



Branched Quantization

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We propose a method for quantization of Lagrangians for which the Hamiltonian, as a function of momentum, is a branched function, possibly with cusps. Appropriate boundary conditions, which we identify, ensure unitary time evolution. In special cases a dual (canonical) transformation maps the problem into a problem of quantum mechanics on singular spaces, which we also develop. Several possible applications are indicated.

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Physically interesting models based on quantum mechanics are often obtained by quantizing classical systems. The construction of a quantum model from a classical one requires a quantization prescription, which should satisfy several guiding principles: it should result in a model that reproduces, approximately, the original classical dynamics in appropriate limits; it should preserve appropriate symmetries; and it should exhibit unitary time evolution. These principles can be applied to the quantization of a wide variety of classical Hamiltonian systems, but they do not guarantee a unique result. (For example, there can be inequivalent quantizations associated with different self-adjoint extensions of the Hamiltonian [1].) There are also important, but less fully developed and possibly less rigorous, procedures using path integrals that allow one to pass directly from classical Lagrangian systems, including some singular ones, to quantum models [2]. In any case, we should regard the construction of quantum models as a creative process, open to innovation. Here we propose methods for quantizing broad classes of classical systems with branched structures in either momentum or position space. We also suggest several applications.

Branched quantization.—Recently [3,4], we were led to consider Lagrangians involving higher than quadratic powers of the time derivatives, and specifically the deceptively simple

$$L = \frac{1}{4}\dot{x}^4 - \frac{\kappa}{2}\dot{x}^2. \quad (1)$$

In the interesting case $\kappa > 0$, the Hamiltonian for this Lagrangian is singular. Since the momentum involves a cubic in velocity,

$$p = \dot{x}^3 - \kappa\dot{x}, \quad (2)$$

we can have either one or three real values of \dot{x} corresponding to a given value of p , depending on the sign of $|\dot{x}| - \sqrt{\kappa/3}$. Thus, the energy function

$$E = \frac{\partial L}{\partial \dot{x}}\dot{x} - L = \frac{3}{4}\dot{x}^4 - \frac{\kappa}{2}\dot{x}^2, \quad (3)$$

expressed in terms of p , is a multivalued function with cusps. See Fig. 1 in Ref. [3].

Because the Hamiltonian based on Eqs. (2) and (3) is not a single-valued function of p , and yet energy must surely qualify as an observable, p does not supply a complete set of commuting observables. Therefore it will not be sufficient to label states with wave functions in (conventional) momentum space. On the other hand, E is a single-valued function of \dot{x} , so we might expect to construct wave functions $\psi(\dot{x})$. As \dot{x} runs monotonically from $-\infty$ to ∞ , the evolution of $p(\dot{x})$ is nonmonotonic, reversing direction at the cusps. This suggests that we consider wave functions that depend on p locally, but accommodate backtracking. Thus, denoting by $p_{\pm} \equiv \pm\sqrt{\kappa/3}$ the cusp points, we have three components to the wave function, namely, $\psi_1(p)$ for $-\infty < p \leq p_+$, $\psi_2(p)$ for $p_- \leq p \leq p_+$, and $\psi_3(p)$ for $p_- \leq p < \infty$. All three components cover the range $p_- \leq p \leq p_+$.

A crucial issue is how the different branches join together; i.e., what are the appropriate boundary

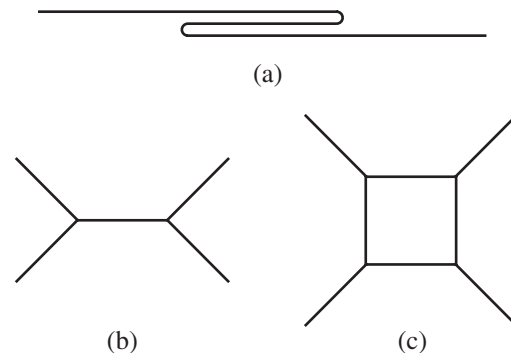


FIG. 1. (a) A wire with kinks. (b) A wire network with two junctions. (c) Box graph for a network with four junctions and a loop.

