^{ikL}) = -\kappa D e^{-\kappa L}. \tag{B6}$$

There exists a nontrivial solution for the coefficients A, B, C, and D if and only if the determinant of the set of linear equations vanishes, yielding the implicit equation

$$e^{2ikL} = \left(\frac{\kappa - ik}{\kappa + ik} \right)^2 \tag{B7}$$

for the energy eigenvalues $\epsilon_n = \hbar^2 k_n^2/(2m) < V_0$ of bound states with discrete values k_n and $\kappa_n = \sqrt{2m(V_0 - \epsilon_n)}\hbar$. The numeration of the states by the integer $n = 1, 2, \ldots$ can be established in the limit $V_0 \to \infty$ when $\kappa \to \infty$ and $e^{2ikL} \to 1$ which yields the wavevectors $k_n = n\pi/L$

with $n \in \mathbb{N}$. It is straightforward to realize that the wavevectors $k_\pm$ satisfying

$$e^{ik_\pm L} = \mp\frac{\kappa_\pm - ik_\pm}{\kappa_\pm + ik_\pm} \tag{B8}$$

with $\kappa_\pm = \sqrt{2mV_0 - k_\pm^2\hbar^2}/\hbar$ in the limit $V_0 \to \infty$ behave as $k_- = 2n'\pi/L$ and $k_+ = (2n'-1)\pi/L$ for $n' = 1, 2, \ldots$.

Eqs. (B3) and (B5) can be used to express A and D via C and D, whereas taking the ratio of the appropriate sides of Eqs. (B3) and (B4) one finds after trivial manipulations

$$C = -\frac{\kappa_\pm - ik_\pm}{\kappa_\pm + ik_\pm}B = \pm e^{ik_\pm L}B \tag{B9}$$

implying $A = B\rho_\pm$ and $D = \pm Be^{\kappa_\pm L}\rho_\pm$ with $\rho_\pm = 1 \pm e^{ik_\pm L}$. The normalization condition $\int_{-\infty}^{\infty} dx|\varphi_n(x)|^2 = \sum_{i=I}^{III}\int_{I_i} dx|\varphi_i(x)|^2 = 1$ with

$$\begin{aligned}\int_{I_{II}} dx|\varphi_{II}(x)|^2 &= |B|^2 2L\left(1 + \frac{\sin k_\pm L}{k_\pm L}\right),\\ \int_{I_i} dx|\varphi_i(x)|^2 &= \frac{|\pm B\rho_\pm|^2}{\kappa_\pm}, \quad i = I,\ III\end{aligned} \tag{B10}$$

yields

$$\begin{aligned}|B|^{-2} &= 2L\left(1 + \frac{\sin k_\pm L}{k_\pm L} + \frac{|\rho_\pm|^2}{2\kappa_\pm L}\right)\\ &\approx 2L\left(1 + \frac{2}{\kappa_\pm L} + \mathcal{O}\left((k/\kappa)^3\right)\right).\end{aligned} \tag{B11}$$

For later use we shall need the coefficients for asymptotically large values of V_0, i.e. those of $\kappa \gg k$ which means $\kappa \gg 1/L$ for sufficiently low lying states. Keeping the terms up to the order $\mathcal{O}\left(\kappa^{-2}\right)$ one obtains

$$\begin{aligned}\rho_\pm &\approx \frac{2ik_\pm}{\kappa_\pm} + \frac{2\kappa_\pm^2}{k_\pm^2} + \mathcal{O}\left((k/\kappa)^3\right),\\ |\rho_\pm|^2 &\approx \frac{4\kappa_\pm^2}{k_\pm^2} + \mathcal{O}\left((k/\kappa)^3\right),\\ \sin k_\pm L &\approx \pm\frac{2k_\pm}{\kappa_\pm} + \mathcal{O}\left((k/\kappa)^3\right),\end{aligned} \tag{B12}$$

and

$$\begin{aligned}B &\approx \frac{1}{\sqrt{2L}}\left(1 \mp \frac{1}{\kappa_\pm L} + \frac{3}{2\kappa_\pm^2 L^2} + \mathcal{O}\left((k/\kappa)^3\right)\right),\\ B\rho_\pm &\approx \frac{1}{\sqrt{2L}}\left(\frac{2ik_\pm}{\kappa_\pm} + \frac{2k_\pm^2}{\kappa_\pm^2} \mp \frac{2ik_\pm}{\kappa_\pm^2 L} + +\mathcal{O}\left((k/\kappa)^3\right)\right),\\ |B\rho_\pm|^2 &\approx \frac{1}{2L}\left(\frac{4k_\pm^2}{\kappa_\pm^2} + \mathcal{O}\left((k/\kappa)^3\right)\right).\end{aligned} \tag{B13}$$

Appendix C: Kinetic energy operator on exponential functions

In general an arbitrary operator function $g(\hat{k}_x)$ operates on a function $f(x)$ as

$$\begin{aligned}g(\hat{k}_x)f(x) &= \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} e^{-ik_x y} g(k_x) e^{ik_x x} f(y)\\ &= \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} g(k_x)\tilde{\tilde{f}}(k_x) e^{ik_x x}\end{aligned} \tag{C1}$$

with the Fourier transform of the function $f(x)$,

$$\tilde{\tilde{f}}(k_x) = \int_{-\infty}^{\infty} dx e^{-ik_x x} f(x) \tag{C2}$$

