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Nelson Diffusions and Nonlinear Schrödinger equations

(Nelson 拡散過程と非線形 Schrödinger 方程式)

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Abstract

This is almost a (personal) memorandum on Nelson's Stochastic Quantization [10, 11] and its possible applications. As Nelson himself mentioned in [11], Fényes also proposed a similar notion of the quantization in [6]. The aim of Nelson's stochastic quantization is to put a probabilistic dynamical law on the path space $\Gamma\equiv C(\mathbb{R};\mathbb{R}^{3})$ to define a probability P which gives us the same prediction as standard Quantum mechanics does. Γ is given a Fréchet topology, and its Borel field will be denoted by $\mathfrak{B}$.

1 Quantum Mechanics.

The fundamental equation for a quantum particle with mass m moving in $\mathbb{R}^{3}$ under the influence of a potential V (a real valued "nice" function) is the following Schrödinger equation:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=-\frac{\hbar^{2}}{2m}\Delta\psi(x,t)+V(x,t)\psi(x,t), \quad (x,t)\in\mathbb{R}^{3}\times\mathbb{R}, \tag{1.1}$$

where $\hbar$ is the planck constant (divided by 2π). Usually, we at least assume that $\psi(\cdot,0)\in L^{2}(\mathbb{R}^{3})$ [*1] so that we can state "Born's probability law" which will soon be explained in the following paragraph.

In quantum mechanics, we can only predict the probability of finding the particle at time t in a region A (a Borel set) of our configuration space, say, $\mathbb{R}^{3}$ (This is so-called Born's probability law). To state this postulate precisely, we introduce here the path space $\Gamma:=C(\mathbb{R};\mathbb{R}^{3})$, which is considered to be the set of all possible path of a (classical) point particle; and we define

[*1] For a "nice" potential function, $\psi(\cdot,0)$ gives rise to the unique solution $\psi\in C(\mathbb{R};L^{2}(\mathbb{R}^{3}))$ such that

$$\|\psi(t)\|^{2}:=\int_{\mathbb{R}^{3}}|\psi(x,t)|^{2}dx=\int_{\mathbb{R}^{3}}|\psi(x,0)|^{2}dx=:\|\psi(0)\|^{2}.$$

"random variables" X_t $(-\infty < t < \infty)$ as follows:

$$\begin{array}{rcccl} X_t: & \Gamma & \longrightarrow & \mathbb{R}^3 & \\ & \Psi & & \Psi & \\ & \gamma & \longmapsto & \gamma(t) & =: X_t(\gamma). \end{array} \tag{1.2}$$

This X_t is just an evaluation map at t; physically this could be regarded as a apparatus measuring the position of the particle at time t. Under this notation above, Born's probability law can be written as:

$$P[X_t \in A] = \int_A \frac{|\psi(x,t)|^2 dx}{\|\psi(0)\|^2}, \tag{1.3}$$

which reads the probability of finding the particle in a region $A \subset \mathbb{R}^3$ at time t is given by the solution of the Schrödinger equation (1.1) in this manner of the right hand side of the formula (1.3) above.*2

Mathematically, we can regard P as a probability measure on Γ and X_t as a random variables with the distribution given by the right hand side of (1.3), provided that such a measure P exists on Γ. However, standard theory of quantum mechanics does not care whether such a measure P actually exists or not.

2 Nelson's Observation: Kinematical part.

Putting $\rho(x,t) = |\psi(x,t)|^2$, we can easily verify that ρ solves both of these two equations:

$$\frac{\partial \rho}{\partial t} + \nabla(b\,\rho) - \frac{\hbar}{2m}\Delta\rho = 0, \tag{2.1}$$

$$\frac{\partial \rho}{\partial t} + \nabla(b_*\,\rho) + \frac{\hbar}{2m}\Delta\rho = 0. \tag{2.2}$$

Here,

$$b := \begin{cases} \dfrac{\hbar}{m}(\Im + \Re)\dfrac{\nabla\psi}{\psi}, & \text{if } \psi \neq 0, \\ 0, & \text{if } \psi = 0, \end{cases} \tag{2.3}$$

and

$$b_* := \begin{cases} \dfrac{\hbar}{m}(\Im - \Re)\dfrac{\nabla\psi}{\psi}, & \text{if } \psi \neq 0, \\ 0, & \text{if } \psi = 0. \end{cases} \tag{2.4}$$

*2 Sometimes the relation (1.3) is symbolically written as

$$P[X_t \in dx] = \frac{|\psi(x,t)|^2 dx}{\|\psi(0)\|^2},$$

which exactly means that a solution ψ of (1.1) gives us the density of distribution of random variables X_t $(t \in \mathbb{R})$.