conditions? It is instructive to consider a more general class of Lagrangians than Eq. (1), bringing in a quadratic potential $V(x) = \frac{1}{2}\alpha x^2$. Directly from the Schrödinger equation we have an equation for the probability density $\rho_\mu(p, t) \equiv \psi_\mu(p, t)^* \psi_\mu(p, t)$, defined on the branch labeled by μ (where $\mu = 1, 2, 3$ for $p_- < p < p_+$, $\mu = 1$ for $p < p_-$, and $\mu = 3$ for $p > p_+$):

$$\begin{aligned} \frac{\partial \rho_\mu}{\partial t} &= i[\psi_\mu^* H \psi_\mu - (H^* \psi_\mu^*) \psi_\mu] \\ &= -\frac{i\alpha}{2} \left(\psi_\mu^* \frac{\partial^2 \psi_\mu}{\partial p^2} - \frac{\partial^2 \psi_\mu^*}{\partial p^2} \psi_\mu \right) \end{aligned} \quad (4)$$

using, in the second step, $V(x) \rightarrow V(i\frac{\partial}{\partial p})$. This substitution implements the basic Heisenberg commutation relation, and also reflects the role of p as the generator of spatial translations. From Eq. (4) we infer an equation of the current-conservation type for $\rho \equiv \sum \rho_\mu$:

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial p} = 0; \quad j \equiv \sum_\mu \frac{i\alpha}{2} \left(\psi_\mu^* \frac{\partial \psi_\mu}{\partial p} - \frac{\partial \psi_\mu^*}{\partial p} \psi_\mu \right). \quad (5)$$

Equation (4) will lead to conservation of the integrated probability $\int \rho$ if we can drop contributions from j at the end points. (Note that j receives contributions from two branches at each end point p_\pm .) We also require our boundary conditions to be linear, so that our Hilbert space will support superposition, and so that they lead to a physically sensible eigenvalue problem for H . The choices

$$\psi_1(p_+) = \psi_2(p_+), \quad \frac{\partial \psi_1}{\partial p}(p_+) = -\frac{\partial \psi_2}{\partial p}(p_+) \quad (6)$$

and their analogues at p_- manifestly give the required cancellation in j . Now consider the eigenvalue problem for the time-independent Schrödinger equation. For $\alpha \neq 0$, we get a second-order differential equation for $\psi(p)$. Thus, on each branch, for each value of energy, there are two disposable constants, making six altogether. Equation (6) gives us four constraints among these constants, and normalizability (absence of growing modes) at $p \rightarrow \pm\infty$ gives us two more (one for each of ψ_1, ψ_3). Thus the number of constraints matches the number of constants, as in conventional quantum potential theory.

If $\alpha = 0$ the derivative conditions in Eq. (6) are not required and should not be imposed, while if V is a higher-order polynomial, we must require augmented boundary conditions. We will discuss those presently, after introducing a different (dual) viewpoint.

Dual viewpoint.—One can hardly fail to notice that the manipulations we performed in momentum space, in connection with probability conservation, resemble manipulations usually performed in position space. Thus it is natural to consider what our models look like after the substitution $p \rightarrow x, x \rightarrow -p$, which preserves the structure of quantum mechanics. After this substitution, our multivalued kinetic

energy becomes something perhaps less unconventional, that is, a multivalued potential. We may think of a wire with kinks, as in Fig. 1(a). Intermediate values of x are triply represented, and physical conditions will be different at different points *along the wire*, even if they are represented by the same x , so a branched wave function is manifestly appropriate to describe this physical system.