In case of exponential functions, however, the Fourier transform is not a well-behaved function, rather a distribution. Therefore, one has to be careful when using the integral representation of various operators on exponential functions. In order to be more definite, one can consider the Fourier transforms of exponential functions as limits of Gaussian integrals. For $f(x) = e^{isx}$ $(s \in \mathbb{R})$, one can write

$$\begin{aligned}\tilde{\tilde{f}}(k_x) &= \lim_{\sigma\to 0^+}\int_{-\infty}^{\infty} dx e^{i(s-k_x)x - \frac{1}{2}\sigma^2 x^2}\\ &= \lim_{\sigma\to 0^+}\sqrt{\frac{2\pi}{\sigma^2}} e^{-\frac{(s-k_x)^2}{2\sigma^2}}\end{aligned} \tag{C3}$$

and similarly for $f(x) = e^{sx}$, $(s \in \mathbb{R})$

$$\begin{aligned}\tilde{f}(k_x) &= \lim_{\sigma\to 0^+}\int_{-\infty}^{\infty} dx e^{-ik_x x + sx - \frac{1}{2}\sigma^2 x^2}\\ &= \lim_{\sigma\to 0^+}\sqrt{\frac{2\pi}{\sigma^2}} e^{\frac{(s-ik_x)^2}{2\sigma^2}},\end{aligned} \tag{C4}$$

and the trivial operation of the powers of $\hat{k}_x$ on exponential functions, $(-i\partial_x)^n e^{isx} = s^n e^{isx}$ and $(-i\partial_x)^n e^{sx} = (-is)^n e^{sx}$, can also be recovered by saddle point integration:

$$\begin{aligned}(-i\partial_x)^n e^{isx} &= \lim_{\sigma\to 0^+}\sqrt{\frac{2\pi}{\sigma^2}}\int_{-\infty}^{\infty}\frac{dk_x}{2\pi} e^{-\frac{(s-k_x)^2}{2\sigma^2}} k_x^n e^{ik_x x}\\ &= \lim_{\sigma\to 0^+}\frac{1}{\sqrt{2\pi\sigma}}(s + i\sigma^2 x)^n e^{isx - \frac{1}{2}\sigma^2 x^2}\\ &\quad\times\int_{-\infty}^{\infty} d\eta e^{-\frac{\eta^2}{2\sigma^2}} = s^n e^{isx}\end{aligned} \tag{C5}$$

and

$$\begin{aligned}(-i\partial_x)^n e^{sx} &= \lim_{\sigma\to 0^+}\sqrt{\frac{2\pi}{\sigma^2}}\int_{-\infty}^{\infty}\frac{dk_x}{2\pi} e^{\frac{(s-ik_x)^2}{2\sigma^2}} k_x^n e^{ik_x x}\\ &= \lim_{\sigma\to 0^+}\frac{1}{\sqrt{2\pi\sigma}}(-is + i\sigma^2 x)^n e^{-\frac{1}{2}\sigma^2 x^2 + sx}\\ &\quad\times\int_{-\infty}^{\infty} d\eta e^{-\frac{\eta^2}{2\sigma^2}} = (-is)^n e^{sx}.\end{aligned} \tag{C6}$$

Then the less trivial action of powers of the operator $|\hat{k}_x|$ can be obtained in a similar manner:

$$|-i\partial_x|^n e^{isx} = \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} |k_x|^n e^{ik_x x} 2\pi\delta(s-k_x) = |s|^n e^{isx} \tag{C7}$$

or otherwise

$$\begin{aligned} |-i\partial_x|^n e^{isx} &= \lim_{\sigma\to 0^+} \sqrt{\frac{2\pi}{\sigma^2}} \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} |k_x|^n e^{ik_x x} e^{-\frac{(s-k_x)^2}{2\sigma^2}} \\ &= \lim_{\sigma\to 0^+} \frac{1}{\sqrt{2\pi}\sigma} |s+i\sigma^2 x|^n e^{isx-\frac{1}{2}\sigma^2 x^2} \\ &\quad \times \int_{-\infty}^{\infty} d\eta e^{-\frac{\eta^2}{2\sigma^2}} = |s|^n e^{isx} \end{aligned} \tag{C8}$$

and

$$\begin{aligned} |-i\partial_x|^n e^{sx} &= \lim_{\sigma\to 0^+} \sqrt{\frac{2\pi}{\sigma^2}} \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} |k_x|^n e^{ik_x x + \frac{(s-ik_x)^2}{2\sigma^2})} \\ &= \lim_{\sigma\to 0^+} \frac{1}{\sqrt{2\pi}\sigma} |-is+i\sigma^2 x|^n e^{sx-\frac{1}{2}\sigma^2 x^2} \\ &\quad \times \int_{-\infty}^{\infty} d\eta e^{-\frac{\eta^2}{2\sigma^2}} = |s|^n e^{sx}. \end{aligned} \tag{C9}$$

The lesson we have learned is the following. Let $\mathcal{T}(v^2, |w|)$ be given as a double Taylor expansion in powers of v^2 and $|w|$, then the operator obtained by inserting $v = w = -i\hbar\alpha\partial_x$ acts on exponential functions as

$$\begin{aligned} &\mathcal{T}(-\hbar^2\alpha^2\partial_x^2, |-i\hbar\alpha\partial_x|)e^{isx} = \mathcal{T}(\hbar^2\alpha^2 s^2, \hbar\alpha|s|)e^{isx}, \\ &\mathcal{T}(-\hbar^2\alpha^2\partial_x^2, |-i\hbar\alpha\partial_x|)e^{sx} = \mathcal{T}(-\hbar^2\alpha^2 s^2, \hbar\alpha|s|)e^{sx} \end{aligned} \tag{C10}$$

for $s \in \mathbb{R}$, or otherwise exponential functions are eigenfunctions of the operator $\mathcal{T}(-\hbar^2\alpha^2\partial_x^2, |-i\hbar\alpha\partial_x|) = [F^{-1}(\hbar\alpha\hat{k}_x)]^2$, i.e. that of the kinetic energy operator. Moreover, the function $[F^{-1}(u)]^2$ is even, so that the eigenvalues of the kinetic energy operator when acting on exponential functions is independent of the sign of s.