If we have a probability measure P on Γ such that we have (1.3), then (2.1) could be considered as the Kolmogorov forward equation for the Itô type stochastic differential equation of the form:

$$dX_t = b(X_t, t)dt + \sqrt{\frac{\hbar}{m}}dB_t, \tag{2.5}$$

where $\{B_t\}_{t\in\mathbb{R}}$ is a standard 3-dimensional Wiener process (Brownian motion) with respect to P. On the other hand, (2.2) corresponds to

$$d_*X_t = b_*(X_t, t)dt + \sqrt{\frac{\hbar}{m}}d_*\widetilde{B}_t \tag{2.6}$$

with another Wiener process $\{\widetilde{B}_t\}_{t\in\mathbb{R}}$. Here we have used the notation that $dX_t = X_{t+dt} - X_t$, $d_*X_t = X_t - X_{t-dt}$ $(dt > 0)$; For $t > s$, $B_t - B_s$ and $\widetilde{B}_t - \widetilde{B}_s$ are independent of $\sigma\{X_\tau | -\infty < \tau \leq s\}$ and $\sigma\{X_\tau | t \leq \tau < \infty\}$, respectively.

So far, the kinematical part of Nelson's stochastic mechanics was discussed.

3 Nelson's Observation: Dynamical part.

We move to the dynamical part of Nelson's stochastic mechanics. We define Nelson's conditional derivatives D and D_* as follows:

$$Df(X_t, t) := \lim_{h\downarrow 0} \mathbb{E}\left[\frac{f(X_{t+h}, t+h) - f(X_t, t)}{h} \middle| \sigma(X_t)\right], \tag{3.1}$$

$$D_*f(X_t, t) := \lim_{h\downarrow 0} \mathbb{E}\left[\frac{f(X_{t-h}, t-h) - f(X_t, t)}{-h} \middle| \sigma(X_t)\right]. \tag{3.2}$$

Here $f \in \mathcal{B}^\infty(\mathbb{R}^3; \mathbb{R})$ (the set of infinitely differentiable bounded functions). Especially, for $X_t \in L^2(\Gamma, \mathfrak{B}, P)$ (finite energy diffusion), taking $f(x) = x$ yields that

$$DX(t) = b(X_t, t), \tag{3.3}$$

$$D_*X(t) = b_*(X_t, t). \tag{3.4}$$

By Itô formula (see, e.g., [7]), we have

$$Df(X_t, t) = \left(\frac{\partial f}{\partial t} + b \cdot \nabla f + \frac{\hbar}{2m}\triangle f\right)(X_t, t), \tag{3.5}$$

$$D_*f(X_t, t) = \left(\frac{\partial f}{\partial t} + b_* \cdot \nabla f - \frac{\hbar}{2m}\triangle f\right)(X_t, t). \tag{3.6}$$

If the process $t \mapsto f(X_t, t)$ is a backward martingale, f should satisfy the backward martingale equation:

$$\frac{\partial}{\partial t} f + b_* \cdot \nabla f - \frac{\hbar}{2m}\triangle f = 0. \tag{3.7}$$

This is a forward diffusion equation with the drift b_*, which is used in [2, 3] to construct a measure P for each solution of (1.1). In "general" situation (see, e.g., [2, 15]), we need the forward martingale equation as well:

$$\frac{\partial}{\partial t} f + b \cdot \nabla f + \frac{\hbar}{2m} \triangle f = 0, \tag{3.8}$$

which is derived by (3.5), while (3.7) by (3.6).

Nelson's observation which led himself to his stochastic mechanics (stochastic quantization) seems to include some interesting ingredients to understand superfluidity and Quantum turbulence (see §6 below).

