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Stationarity-Based Representation for the Coulomb Potential and a Diffusion Representation for Solution of the Schrödinger Equation

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I. General Discussion

Diffusion representations have long been utilized in the study of Hamilton-Jacobi partial differential equations (HJ PDEs), cf. [5], [10], [13] among many others. The bulk of such results apply to real-valued HJ PDEs, that is, to HJ PDEs where the coefficients and solutions are real-valued. The Schrödinger equation is complex-valued, although generally defined over a real-valued space domain, which presents difficulties for the development of stochastic control representations. There is substantial existing work on the relation of stochastic processes to the Schrödinger equation, cf. [11], [15], [25], [26], [27]. The approach considered here is in the spirit of the Feynman path-integral interpretation [6], [7], where in particular, one looks at a certain action-based functional, S, where $\psi = \exp\{\frac{i}{\hbar}S\}$ and $\hbar$ denotes Planck's constant. One seeks a representation for S in the form of a value function for a stochastic control problem where the action functional is the payoff, cf. [2], [3], [6], [7], [8], [14], [17]. We note that this latter approach is also sometimes employed in analysis of semiclassical limits, cf. [1], [3], [8], [14].

An issue that arises in such approaches is that control has traditionally considered classical optimization (minimization or maximization) of some payoff. Implicit in that is an assumption that the payoff is real valued. In [4], [22], [24], the authors consider a least-action approach to obtaining fundamental solutions to two-point boundary value problems (TPBVPs) for conservative dynamical systems. However, that formulation, which was in terms of minimization of the action, induced duration limits on the problems which could be addressed, where those limits were also similar to duration limits present in existing results on the Schrödinger equation representation in terms of action, cf. [2], [3], [8]. We note that the duration limits are related to a loss of convexity of the payoff as the time horizon is extended. While in [4], [22], [24], the least-action principle was applied, the more generally applicable form is the stationary-action principle, which coincides with the least-action principle when the action functional is convex and coercive. Consequently and more recently, the notion of "staticization" was introduced for such TPBVPs, in which case one seeks a stationary point of the action over the space of control inputs. The extension to stationarity removes the restriction on problem duration. This yields a dynamic program which takes the form of an HJ PDE in the case of continuous-time/continuous-space processes, where these were studied in the context of deterministic dynamics in [20], [21], [23].

As staticization seeks points where the derivative of a functional is zero, as opposed to optimization of the functional, it is easily extended to the case of complex-valued systems. The extension to stochastic dynamics is easily made as well. Also, as staticization does not require the imposition of duration limits on the problems, one can apply this new tool to the stochastic-control representation problem for the dequantized Schrödinger equation, and that is the topic considered herein.

In order to clarify the details in the above, we recall the Schrödinger initial value problem, given as

$$0 = i\hbar\psi_t(s,y) + \frac{\hbar^2}{2m}\Delta\psi(s,y) - \psi(s,y)V(y), \ \ (s,y) \in \mathcal{D}, \tag{1}$$

$$\psi(0,y) = \psi_0(y), \quad y \in \mathbb{R}^n, \tag{2}$$

where $m \in (0,\infty)$ denotes mass, initial condition ψ_0 takes values in $\mathbb{C}$, V denotes a known potential function, Δ denotes the Laplacian with respect to the space (second) variable, $\mathcal{D} \doteq (0,t) \times \mathbb{R}^n$, and subscript t will denote the derivative with respect to the time variable (the first argument of ψ here) regardless of the symbol being used for time in the argument list. We also let $\overline{\mathcal{D}} \doteq (0,t] \times \mathbb{R}^n$. We consider what is sometimes referred to as the Maslov dequantization of the solution of the Schrödinger equation (cf. [16]), which as noted above, is $S : \overline{\mathcal{D}} \to \mathbb{C}$ given by $\psi(s,y) = \exp\{\frac{i}{\hbar}S(s,y)\}$. The Maslov dequantization is clearly similar to the logarithmic transform (cf. [9]), but with a modification induced through multiplication by an imaginary constant. Note that $\psi_t = \frac{i}{\hbar}\psi S_t$, $\psi_y = \frac{i}{\hbar}\psi S_y$ and $\Delta\psi = \frac{i}{\hbar}\psi\Delta S - \frac{1}{\hbar^2}\psi|S_y|_c^2$ where for $x \in \mathbb{C}^n$, $|x|_c^2 \doteq \sum_{j=1}^n x_j^2$. (We remark that notation $|\cdot|_c^2$ is not intended to indicate a squared norm; the range is complex.) We find that (1)–(2) become

$$0 = -S_t(s,y) + \frac{i\hbar}{2m}\Delta S(s,y) + H(y, S_y(s,y)), \tag{3}$$

$$S(0,y) = \phi(y), \quad y \in \mathbb{R}^n, \tag{4}$$

where $H : \mathbb{R}^n \times \mathbb{C}^n \to \mathbb{C}$ is the Hamiltonian given by

$$\begin{aligned} H(y,p) &= -\left[\tfrac{1}{2m}|p|_c^2 + V(y)\right] \\ &= \operatorname*{stat}_{u^0 \in \mathbb{C}^n} \left\{(u^0)^T p + \tfrac{m}{2}|u^0|_c^2 - V(y)\right\}, \end{aligned} \tag{5}$$

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stat will be defined in the next section, and throughout, superscript T denotes transpose. We look for solutions in the space

$$\mathcal{S} \doteq \{S : \overline{\mathcal{D}} \to \mathbb{C} \,|\, S \in C_p^{1,2}(\mathcal{D}) \cap C(\overline{\mathcal{D}})\}, \tag{6}$$

where $C_p^{1,2}$ denotes the space of functions which are continuously differentiable once in time and twice in space, and which satisfy a polynomial-growth bound. We will find it helpful to reverse the time variable, and hence we look instead, and equivalently, at the Hamilton-Jacobi partial differential equation (HJ PDE) problem given by

$$0 = S_t(s,y) + \frac{i\hbar}{2m}\Delta S(s,y) + H(y, S_y(s,y)), \;\; (s,y) \in \mathcal{D}, \tag{7}$$

$$S(t,y) = \phi(y), \quad y \in \mathbb{R}^n. \tag{8}$$

Working mainly with this last form, we will fix $t \in (0,\infty)$, and allow s to vary in $(0,t]$.