Appendix D: Evaluation of v_{nn}

The independent integrals $v_{i,j}$ contributing to the matrix element v_{nn} are

$$\begin{aligned} &v_{I,I} = |B\rho_\pm|^2 V_0 \\ &\times \left[\int_{-\infty}^{0} dx e^{\kappa_\pm x} \int_{-\infty}^{0} dy e^{\kappa_\pm y} \Pi(x-y) - \frac{1}{2\kappa_\pm} \right], \\ &v_{I,III} = \pm|B\rho_\pm|^2 V_0 \\ &\times \int_{-\infty}^{0} dx e^{\kappa_\pm x} \int_{L}^{\infty} dy e^{\kappa_\pm (L-y)} \Pi(x-y), \\ &v_{I,II} = \frac{1}{2}|B|^2 \rho_\pm^* V_0 \\ &\times \int_{-\infty}^{0} dx e^{\kappa_\pm x} \int_{0}^{L} dy (e^{ik_\pm y} \pm e^{ik_\pm (L-y)}) \Pi(x-y). \end{aligned} \tag{D1}$$

We shall determine these integrals in the asymptotic limit $V_0 \to \infty$ implying $\kappa \to \infty$. (Let us suppress the lower index $\pm$ still it is not disturbing.) Then the main contribution to the x integral comes in each cases from $x = 0$ due to the extremely rapidly falling off factors $e^{\kappa x}$ in the integrands. Therefore, we can expand the slowly variing x-dependent factor $\Pi(x-y)$ of the integrand at $x = 0$ and recast the integral over x like

$$\begin{aligned} &\int_{-\infty}^{0} dx e^{\kappa x} \Pi(x-y) \\ &\approx \int_{-\infty}^{0} dx e^{\kappa x} [\Pi(-y) + x\Pi'(-y) + \mathcal{O}\left(x^2\right)] \\ &\approx [\Pi(-y) + \Pi'(-y)\partial_\kappa + \mathcal{O}\left(\partial_\kappa^2\right)] \int_{-\infty}^{0} dx e^{\kappa x} \\ &\approx [\Pi(-y) + \Pi'(-y)\partial_\kappa + \mathcal{O}\left(\partial_\kappa^2\right)] \kappa_\pm^{-1} \\ &\approx \kappa^{-1}\Pi(-y) + \kappa^{-2}\Pi'(-y) + \mathcal{O}\left(\kappa^{-3}\right) \end{aligned} \tag{D2}$$

with the notations $\Pi'(u) = d\Pi(u)/du$, $\Pi''(u) = d^2\Pi(u)/du^2$. Thus we get an expansion of the integral in powers of $1/\kappa$. In the limit $V_0 \to \infty$, i.e. $k/\kappa \to 0$ one is only interested in the leading order terms of $v_{i,j}$'s.

With similar logic, one can expand the integrals over y in the expressions of $v_{I,I}$ and $v_{I,III}$ also in powers of $1/\kappa$. Since the even and odd derivatives of $\Pi(u)$ at $u = 0$ are finite and zero, respectively, (e.g. $\Pi(0) = K/\pi$, $\Pi'(0) = 0$, $\Pi''(0) = -K^3/\pi$) the following well-defined expansion occurs in the expression of $v_{I,I}$,

$$\begin{aligned} &\int_{-\infty}^{0} dy e^{\kappa y} \left(\kappa^{-1}\Pi(-y) + \kappa^{-2}\Pi'(-y) + \mathcal{O}\left(\kappa^{-3}\right) \right) \\ &\approx \left(\kappa^{-1}\Pi(0) + \kappa^{-2}\Pi'(0) + \mathcal{O}\left(\kappa^{-3}\right) \right) \kappa^{-1} \\ &\approx \kappa^{-2}\Pi(0) + \mathcal{O}\left(\kappa^{-3}\right) \end{aligned} \tag{D3}$$

which implies

$$\begin{aligned} v_{I,I} &\approx |B\rho|^2 V_0 \left(\frac{\Pi(0)}{\kappa^2} - \frac{1}{2\kappa} + \mathcal{O}\left(\kappa^{-3}\right) \right) \\ &\approx |B\rho|^2 V_0 \left(-\frac{1}{2\kappa} + \mathcal{O}\left(\kappa^{-2}\right) \right). \end{aligned} \tag{D4}$$