4 Nelson's Observation: Dynamical part continues.

According to Nelson, we define the stochastic acceleration (SA) by:

$$\alpha(X_t) :\stackrel{\text{def}}{=} \left(\frac{DD_* + D_*D}{2} \right) X_t \tag{4.1}$$

Here we introduce the current velocity

$$v := \frac{b + b_*}{2} \tag{4.2}$$

and the osmotic velocity

$$u := \frac{b - b_*}{2}. \tag{4.3}$$

Then, we see by a tedious calculation that (SA) is given by:

$$\alpha(X_t) = \frac{\partial v}{\partial t} - (u \cdot \nabla)u + (v \cdot \nabla)v - \frac{\hbar}{2m} \triangle u, \tag{4.4}$$

where u and v stand for $u(X_t, t)$ and $v(X_t, t)$, respectively. On the other hand, setting $\psi = \exp(R + iS)$ $(\rho = \exp 2R)$, we have

$$\alpha(X_t) = \hbar \nabla \left(\frac{\partial S}{\partial t} - \frac{\hbar}{2m} |\nabla R|^2 + \frac{\hbar}{2m} |\nabla S|^2 - \frac{\hbar}{2m} \triangle R \right). \tag{4.5}$$

Here we have used the fact that $u = \frac{\hbar}{m} \nabla R$, $v = \frac{\hbar}{m} \nabla S$. By noting that fact that both u and v are defined through the wave function ψ solving Schrödinger equation (1.1), one can obtain

$$m\,\alpha(X_t) = -(\nabla V)(X_t, t), \tag{4.6}$$

which is Nelson's amazing result. This equation can be regarded as a stochastic version of Newton's second law of motion.

5 Nelson's Stochastic Quantization I.

Nelson's stochastic quantization (or stochastic mechanics) consists of the reverse procedures of those in the previous sections. Our fundamental assumption is that we have a probability measure P on Γ which gives us the same prediction as standard quantum mechanics does.

In order to characterize the measure P, Nelson first write down Itô type SDEs (2.5) and (2.6) for the evaluation map $X_t : \Gamma \ni \gamma \mapsto \gamma(t) \in \mathbb{R}^3$. This is the kinematical part of Nelson's stochastic mechanics. The dynamical part of his quantization is the stochastic version of the equation of Newton's 2nd law of motion (4.6), i.e.,

$$\frac{Db_*(X_t,t) + D_*b(X_t,t)}{2} = -(\nabla V)(X_t,t). \tag{5.1}$$

This equation (5.1) togerther with (2.5), (2.6) is governing the drifts b and b_*, and the probability P as well. In other words, the osomotic velocity u, the current velocity v and the density ρ will be determined through (2.5), (2.6) and (5.1).

6 Nelson's Stochastic Quantization II.

We shall derive a set of equations which govern u, v and ρ. Subtracting (2.2) from (2.1), we have:

$$u = \frac{\hbar}{2m}\nabla \log \rho. \tag{6.1}$$

Adding (2.1) and (2.2) gives us:

$$\frac{\partial \rho}{\partial t} + \nabla(v\rho) = 0. \tag{6.2}$$

Differentiate (6.1) with respect to t, we have by the aid of (6.2) that

$$\frac{\partial u}{\partial t} = -\nabla(v \cdot u) - \frac{\hbar}{2m}\nabla(\nabla \cdot v). \tag{6.3}$$

Besides we obtain from (4.4) and (4.6) that

$$\frac{\partial v}{\partial t} = (u \cdot \nabla)u - (v \cdot \nabla)v + \frac{\hbar}{2m}\Delta u - \nabla V. \tag{6.4}$$

These two equations (6.3) and (6.4) make a system of PDEs. The distribution ρ is determined by (6.2).

In a formal level, we obtain Euler-like-system in the semi-classical limit ($\hbar \to 0$):

$$\begin{cases} \dfrac{\partial v}{\partial t} + (v \cdot \nabla)v = -\nabla V, \\ \dfrac{\partial \rho}{\partial t} + \nabla(v\rho) = 0. \end{cases} \tag{6.5}$$

7 Nelson to Schrödinger

We suppose that we have current velocity v and osmotic velocity u which satisfy (6.3) and (6.4). Define a wave function ψ by

$$\psi := \sqrt{\rho}\exp(i\widetilde{S}/\hbar), \tag{7.1}$$

where $\widetilde{S} = \hbar S$, so that we have $v = \dfrac{1}{m}\nabla\widetilde{S}$. Then, by changing the phase factor of ψ which depends on only t-variable,*3 we can see that ψ in (7.1) solves (1.1) through the relations (6.1) and (6.2). Thus, we have derived the Schrödinger equation (1.1) from the equation of Newton's 2nd law of motion (4.6).