From this dual point of view our quadratic potential $V(x) \rightarrow V(p) = \frac{1}{2}\alpha p^2$ becomes the conventional kinetic energy of a particle with mass $m = 1/\alpha$, and the branched kinetic term becomes a multivalued potential $W(x)$ in position space. Thus we have wave functions $\psi_1(x)$ defined for $-\infty < x \leq x_+$ subject to $W_1(x)$, $\psi_2(x)$ defined for $x_- \leq x \leq x_+$ subject to $W_2(x)$, and $\psi_3(x)$ defined for $x_- \leq x < \infty$ subject to $W_3(x)$, and boundary conditions similar to Eq. (6), after the obvious substitutions of x for p .

Now let us consider a quartic potential $V(x) = x^4 + \alpha x^3 + \beta x^2 + \gamma x$. In dual variables this leads to a kinetic energy that is a quartic polynomial in p , $H = p^4 - \alpha p^3 + \beta p^2 - \gamma p + W(x)$. We find a probability current (in the dual x space)

$$\begin{aligned} j &= \frac{1}{i} \left(\psi^\dagger \frac{\partial^3 \psi}{\partial x^3} - \frac{\partial \psi^\dagger}{\partial x} \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi^\dagger}{\partial x^2} \frac{\partial \psi}{\partial x} - \frac{\partial^3 \psi^\dagger}{\partial x^3} \psi \right) \\ &\quad - \alpha \left(\psi^\dagger \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial \psi^\dagger}{\partial x} \frac{\partial \psi}{\partial x} + \frac{\partial^2 \psi^\dagger}{\partial x^2} \psi \right) \\ &\quad + i\beta \left(\psi^\dagger \frac{\partial \psi}{\partial x} - \frac{\partial \psi^\dagger}{\partial x} \psi \right) + \gamma \psi^\dagger \psi, \end{aligned} \quad (7)$$

where ψ is a column vector with the requisite number of components ψ_μ in each momentum range. We will ensure conservation of probability with the boundary conditions

$$\frac{\partial^n \psi_1}{\partial x^n} = (-1)^n \frac{\partial^n \psi_2}{\partial x^n}, \quad 0 \leq n \leq 3, \quad (8)$$

at the kinks, provided that α and γ change sign between the branches. This augmentation of the boundary conditions also leads to a good eigenvalue problem, since we have both twice as many disposable constants and twice as many conditions as in the quadratic case.

Inspired by the wire analogy it is natural to consider networks analogous to the geometries of electric circuit theory, where we put quantum dynamics on graphs [5,6]. Let us consider what is required to ensure no flow of probability into a node where several lines indexed by μ come together. If the momentum dependence on each line is simply p^2 , and we orient each line so all coordinates x^μ flow into the node, then the ‘‘Kirchhoff’’ boundary conditions

$$\psi_1 = \psi_2 = \dots, \quad \sum_\mu \frac{\partial \psi_\mu}{\partial x^\mu} = 0, \quad (9)$$

ensure that no probability accumulates at the node. These natural conditions give good eigenvalue problems for the ‘‘Compton’’ tree graph and the box graph displayed in

Figs. 1(b) and 1(c) (and many others). In the Compton graph, Eq. (9) yields $2 \times 3 = 6$ conditions at the two nodes, which together with four conditions at infinity for the external legs gives 10 conditions, as is appropriate to five lines with two disposable constants each. In the box graph, Eq. (9) yields $4 \times 3 = 12$ conditions at the four nodes, which together with four conditions at infinity gives 16 conditions, as is appropriate for eight lines with two disposable constants each. Though it is simple and natural, this is by no means the only possible setup consistent with the general requirements of the framework of quantum mechanics [5]. We can vary both the Hamiltonians and the boundary conditions.