Similarly, expanding the y-dependent factor of the integrand of $v_{I,III}$ at $y = L$, the leading order term provides

$$v_{I,III} = \pm|B\rho|^2 V_0 \left(\frac{\Pi(-L)}{\kappa^2} + \mathcal{O}\left(\kappa^{-3}\right) \right) \tag{D5}$$

in the limit $V_0 \to \infty$ (with the sign $\pm$ when the lower index $\pm$ is everywhere restored). Furthermore, the integral $v_{I,II}$ can be recasted as

$$\begin{aligned} v_{I,II} &\approx \frac{1}{2\kappa}|B|^2 V_0 \rho^* \\ &\int_{0}^{L} dy (e^{iky} \pm e^{ik(L-y)}) [\Pi(-y) + \mathcal{O}\left(\kappa^{-1}\right)] \\ &\approx \frac{1}{2\kappa i}|B|^2 V_0 \rho^* \end{aligned}$$

$$\int_{-K}^{K}\frac{dq}{2\pi}\left(\frac{e^{i(k-q)L}-1}{k-q}\mp e^{ikL}\frac{e^{-i(k+q)L}-1}{k+q}\right)$$
$$\approx\frac{1}{2\kappa i 2\pi}|B|^2V_0\rho^*\left(\int_{-KL-kL}^{KL-kl}du\frac{1-e^{-iu}}{u}\right.$$
$$\left.\pm e^{ikL}\int_{-KL+kL}^{KL+kL}du\frac{1-e^{-iu}}{u}\right) \quad \text{(D6)}$$

for asymptotically large values of κ. Here the expression in the bracket can be recasted into the sum

$$\Big(\ldots\Big)=I_{c-}+iI_{s-}\pm e^{ikL}(I_{c+}+iI_{s+})$$
$$=[\pm e^{ikL}-1]I_{c+}+i[1\pm e^{ikL}]I_{s+} \quad \text{(D7)}$$

with

$$I_{c\pm}=\int_{-KL\pm kL}^{KL\pm kL}du\frac{1-\cos u}{u},$$
$$I_{s\pm}=\int_{-KL\pm kL}^{KL\pm kL}du\frac{\sin u}{u}. \quad \text{(D8)}$$

and $I_{c-}=-I_{c+}$, $I_{s-}=I_{s+}$. For the low-lying excited states we can Taylor-expand these integrals in the small parameter $k/K\ll 1$,

$$I_{c+}\approx\frac{k}{K}\left(4\sin^2\frac{KL}{2}+(kL)^2\cos(KL)\right.$$
$$\left.+\mathcal{O}\left((kL)^4\right)\right)+\mathcal{O}\left((k/K)^2\right),$$
$$I_{s+}\approx\int_{-KL}^{KL}du\frac{\sin u}{u}+\mathcal{O}\left((k/K)^2\right). \quad \text{(D9)}$$

Making use of the asymptotic relations $\kappa_\pm\approx\sqrt{2mV_0}/\hbar$, $\pm e^{ik_\pm L}\to -1$ and those in Eqs. (B12) and (B13), one easily establishes the order-of-magnitude relations $v_{I,I}\sim\mathcal{O}\left(\kappa^{-1}\right)$, $v_{I,III}\sim\mathcal{O}\left(\kappa^{-2}\right)$, and the leading order contribution comes from

$$v_{I,II}\approx\frac{\hbar^2k}{4mL\pi}I_{c+}, \quad \text{(D10)}$$

One can write $KL=2\pi(N+\nu)$ where N and $0\le\nu<1$ stand for the integer and fractional parts of the ratio $KL/(2\pi)$, respectively. Consequently, one finds $\sin^2(KL/2)=\sin^2(\nu\pi)$ and

$$I_{c+}=\frac{k}{K}[4\sin^2(\nu\pi)+(n\pi)^2\cos(2\nu\pi)+\mathcal{O}\left(n^4\right)]$$
$$+\mathcal{O}\left((k/K)^2\right) \quad \text{(D11)}$$

which has the order of magnitude $k/K\sim n(\ell_P/L)$.

Summing the contributions of leading order in $1/\kappa$, and making use of $v_{III,II}=\pm v_{I,II}$, finally one obtains for the matrix element v_{nn},

$$v_{nn}\approx v_{I,II}+v_{II,I}+v_{III,II}+v_{II,III}$$
$$\approx 2(v_{I,II}+v_{III,II})$$
$$\approx\begin{cases}4v_{I,II} & \text{for } n \text{ odd}\\ 0 & \text{for } n \text{ even}\end{cases} \quad \text{(D12)}$$

The vanishing of the potential energy shift for n even is the consequence of the sign difference of the wavefunction in the outer regions I_I and I_{III}, i.e. that of the coefficients A and D implying $v_{III,II}=-v_{I,II}$ in that case.

Appendix E: Evaluation of t_{nn}

The independent integrals contributing to the kinetic energy shift t_{nn} arising due to the finite band width are as follows:

$$t_{I,I}=\frac{|B\rho|^2}{2m\alpha^2}\int_{-\infty}^{0}dxe^{\kappa x}[F^{-1}(-i\alpha\hbar\partial_x)]^2$$
$$\times\left(\int_{-\infty}^{0}dy\Pi(x-y)e^{\kappa y}-e^{\kappa x}\right),$$
$$t_{II,I}=\frac{|B|^2\rho}{2m\alpha^2}\int_0^L dx(e^{-ikx}\pm e^{-ik(L-x)})[F^{-1}(-i\alpha\hbar\partial_x)]^2$$
$$\times\int_{-\infty}^{0}dy\Pi(x-y)e^{\kappa y},$$
$$t_{III,I}=\pm\frac{|B\rho|^2}{2m\alpha^2}\int_L^{\infty}dxe^{\kappa(L-x)}[F^{-1}(-i\alpha\hbar\partial_x)]^2$$
$$\times\int_{-\infty}^{0}dy\Pi(x-y)e^{\kappa y},$$
$$t_{II,II}=\frac{|B|^2}{2m\alpha^2}\int_0^L dx(e^{-ikx}\pm e^{-ik(L-x)})[F^{-1}(-i\alpha\hbar\partial_x)]^2$$
$$\times\left(\int_0^L dy\Pi(x-y)(e^{iky}\pm e^{ik(L-y)})\right.$$
$$\left.-(e^{ikx}\pm e^{ik(L-x)})\right). \quad \text{(E1)}$$