8 Carlen's Works [2, 3, 5]

For each solution $\psi \in C(\mathbb{R}; H^1(\mathbb{R}^3))$ of (1.1),*4 Carlen constructs a probability measure P on the path space Γ, which gives us the same prediction as standard Quantum Mechanics does. That is, we have (1.3). Unlike the notorious Feynman measure, which cannot exist as a genuine measure on Γ (see. e.g.,[9]), this measure P does exist for each solution ψ of (1.1).*5

The desired measure P is characterized as follows: P makes the functional

$$B_t \overset{\text{def}}{:=} \sqrt{\frac{m}{\hbar}}\left(X_t - X_0 + \int_0^t b(X_\tau, \tau)d\tau\right) \tag{8.1}$$

a standard brownian motion on $\mathbb{R}^3$, where X_t ($t \in \mathbb{R}$) are given evaluation maps defined by (1.2). Hence, this is a kind of a martingale problem, that is, P is a weak solution of the SDE (2.5).

The key ingredient of his proof is the following fact: the propagator $P_{t,s}$ ($s < t$) of (3.7) is given by

$$(P_{t,s}f_s)(X_t) = \mathbb{E}\left[f(X_s, s)\middle|\sigma(X_t)\right], \tag{8.2}$$

where $f_s(y) = f(y, s)$.*6 That is, $u(x,t) := (P_{t,s}f_s)(x)$ solves (3.7) with $u(x,s) = f_s(x)$. Analogously, we can construct the propagator $Q_{s,t}$ ($s < t$) for (3.8), that is, $u(x,s) := (Q_{s,t}f_t)(x)$ solves (3.7) with $u(x,t) = f_t(x)$.

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*3 This is a kind of gauge transformations.

*4 In [2], Carlen also assume that $\psi \in C(\mathbb{R}; L^2(\mathbb{R}^3; |x|^2dx))$.

*5 It is worth while noting here that Carlen consider the Schrödinger equation (1.1) on any space dimension d in [2, 3].

*6 In other words, (8.2) means:

$$f(X_t, t) = (P_{t,s}f_s)(X_t) = \int_{\mathbb{R}^3} f(x,s)P(X_s \in dx|X_t) = \int_{\mathbb{R}^3} f(x,s)p(X_t, t; dx, s)$$

Even for very "singular" drifts b and b_*, Carlen succeeded in construction of these propagators such that: for $s < t$

$$P_{t,s} : L^2(\mathbb{R}; \rho(x,s)dx) \longrightarrow L^2(\mathbb{R}; \rho(x,t)dx), \tag{8.3}$$

$$Q_{s,t} : L^2(\mathbb{R}; \rho(x,t)dx) \longrightarrow L^2(\mathbb{R}; \rho(x,s)dx), \tag{8.4}$$

and we have that for $f,\ g \in \mathcal{B}^\infty(\mathbb{R}^3, \mathbb{R})$

$$(P_{t,s}f, g)_t = (f, Q_{s,t}g)_s, \tag{8.5}$$

where $(\cdot,\cdot)_t$ is a standard inner product of $L^2(\mathbb{R}^3; \rho(x,t)dx)$, which implies:

$$\mathbb{E}\left[(P_{t,s}f)(X_t)g(X_t)\right] = \mathbb{E}\left[f(X_s)g(X_t)\right] = \mathbb{E}\left[f(X_s)(Q_{s,t}g)(X_s)\right]. \tag{8.6}$$