Unfolding.—Quadratic models with branching in the dual viewpoint can be unfolded, upon which the eigenvalue problem assumes a conventional form. In equations: If we define a real variable χ with

$$\begin{aligned}\chi &\equiv x - x_+ + x_- & \text{for } \chi \leq x_-, \\ \chi &\equiv -x + x_+ + x_- & \text{for } x_- \leq \chi \leq x_+, \\ \chi &\equiv x + x_+ - x_- & \text{for } x_+ \leq \chi,\end{aligned}\quad (10)$$

then as χ evolves monotonically from $-\infty$ to ∞ it covers each branch of x uniquely (as \dot{x} covered p in our earlier discussion). The boundary conditions Eq. (6), with $p \rightarrow x$ become, upon transcription into the unfolding variable χ , the statement that $\psi(\chi)$ and its derivative are continuous. Similarly, the boundary conditions Eq. (8) for quartics unfold into continuity for $\psi(\chi)$ and its first three derivatives.

Potentials.—Now we return to our original problem, the issue of quantizing the kinetic Lagrangian of Eq. (1) allowing for a general potential $V(x)$. Inspired by the preceding unfolding procedure, we formulate our wave function in terms of a variable that locally reduces to $\pm p$ plus a c number, but covers all three branches following the same flow directions as ϕ . Thus we introduce

$$\begin{aligned}\xi &\equiv p - p_+ + p_- & \text{for } \xi \leq p_-, \\ \xi &\equiv -p + p_+ + p_- & \text{for } p_- \leq \xi \leq p_+, \\ \xi &\equiv p + p_+ - p_- & \text{for } p_+ \leq \xi,\end{aligned}\quad (11)$$

and the decomposition of wave functions

$$\begin{aligned}\psi(\xi) &= \psi(\xi)[1 - H(\xi - p_-)] + \psi(\xi)[H(\xi - p_-) \\ &\quad - H(\xi - p_+)] + \psi(\xi)H(\xi - p_+) \\ &\equiv \psi_1(\xi) + \psi_2(\xi) + \psi_3(\xi),\end{aligned}\quad (12)$$

where H is the Heaviside function. In this formulation p is realized (piecewise) as a modified multiplication operator, with slightly different modifications on each branch. We can use that fact to write the operator V as an explicit kernel in ξ space. Thus we transform $\psi_1(\xi)$ to x space, where V acts as multiplication, and transform back as follows:

$$\begin{aligned}u(x) &\equiv \int e^{ipx} \psi_1(p) \frac{dp}{2\pi} = \int e^{i(\xi' + p_+ - p_-)x} \psi_1(\xi') \frac{d\xi'}{2\pi}, \\ (\hat{V}u)(x) &= V(x)u(x), \\ (\hat{V}\psi_1)(\xi) &= \int e^{-ipx} (\hat{V}u)(x) dx = \int_{-\infty}^{p_-} K_1(\xi - \xi') \psi(\xi') \frac{d\xi'}{2\pi}, \\ K_1(\xi - \xi') &= \int e^{-i(\xi - \xi')x} V(x) dx.\end{aligned}\quad (13)$$

Note that the result of \hat{V} acting on ψ_1 generally does not vanish for $\xi > p_-$. It is realized as an operator of the Wiener-Hopf type.

Performing the same manipulations in the other intervals, we arrive at $K_2 = K_1^*$, $K_3 = K_1$, and

$$\begin{aligned}(\hat{V}\psi)(\xi) &= \int [K_1(\xi - \xi') \psi_1(\xi') + K_2(\xi - \xi') \psi_2(\xi') \\ &\quad + K_3(\xi - \xi') \psi_3(\xi')] d\xi'.\end{aligned}\quad (14)$$

The peculiarity of K_2 arises from the reversed flow of p , as a function of ξ , in the medial interval. In the symmetric case $V(x) = V(-x)$ all the K 's are real and equal, and \hat{V} becomes an ordinary convolution operator.