Let us expand the integrals over y in $t_{I,I}$, $t_{II,I}$ and $t_{III,I}$ in powers of κ^{-1} similarly to what we did in App. D for the x-integrals,

$$\int_{-\infty}^{0}dy\Pi(x-y)e^{\kappa y}$$
$$\approx\int_{-\infty}^{0}dy[\Pi(x)-y\Pi'(x)+\mathcal{O}\left(y^2\right)]e^{\kappa y}$$
$$\approx[\Pi(x)-\Pi'(x)\partial_\kappa+\mathcal{O}\left(\partial_\kappa^2\right)]\kappa^{-1}$$
$$\approx\kappa^{-1}\Pi(x)+\mathcal{O}\left(\kappa^{-2}\right). \quad \text{(E2)}$$

Then a similar $(1/\kappa)$-expansion of the integrals over x occurring in $t_{I,I}$ and $t_{III,I}$, respectively, is possible:

$$\kappa^{-1}\int_{-\infty}^{0}dxe^{\kappa x}G_\Pi(x)\approx\kappa^{-2}G_\Pi(0)+\mathcal{O}\left(\kappa^{-3}\right),$$
$$\kappa^{-1}\int_L^{\infty}dxe^{\kappa(L-x)}G_\Pi(x)\approx\kappa^{-2}G_\Pi(L)+\mathcal{O}\left(\kappa^{-3}\right) \quad \text{(E3)}$$

with $G_\Pi(x)=[F^{-1}(-i\alpha\hbar\partial_x)]^2\Pi(x)$. Then one finds in the leading order of $1/\kappa$,

$$t_{I,I}\approx\frac{|B\rho|^2}{2m\alpha^2}\left(\kappa^{-2}G_\Pi(0)-\frac{[F^{-1}(-i\alpha\hbar\kappa)]^2}{2\kappa}+\mathcal{O}\left(\kappa^{-3}\right)\right)$$

$$\approx \mathcal{O}\left(\kappa^{-3}\right),$$
$$t_{III,I} \approx \pm\frac{|B\rho|^2}{2m\alpha^2}[\kappa^{-2}G_\Pi(L)+\mathcal{O}\left(\kappa^{-3}\right)]$$
$$\approx \mathcal{O}\left(\kappa^{-4}\right), \tag{E4}$$

where we made use of our particular choice of the deformation function $f(u)$. The leading order terms of $t_{II,I}$ are given as

$$t_{II,I} \approx \frac{|B|^2\rho}{2m\alpha^2}\kappa^{-1}\int_0^L dx(e^{-ikx}\pm e^{-ik(L-x)})G_\Pi(x)$$
$$\approx \mathcal{O}\left(\kappa^{-2}\right). \tag{E5}$$

Therefore the only independent integral contributing to t_{nn} in the limit $\kappa\to\infty$ is $t_{II,II}$.

As to the next we try to estimate the integral $t_{II,II}$ in the limit $\kappa\to\infty$. Let $\chi_{[0,L]}(x)$ be the characteristic function of the interval $x\in[0,L]$. In order to perform the integral over y, let us first rewrite the trivial integral $\int_0^L dy\delta(x-y)e^{iky}=e^{ikx}\chi_{[0,L]}(x)$ as a limit,

$$\int_0^L dy\delta(x-y)e^{iky}$$
$$=\lim_{\Lambda\to\infty}\int_{-\Lambda}^{\Lambda}\frac{dq}{2\pi}e^{iqx}\int_0^L dye^{-i(q-k)y}$$
$$=e^{ikx}\lim_{\Lambda\to\infty}\int_{-\Lambda}^{\Lambda}\frac{dq}{2\pi}e^{i(q-k)x}i\frac{e^{-i(q-k)L}-1}{q-k}$$
$$=e^{ikx}\lim_{\Lambda\to\infty}\int_{-\Lambda}^{\Lambda}\frac{dp}{2\pi}e^{ipx}i\frac{e^{-ipL}-1}{p}$$
$$=e^{ikx}\lim_{\Lambda\to\infty}\int_{-\Lambda}^{\Lambda}\frac{dp}{2\pi}\left[\frac{\sin pL}{p}\cos px-[\cos(pL)-1]\frac{\sin px}{p}\right]$$
$$=e^{ikx}\lim_{\Lambda\to\infty}\frac{1}{2}\int_{-1}^{1}ds\left[\frac{\sin[s\Lambda(L-x)]}{s\pi}+\frac{\sin(s\Lambda x)}{s\pi}\right]$$
$$=e^{ikx}\frac{1}{2}\int_{-1}^{1}ds\Big[\chi_{[0,L]}(x)\Big(\delta(s)+\delta(s)\Big)$$
$$+\Theta(L-x)\Big(-\delta(s)+\delta(s)\Big)$$
$$+\Theta(-x)\Big(\delta(x)-\delta(x)\Big)\Big]$$
$$=e^{ikx}\chi_{[0,L]}(x)\frac{1}{2}\int_{-1}^{1}ds\Big(\delta(s)+\delta(s)\Big)$$
$$=e^{ikx}\chi_{[0,L]}(x). \tag{E6}$$