Once we get the Markovian propagator $P_{t,s}$, we can construct the desired measure P through the functional:*7

$$P(F) := (1, P_{T,t_n}f_nP_{t_n,t_{n-1}}f_{n-1}\cdots P_{t_2,t_1}f_1)_T \quad (t_1 < t_2 < \cdots < t_n < T) \tag{8.7}$$

for $F(\cdot) = \prod_{i=1}^{n} f_i(X_{t_i}(\cdot)) \in C(\overline{\Gamma})$ where $\overline{\Gamma} := (\mathbb{R}^3 \cup \{\infty\})^{\mathbb{R}}$ with the product topology, and $f_i \in C^\infty(\mathbb{R}^d \cup \{\infty\})$ $(i = 1, 2, \ldots, n)$. One can extend this functional P to the one defined on the whole space of $C(\overline{\Gamma})$. We can safely say that this is a standard procedure to obtain the desired measure. Here the important thing is that the support of P lies on $C(\Gamma)$; proving this fact is an ingredient of Carlen's proof in [3] (see also Yoshida [15]), where the backward propagator $Q_{s,t}$ also plays an important role. Finally, Levy's characterization of Brownian motion (see, e.g., [7]) tells us that (8.1) is a standard Brownian motion ([3, 15]).

9 NLS and Nelson diffusions

We consider the Cauchy problem*8 for the nonlinear Schrödinger equation (abbreviated to NLS) of the form:

$$\begin{cases} 2i\dfrac{\partial\psi}{\partial t} + \triangle\psi + |\psi|^{p-1}\psi = 0, & (x,t) \in \mathbb{R}^d \times \mathbb{R}_+, \\ \psi(0) = \psi_0 \in H^1(\mathbb{R}^d). \end{cases}$$

Here, the index p in the nonlinear term satisfies: $p \in (1, 2^* - 1)$, where $2^* = \dfrac{2d}{d-2}$ for $d \geqq 3$; $2^* = \infty$ for $d = 1, 2$.

The unique local existence theorem is well known (see, e.g., [14]): for any $\psi_0 \in H^1(\mathbb{R}^d)$, there exists a unique solution ψ in $C([0, T_{\max}); H^1(\mathbb{R}^d))$ for some $T_{\max} \in (0, \infty]$ (maximal

*7 Here we abuse the notation. This functional P will be identified with desired probability measure.

*8 For simplicity, we consider the forward time only.

existence time) such that ψ satisfies the following three conservation laws of L^2-norm (or charge), momentum, energy (or Hamiltonian) in this order:

$$\|\psi(t)\|^2 = \|\psi(0)\|^2, \tag{9.1}$$

$$\Im \int_{\mathbb{R}^d} \overline{\psi(x,t)} \nabla\psi(x,t)dx = \Im \int_{\mathbb{R}^d} \overline{\psi_0(x)} \nabla\psi_0(x)dx =: \Im\left(\psi_0, \nabla\psi_0\right), \tag{9.2}$$

$$\mathcal{H}_{p+1}(\psi(t)) \stackrel{\text{def}}{:=} \|\nabla\psi(t)\|^2 - \frac{2}{p+1}\|\psi(t)\|_{p+1}^{p+1} = \mathcal{H}_{p+1}(\psi_0). \tag{9.3}$$

Here, $\|\cdot\|_{p+1}$ denotes the L^{p+1}-norm of $\psi(\cdot,t)$:

$$\|\psi(t)\|_{p+1} := \left(\int_{\mathbb{R}^d} |\psi(x,t)|^{p+1}dx\right)^{\frac{1}{p+1}}.$$

It is worth while noting that a certain number $p > 1$ (the index appearing in the nonlinear term) divides the world of solutions of NLS into two parts:

- When $1 < p < 1 + \frac{4}{d}$, every solution exists globally in time, i.e., $T_{\max} = \infty$.

  For: we have an a priori bound on $\|\nabla\psi(t)\|$ by virtue of the energy conservation law and the Gagliardo-Nirenberg inequality:

  $$\|f\|_{p+1}^{p+1} \leqq C_{p,d}\|f\|^{p+1-\frac{d}{2}(p-1)}\|\nabla f\|^{\frac{d}{2}(p-1)}.$$

- When $2^* - 1 > p \geqq 1 + \frac{4}{d}$, there exists a class of initial data which give rise to blowup solutions, that is,

  $$T_{\max} < \infty \quad \text{and} \quad \lim_{t\uparrow T_{\max}} \|\nabla\psi(t)\| = \infty.$$