If $V(x)$ is not symmetric, however, we must reconsider our procedure, because the \hat{V} defined in Eq. (14) is not Hermitian. Indeed, although each K_j satisfies the Hermiticity condition $K_j(\xi', \xi) = K_j^*(\xi, \xi')$, the full kernel

$$\begin{aligned}K(\xi', \xi) &= K_1(\xi', \xi)[1 - H(\xi - p_-)] + K_2(\xi', \xi)[H(\xi - p_-) \\ &\quad - H(\xi - p_+)] + K_3(\xi', \xi)H(\xi - p_+)\end{aligned}\quad (15)$$

does not. Thus, to reach a consistent quantization we must impose $K_2 = K_1$ also (and not $K_2 = K_1^*$). The sign changes for α and γ required in Eq. (8) foreshadowed this conclusion. By adopting this modified quantization condition, we lose the Heaviside functions and arrive at a (manifestly Hermitian) convolution. The modified quantization condition entails that the basic commutation relation $[\xi, x] = -i$ involves the unfolded ξ , not the mechanical p .

For long-range potentials $V(x)$ the formal definition of \hat{V} by Fourier transformation leads to derivatives of δ functions, which must be defined through integration by parts on the momentum-space wave functions. In this way we make contact with our earlier discussion of polynomial potentials, and see why smoothness conditions connecting the different zones in ψ are required, that become more demanding as the order of V increases.

After this work, the mathematical eigenvalue problem is well defined and amenable to standard mathematical techniques. Several examples of branched quantization are analyzed quantitatively in Ref. [7].

Another unfolding method.—An alternative and natural choice of an unfolding coordinate for p is \dot{x} . The phase space coordinates (x, \dot{x}) are noncanonical, but one can formulate a symplectic structure, Hamiltonian, and Poisson bracket for them [8], which reduce to the following

forms in the momentum range for which the map between \dot{x} and p is invertible:

$$\{F, G\} = \frac{1}{3\dot{x}^2 - \kappa} \left[\frac{\partial F}{\partial x} \frac{\partial G}{\partial \dot{x}} - \frac{\partial F}{\partial \dot{x}} \frac{\partial G}{\partial x} \right], \quad (16)$$

$$H(x, \dot{x}) = \frac{3}{4}\dot{x}^4 - \frac{\kappa}{2}\dot{x}^2 + V(x).$$

With this structure Hamilton's equation $\dot{F} = \{F, H\}$ reproduces the equation of motion derived from Eq. (1). In this Hamiltonian formulation time evolution is uniquely defined except at $\dot{x} = \pm\sqrt{\kappa/3}$, where the symplectic structure degenerates and nondeterministic motion may occur [3]. The Poisson bracket in Eq. (16) suggests an alternative approach to quantization [9].

First-order Lagrangians.—Other wide classes of simple, regular Lagrangians lead to Hamiltonians with cusps or multivaluedness. Consider specifically

$$L(\psi^*, \psi) = f(\psi^*, \psi) \partial_t \psi - V(\psi^*, \psi). \quad (17)$$

The canonical momentum associated with ψ is $\pi_\psi = f(\psi^*, \psi)$ while the Hamiltonian is numerically $V(\psi^*, \psi)$, but expressed as a function $H = V(\psi, \pi_\psi)$ of the dynamical variable ψ and its conjugate momentum π_ψ . We may also require that L be real up to a total time derivative, formally motivated by Hermiticity, or unitarity in the path integral formulation. The simplest, most conventional form, widely used in many-body physics [10], is $f = i\psi^*$. But we can also have, for example,

$$f_n = i\psi^{*n}\psi^{n-1}, \quad (18)$$

$$f_{\bar{n}} = \alpha\psi^{*n}\partial_t\psi - n\alpha^*\psi^*\psi^{n-1}\partial_t\psi,$$

or (real) linear combinations thereof. At points where the implicit function theorem fails, i.e., $\partial f/\partial\psi^* = 0$, we can expect to have singularities in $H(\pi_\psi, \psi)$.