Now let us evaluate $\int_0^L dy\Pi(x-y)e^{iky}$ in a similar manner, where the limit $\Lambda\to\infty$ is removed and Λ replaced by the finite cutoff K,

$$\int_0^L dy\Pi(x-y)e^{iky}$$
$$=\int_{-K}^{K}\frac{dq}{2\pi}e^{iqx}\int_0^L dye^{-i(q-k)y}$$
$$=e^{ikx}\frac{1}{2}\int_{-1}^{1}ds\left[\frac{\sin[sK(L-x)]}{s\pi}+\frac{\sin(sKx)}{s\pi}\right]$$
$$=e^{ikx}\mathcal{I}_K(x). \tag{E7}$$

Making use of this and the limit $\pm e^{ik_\pm L}\to-1$ for $\kappa\to\infty$, one can recast the integral $t_{II,II}$ in the form

$$t_{II,II}=-\frac{|B|^2}{2m\alpha^2}\int_0^L dx(e^{ikx}-e^{-ikx})[\mathcal{I}_K(x)-1]$$
$$\times[F^{-1}(-i\alpha\hbar\partial_x)]^2(e^{ikx}-e^{-ikx}). \tag{E8}$$

In order to obtain an order-of-magnitude estimate for $t_{II,II}$, let us note that the integral $\mathcal{I}_K(x)$ for sufficiently large cutoff K should be a rather smooth function of x because it is independent of x for $K\to\infty$, $\mathcal{I}_{K\to\infty}(x)\to 1$. Then the following approximations seem to be justified: (i) the replacement of the kinetic energy operator by its eigenvalue when acting on the functions $e^{\pm ikx}$ (c.f. App. C), (ii) replacement of $\mathcal{I}_K(x)$ by $\mathcal{I}_K(L/2)$. The integral over x reduces then to

$$\int_0^L dx\sin^2(kx)=\frac{1}{2}L \tag{E9}$$

for $kL=n\pi$ with any $n=1,2,\ldots$ and one finds

$$t_{II,II}\approx\frac{[F^{-1}(\alpha\hbar k)]^2}{2m\alpha^2}[\mathcal{I}_K(L/2)-1] \tag{E10}$$

with

$$\mathcal{I}_K(L/2)-1=\frac{2}{\pi}\int_0^{KL/2}du\frac{\sin u}{u}-1, \tag{E11}$$

where the new integration variable $u=sKL/2$ has been introduced.

Let N' and $\nu'\in[0,1)$ the integer and fractional parts of $KL/(4\pi)$, respectively. The integral (E11) can be rewritten as

$$\mathcal{I}_K(L/2)-1=-\frac{2}{\pi}\int_{KL/2}^{\infty}du\frac{\sin u}{u}$$
$$\approx-\frac{2}{\pi}\frac{2}{KL}\int_{\nu 2\pi}^{2\pi}du\sin u$$
$$\approx\frac{4}{KL\pi}[1-\cos(2\nu\pi)]. \tag{E12}$$

Here one has split the interval $u\in[KL/2,\infty)$ into subintervals $[(N'+\nu')2\pi,(N'+1)2\pi]$, $[2(N'+j)\pi,2(N'+j+1)\pi]$ with $j=1,2,\ldots$ and replaced the factor $1/u$ in the integrand by $[(N'+\nu')2\pi]^{-1}$, $[(N'+j)2\pi]^{-1}$ with $j=1,2,\ldots$, respectively in the subsequent intervals.

Appendix F: Maximally localized states

Following the method of Detournay, Gabriel, and Spindel [18] we construct the maximally localized state centered at position $\bar{x}$ for arbitrary deformation function. One should look for the state $|\phi\rangle$ with a given undetermined position uncertainty μ, i.e. the state satisfying

$$\mu^2=\langle\phi|\hat{x}^2-\bar{x}^2|\phi\rangle \tag{F1}$$

and the subsidiary conditions

$$\langle\phi|\hat{x}|\phi\rangle = \bar{x} \tag{F2}$$

and $\langle\phi|\phi\rangle = 1$. Then one selects out the state $|\varphi_{\bar{x}}\rangle$ with the minimal value of μ. In the wavevector representation, the variational problem is equivalent with the solution of the differential equation

$$0 = [(i\partial_{k_x})^2 - \bar{x}^2 - \mu^2 - 2\lambda(i\partial_{k_x} - \bar{x})]\tilde{\tilde{\phi}}(k_x), \tag{F3}$$

where the wavefunction $\tilde{\tilde{\phi}}(k_x)$ should satisfy Dirichlet's boundary conditions $\tilde{\tilde{\phi}}(\pm K) = 0$ and be normalized, $\int_{-K}^{K} \frac{dk_x}{2\pi}|\tilde{\tilde{\phi}}(k_x)|^2 = 1$; $\lambda \in \mathbb{R}$ is a Lagrange-multiplier that should be determined from the subsidiary condition (F2). Looking for the solutions in exponential form, one finds two independent solutions, $\tilde{\tilde{\phi}}_{\pm} = e^{ik_x\sigma_{\pm}}$ with $\sigma_{\pm} = -\lambda \pm \sqrt{(\lambda-\bar{x})^2+\mu^2}$. Then the general solution of Eq. (F3) is given as $\tilde{\tilde{\phi}}(k_x) = Ae^{ik_x\sigma_+} + Be^{ik_x\sigma_-}$ and one gets from Dirichlet's boundary conditions, $\tilde{\tilde{\phi}}(\pm K) = 0$, that

$$\begin{aligned} K(\sigma_+ - \sigma_-) = 2\sqrt{(\lambda-\bar{x})^2+\mu^2} = N\pi, \quad N \in \mathbb{N} \\ B = -Ae^{iN\pi}. \end{aligned} \tag{F4}$$