Recall that in semiclassical limit analysis, one views $\hbar$ as a small parameter, and examines the limit as $\hbar \downarrow 0$. Applying this in (7)–(8) yields an HJ PDE problem of the form

$$0 = S_t(s,y) + H(y, S_y(s,y)), \quad (s,y) \in \mathcal{D}, \tag{9}$$

$$S(t,y) = \phi(y), \quad y \in \mathbb{R}^n. \tag{10}$$

Recalling the above-noted recent work on least-action and stationary-action formulations of certain TPBVPs [4], [20], [22], [24], [21], [23], it was found that the associated HJ PDEs for such problems also take the form (9)–(10). This was the original motivation for the effort here, where we develop a stationary-action based representation for the solution of (7)–(8) (and consequently (1)–(2)). Due to the complex multiplier on the Laplacian, this representation is in terms of a stationary-action stochastic control problem with a complex-valued diffusion coefficient.

II. Stationarity-Based Representation

The use of stationarity rather than optimization allows for the extension of the stochastic representation to arbitrary duration problems. The efforts to date have assumed a smooth potential that may be extended to a holomorphic potential over $\mathbb{C}^n$ [18], [19]. This precludes the Coulomb potential. In a parallel effort on the application of stationary action to conservative dynamics, specifically including the n-body problem, a staticization-based representation for the gravitational potential proved to be of critical importance [22], [23], [24]. Here, we will obtain a staticization-based representation for an extension of the Coulomb potential to $\mathbb{C}^n$.

In order to indicate this representation, we first need to define the staticization operator, [20], [21]. Suppose $(\mathcal{U}, |\cdot|)$ is a generic normed vector space with $\mathcal{G} \subseteq \mathcal{U}$, and suppose $F : \mathcal{G} \to \mathbb{R}$. We say $\bar{v} \in \operatorname{argstat}\{F(v) \,|\, v \in \mathcal{G}\}$ if $\bar{v} \in \mathcal{G}$ and either

$$\limsup_{v \to \bar{v}, v \in \mathcal{G}\setminus\{\bar{v}\}} |F(v) - F(\bar{v})|/|v - \bar{v}| = 0,$$

or there exists $\delta > 0$ such that $\mathcal{G} \cap B_\delta(\bar{v}) = \{\bar{v}\}$. If $\operatorname{argstat}\{F(v) \,|\, v \in \mathcal{G}\} \neq \emptyset$, we define the possibly set-valued stat^s operation by

$$\operatorname*{stat}^s_{v \in \mathcal{G}} F(v) \doteq \big\{F(\bar{v}) \,\big|\, \bar{v} \in \operatorname{argstat}\{F(v) \,|\, v \in \mathcal{G}\}\big\}.$$

If $\operatorname{argstat}\{F(v) \,|\, v \in \mathcal{G}\} = \emptyset$, $\operatorname{stat}^s_{v\in\mathcal{G}} F(v)$ is undefined. Where applicable, we are also interested in a single-valued stat operation (note the absence of superscript s). In particular, if there exists $a \in \mathbb{R}$ such that $\operatorname{stat}^s_{v\in\mathcal{G}} F(v) = \{a\}$, then $\operatorname{stat}_{v\in\mathcal{G}} F(v) \doteq a$; otherwise, $\operatorname{stat}_{v\in\mathcal{G}} F(v)$ is undefined.

Note that in the case where $\mathcal{U}$ is a Hilbert space, $\mathcal{G}$ is open, and $F : \mathcal{G} \to \mathbb{R}$ is Fréchet differentiable at $\bar{v} \in \mathcal{G}$ with derivative denoted by $F_v(\bar{v})$, $\bar{v} \in \operatorname{argstat}\{F(y) \,|\, y \in \mathcal{G}\}$ if and only if $F_v(\bar{v}) = 0$.

With the staticization operator in hand, we may indicate the staticization-based representation for the extension of the Coulomb potential. More specifically, for $x \in \mathbb{C}^n$, this representation is given by

$$\begin{aligned} -V(x) &= \exp\left\{\tfrac{-1}{2}\log\left(|x|_c^2\right)\right\} \\ &= \left(\tfrac{3}{2}\right)^{3/2} \operatorname*{stat}_{\alpha\in\mathcal{A}^R} \left\{\alpha - \frac{\alpha^3 |x|_c^2}{2}\right\}, \end{aligned}$$

where

$$\mathcal{A}^R \doteq \left\{\alpha = r[\cos(\theta) + i\sin(\theta)] \in \mathbb{C} \,\middle|\, r \geq 0,\, \theta \in \left(\tfrac{-\pi}{2}, \tfrac{\pi}{2}\right)\right\}.$$

In the simple one-dimensional case, the resulting function on $\mathbb{C}$ has a branch cut along the negative imaginary axis, and this generalizes to the higher-dimensional case in the natural way. Recall that the observable portion of the solution lies entirely on the real domain. This representation for the potential results in a diffusion representation for the solution of the Schrödinger equation that takes the form of an iterated staticization operator. In the gravitational case, a reordering of these operators on short time-horizons plays a critical role in generating fundamental solutions. The extension to the Coulomb potential and Schrödinger equation will be explored here.

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