To make contact with our earlier discussion, let us consider

$$L = i(\psi^{*2}\psi - \kappa\psi^*)\partial_t\psi - V(\psi^*, \psi), \quad (19)$$

$$V = -a\psi^*\psi + b\psi^{*2}\psi^2,$$

so that $\pi_\psi = i(\psi^{*2}\psi - \kappa\psi^*)$. Upon going to the real section $\psi^* = \psi$, we reproduce the momentum of Eq. (2) (with a conventional factor i). Taking $(a, b) = (\frac{\kappa}{2}, \frac{3}{4})$ would reproduce the corresponding Hamiltonian derived from the Lagrangian of Eq. (1), with its cuspidal form. Now, however, we are invited to consider more general values of those parameters. We find that multivaluedness of the Hamiltonian is generic for κ positive (but not for $\kappa < 0$), while occurrence of cusps is special. Cusps can occur when the condition $\frac{\partial f}{\partial\psi^*} = 0$ occurs together with $\frac{\partial H}{\partial\psi^*} = 0$. Generically the “singular” behavior, where the tangent is vertical, occurs at different points from the minimum of the

energy. (There are also multiple points, where branches intersect transversally.) The fact that in this broader context the “singularities” are quite mild—from the point of view of intrinsic curve theory, they are essentially coordinate singularities—further recommends our quantization procedure, which patches the branches together smoothly.

Comments:

1. A very common and fruitful procedure in analyzing quantum many-body problems is to model the effect of interactions on a given particle by an effective one-body Hamiltonian (or Lagrangian), solving the one-body problem, and constructing a many-body wave function as a suitable product, e.g., a Slater determinant. By widening the class of candidate one-body Hamiltonians, we can hope to extend this sort of analysis to wider classes of systems. Dynamical mean field theory [11] generates complicated time dependence in a time-translation invariant energy functional, as a consequence of interactions. Polynomial truncation of such time dependence, using substitutions of the type $[x(t) - x(t - \delta)]^n \rightarrow \delta^n \dot{x}^n$ [3], with retention of spatial structure, brings us to the sort of models considered above.

2. More generally, we might model specific examples of quasiparticles this way. “Swallowtail” structures [12] similar to Fig. 1 in Ref. [3] have appeared in the description of Bose-Einstein condensates in lattice traps [13] and in studies of Lieb-Lininger models [14]. In this context the first-order Lagrangians discussed above are very plausible effective field theories, since their structure is quite similar to that of the microscopic model.

3. A particularly interesting case arises for periodic potentials $V(x)$. In that case, famously, conventional kinetic terms lead to band structures: The energy becomes a multivalued function of the quasimomentum. Our branched Hamiltonian already for $V = 0$ has a sort of band structure, associated with the branches, in a region of momentum $p_- < p < p_+$ where the limiting p_- , p_+ are determined by the form of the kinetic energy, not by any spatial periodicity. With a periodic potential added, both sources of banding are effective. Especially interesting is the possibility of describing dynamically induced insulating behavior (Mott phenomenon) at filling fractions determined dynamically by the value of κ .

4. Our earlier work on time crystals was somewhat schizophrenic. In the classical case [3], we found systems with motion in their ground state using kinetic Lagrangians of the type considered above. In the quantum case [4], not knowing how to treat such Lagrangians, we used a different mechanism, based on a more conventional kinetic term, that depended on the discreteness of (generalized) quantum angular momentum. A possible experimental realization has been proposed [15]. With the method here described we can quantize the classical time crystals, and thereby construct much more general candidate models of quantum time crystals.

5. We initially passed to the dual models to guide our intuition, but they appear to have considerable independent interest. The central observation is that appropriate, fairly simple boundary conditions, both on wave functions and (odd) interactions, appear to allow construction of unitary quantum mechanics on a wide variety of singular manifolds. One can even relax the boundary conditions, at the cost of allowing probability to flow into and out of the designated points—in other words, by allowing the points to have internal degrees of freedom. This procedure appears natural, specifically, in the modeling of black holes, where (in the Euclidean formalism) the horizon appears as a sphere attached to a point.

To summarize: We have proposed a method for quantizing a broad class of classical models that previously eluded consistent theoretical treatment. To do so we had to address some fundamental issues, and even to tinker with the usual Heisenberg commutation relations. We also indicated, with useful concreteness, some immediately promising applications.

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