Thus one finds the sets of solutions:

$$\begin{aligned} \tilde{\tilde{\phi}}_{N=2n}(k_x) &= 2iAe^{-ik_x\lambda}\sin\left(\frac{n\pi}{K}k_x\right), \\ \tilde{\tilde{\phi}}_{N=2n-1}(k_x) &= 2Ae^{-ik_x\lambda}\cos\left(\frac{(2n-1)\pi}{2K}k_x\right) \end{aligned} \tag{F5}$$

with $n \in \mathbb{N}$, again. For both sets the subsidiary condition (F2) yields $\lambda = \bar{x}$ that implies

$$\mu^2 = \left(\frac{N\pi}{2K}\right)^2 \tag{F6}$$

Therefore, the state centered at $x = \bar{x}$ with minimal position uncertainty is the one with $N = 1$,

$$\tilde{\tilde{\varphi}}_{\bar{x}}(k_x) = \tilde{\tilde{\phi}}_{N=1}(k_x) = \sqrt{2a}e^{-ik_x\bar{x}}\cos\left(\frac{k_x a}{2}\right) \tag{F7}$$

with $a = \pi/K$ after normalization. What one has to check yet that this state is of finite energy. For a particle with the usual kinetic energy $\frac{\hat{p}_x^2}{2m}$ the integral

$$\int_{-\infty}^{\infty} \frac{dp_x}{2\pi f(\alpha|p_x|)} p_x^2 \cos^2\left(\frac{k_x(p_x)a}{2}\right) \tag{F8}$$

should converge, which happens if the deformation function increases for $|p_x| \to \infty$ faster than p_x^2, a condition satisfied by the deformation functions $f = \exp(\alpha^2 p_x^2)$, and $f = \exp(\alpha|p_x|)$ cited in Sect. I, except of the case with $f = 1 + \alpha^2 p_x^2$, although the latter might be a good low-momentum approximation of some realistic deformation function. The function (F7) and its derivatives with respect to k_x are bounded functions of k_x. Therefore, any potential energy which can be approximated with a sequence of polynomials will have finite expectation value in the state given by Eq. (F7). Therefore, we can consider the wavefunction in Eq. (F7) for the particular class of the deformation functions as that of the physical state of a particle centered at $\bar{x}$ with the minimal position uncertainty, indeed. It is an advantage of the wavevector representation as compared to the canonical momentum representation that the wavevector wavefunctions of the states maximally localized at various positions do not depend on the explicit form of the deformation function.

Appendix G: Reconstruction of a continuous bandlimited potential from sampled values of Dirac-delta potential

First, we give a unique definition of the sum $\sum_{n=-\infty}^{\infty} e^{iqna}$ which turns out to be useful for the determination of reconstructed bandlimited potentials. We settle the ordering of the terms in the sum via

$$\sum_{n=-\infty}^{\infty} e^{iqna} = \lim_{N\to\infty}\left(\sum_{n=0}^{N} e^{-iqna} + \sum_{n=0}^{N} e^{inqa} - 1\right), \tag{G1}$$

i.e. in the manner that ensures the completeness of the eigenstates $\tilde{\tilde{\psi}}_{x_n}(k_x) = \sqrt{a}e^{-ik_x x_n}$ ($x_n = na + \theta$, $\theta \in [0, a)$, $n \in \mathbb{Z}$) of an arbitrarily chosen self-adjoint extension $\hat{x}_\theta$ of the coordinate operator $-i\partial_{k_x}$ in the bandlimited Hilbert space $\mathcal{H}$. Then one finds

$$\begin{aligned} &\sum_{n=-\infty}^{\infty} e^{iqna+iq\theta} \\ &= \lim_{N\to\infty} e^{iq\theta}\left(\frac{e^{-iq(N+1)a}-1}{e^{-iqa}-1} + \frac{e^{iq(N+1)a}-1}{e^{iqa}-1} - 1\right) \\ &= \lim_{N\to\infty} e^{iq\theta}\frac{\cos(Nqa) - \cos[(N+1)qa]}{1-\cos(qa)} \\ &= \pi qae^{iq\theta}\lim_{N\to\infty}\left(\frac{\cos(Nqa)}{\pi qa} + \frac{\sin(qa)}{1-\cos(qa)}\frac{\sin(Nqa)}{\pi qa}\right) \\ &= \pi qa\left(-1 + \frac{\sin(qa)}{1-\cos(qa)}\right)\delta(qa) \\ &= \frac{2\pi}{a}\delta(q). \end{aligned} \tag{G2}$$

Let us emphasize that the definition of the sum does not depend on the choice of θ, i.e. that of the self-adjoint extension of the coordinate operator. Hence the completeness relation of the coordinate eigenstates $|x_n^\theta\rangle$ in the bandlimited Hilbert space $\mathcal{H}$ takes the form

$$\begin{aligned} \sum_{n=-\infty}^{\infty} \tilde{\tilde{\psi}}_{x_n^\theta}^{\,*}(k_x)\tilde{\tilde{\psi}}^{\theta}{}_{x_n}(k'_x) &= a\left(\sum_{n=-\infty}^{\infty} e^{i(k_x-k'_x)(na+\theta)}\right) \\ &= 2\pi\delta(k_x - k'_x) \end{aligned} \tag{G3}$$

in the wavevector representation.