Hence, (NLS) with $p = 1 + \frac{4}{d}$ *9 is the borderline case for the existence of blowup solutions. This fact can be easily seen in a weighted energy space $H^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d; |x|^2dx)$ *10: If we assume in addition that $|x|\psi_0 \in L^2(\mathbb{R}^d)$, then the corresponding solution ψ of NLS satisfies

$$|x|\psi(\cdot) \in C([0,T_{\max}); L^2(\mathbb{R}^d))$$

and

$$\begin{aligned}\||x|\psi(t)\|^2 =& \||x|\psi(0)\|^2 + 2t\Im\left(\psi(0), x\cdot\nabla\psi(0)\right) + t^2\mathcal{H}_{p+1}(\psi(0)) \\ &- \frac{d}{p+1}\left(p+1-\left(2+\frac{4}{d}\right)\right)\int_0^t (t-\tau)\|\psi(\tau)\|_{p+1}^{p+1}d\tau.\end{aligned} \tag{9.4}$$

From this identity (sometimes called the virial identity), one can show that every negative energy solution has to blow up in a finite time, provided that $p \geq 1 + \frac{4}{d}$. *11

*9 This equation is invariant under the pseudo-conformal transformations (see, e.g., [14]).

*10 The form domain of harmonic oscillators, $-\Delta + c|x|^2$ $(c > 0)$.

*11 For $p = 1 + \frac{4}{d}$, the last term in the right hand side vanishes; this is one of the manifestation of the invariance property of the equation under the pseudo-conformal transformations.

E. Carlen's method is translatable for nonlinear cases.*12 For each solution $\psi \in C(\mathbb{R}; H^1(\mathbb{R}^d))$ of (NLS), we can prove:

Theorem 1. *Let u, v, and b be analogously defined by* (4.3), (4.2) *and* (2.3), *respectively, through the solution ψ of* (NLS) *on $[0, T_{\max})$. We associate $\Gamma_{\rm loc} := C([0, T_{\max}); \mathbb{R}^d)$ with its Borel σ-algebra $\mathcal{F}$ with respect to the Fréchet topology. Let $(\Gamma_{\rm loc}, \mathcal{F}, \mathcal{F}_t, X_t)$ be evaluation stochastic process $X_t(\gamma) := \gamma(t)$ for $\gamma \in \Gamma_{\rm loc}$ with natural filtration $\mathcal{F}_t = \sigma(X_s, s \leqq t)$. Then there exists a Borel probability measure P on $\Gamma_{\rm loc}$ such that:*

(i) *$(\Gamma_{\rm loc}, \mathcal{F}, \mathcal{F}_t, X_t, P)$ is a Markov process,*

(ii) *the probability that X_t is in a measurable set $A \subset \mathbb{R}^d$ is given by*

$$P[X_t \in A] = \int_A \frac{|\psi(x,t)|^2 dx}{\|\psi(0)\|^2}, \tag{9.5}$$

(iii) *the following process B_t is a $(\Gamma_{\rm loc}, \mathcal{F}_t, P)$-Brownian motion:*

$$B_t :\stackrel{def}{=} X_t - X_0 - \int_0^t b(X_\tau, \tau) d\tau. \tag{9.6}$$

Even though the weak solution of (9.6), once we have a Brownian motion, we can utilize it for further investigation of properties of the solution of (NLS). Some nature of blow up solutions of (NLS) with $p = 1 + \frac{4}{d}$ and the properties of the corresponding process $\{X_t\}_{t \in [0, T_{\max})}$ was discussed in [13, 12]. This is still an ongoing research project of the author.

Akahori and the author [1] consider the scattering and blowup problem of (NLS) with $p > 1 + \frac{4}{d}$. The scattering part is investigated in the spilit of Kenig-Merle [8], which is based on high-level reductio ad absurdum. We believe that we could give another direct proof for the scattering part by investigating the behavior of $\frac{X_t}{t}$ $(t \to \infty)$ (as in [4] for linear problem (1.1)) through (9.4) or its truncated version for our nonlinear problem.

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*12 In fact, he considered (1.1) on $\mathbb{R}^d \times \mathbb{R}$ in [2, 3, 5], and his arguments works well for "nice" time dependent potentials $V = V(x,t)$ as well.

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