As to the next, we determine the bandlimited continuous potential $\bar{V}(\bar{x})$ reconstructed from discrete sampled values $\bar{V}_n$ (with the notations of Sect. IV) of the Dirac-delta like potential $V(x) = V_0 a\delta(x)$. Making use of the reconstruction formula in Eq. (20), the sample (26), and the rule to evaluate the sum like in Eq. (G2), one reconstructs the following continuous bandlimited potential,

$$\begin{aligned}
&\bar{V}(\bar{x}) \\
&= \frac{V_0 a^3}{2} \sum_{n=-\infty}^{\infty} [\Pi(x_n - \frac{1}{2}a) + \Pi(x_n + \frac{1}{2}a)]^2 \Pi(\bar{x} - x_n) \\
&= \frac{V_0 a^3}{2} \sum_{n=-\infty}^{\infty} \int_{-K}^{K} \frac{dk_1}{2\pi} [e^{ik_1(x_n - \frac{1}{2}a)} + e^{ik_1(x_n + \frac{1}{2}a)}] \\
&\quad \times \int_{-K}^{K} \frac{dk_2}{2\pi} [e^{ik_2(x_n - \frac{1}{2}a)} + e^{ik_2(x_n + \frac{1}{2}a)}] \\
&\quad \times \int_{-K}^{K} \frac{dq}{2\pi} e^{iq(\bar{x} - x_n)} \\
&= \frac{V_0 a^3}{2} \int_{-K}^{K} \frac{dk_1}{2\pi} \int_{-K}^{K} \frac{dk_2}{2\pi} \int_{-K}^{K} \frac{dq}{2\pi} [e^{-ik_1 \frac{1}{2}a} + e^{ik_1 \frac{1}{2}a}] \\
&\quad \times [e^{-ik_2 \frac{1}{2}a} + e^{ik_2 \frac{1}{2}a}] e^{iq\bar{x}} \sum_{n=-\infty}^{\infty} e^{i(k_1 + k_2 - q)x_n} \\
&= \frac{V_0 a^2}{2(2\pi)^2} \int_{-K}^{K} dk_1 \int_{-K}^{K} dk_2 [e^{-ik_1 \frac{1}{2}a} + e^{ik_1 \frac{1}{2}a}] \\
&\quad \times [e^{-ik_2 \frac{1}{2}a} + e^{ik_2 \frac{1}{2}a}] \int_{-K}^{K} dq e^{iq\bar{x}} \delta(k_1 + k_2 - q) \\
&= \frac{V_0 a^2}{2(2\pi)^2} \int_{-K}^{K} dk_1 \int_{-K}^{K} dk_2 [e^{-ik_1 \frac{1}{2}a} + e^{ik_1 \frac{1}{2}a}] \\
&\quad \times [e^{-ik_2 \frac{1}{2}a} + e^{ik_2 \frac{1}{2}a}] e^{i(k_1 + k_2)\bar{x}} \\
&\quad \times \Big(\Theta(k_1 + k_2 + K) - \Theta(K - k_1 - k_2) \Big) \\
&= \frac{V_0 a^2}{2(2\pi)^2} [I(\bar{x}) + J(\bar{x})] \qquad \text{(G4)}
\end{aligned}$$

with

$$\begin{aligned}
I(\bar{x}) &= \int_{-K}^{0} dk_1 \int_{-K-k_1}^{K} dk_2 [e^{-ik_1 \frac{1}{2}a} + e^{ik_1 \frac{1}{2}a}] \\
&\quad \times [e^{-ik_2 \frac{1}{2}a} + e^{ik_2 \frac{1}{2}a}] e^{i(k_1 + k_2)\bar{x}}, \\
J(\bar{x}) &= \int_{0}^{K} dk_1 \int_{-K}^{K-k_1} dk_2 [e^{-ik_1 \frac{1}{2}a} + e^{ik_1 \frac{1}{2}a}] \\
&\quad \times [e^{-ik_2 \frac{1}{2}a} + e^{ik_2 \frac{1}{2}a}] e^{i(k_1 + k_2)\bar{x}} \\
&= I(-\bar{x}). \qquad \text{(G5)}
\end{aligned}$$

Then a somewhat lengthy but straightforward calculation yields

$$\begin{aligned}
\bar{V}(\bar{x}) = V_0 \frac{a^2}{(2\pi)^2 [\bar{x}^2 - (a/2)^2]} \Big(&\frac{a^2}{\bar{x}^2 - (a/2)^2} \\
&- \frac{2a\bar{x} \sin(K\bar{x})}{\bar{x}^2 - (a/2)^2} + \frac{4\bar{x}}{a} \sin K\bar{x} - \pi \cos K\bar{x} \Big). \qquad \text{(G6)}
\end{aligned}$$

This function turns out to be a unique even function of $\bar{x}$ in all of the various θ sectors. It takes the typical values $\bar{V}(0) = V_0 \frac{4+\pi}{\pi^2} \approx 0.72 V_0$, $\bar{V}(\pm\frac{1}{2}a) = V_0 \frac{1+5(\pi/4)^2}{\pi^2} \approx 0.41 V_0$ and falls off rapidly outside the interval $\bar{x} \in [-\frac{1}{2}a, \frac{1}{2}a]$ in an oscillatory manner.