# New Phase Space Formulations and Quantum Dynamics Approaches

## Article Type:

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It is important to note that, in general $\frac{\partial d_{mn}^{(J)}(\tilde{\mathbf{R}})}{\partial \tilde{R}_I} - \frac{\partial d_{mn}^{(I)}(\tilde{\mathbf{R}})}{\partial \tilde{R}_J} = 0$ does not always hold for $I \neq J$, except for two-electronic-state systems. So eq 115 is not always equal to zero. The term of eq 115 cancels out the third term of eq 113. The last term of the RHS of eq 113 can be recast into

$$\begin{aligned} &\sum_{n,m=1}^{F} \left( E_n(\tilde{\mathbf{R}}) \tilde{x}^{(n)} \tilde{x}^{(m)} - E_m(\tilde{\mathbf{R}}) \tilde{p}^{(m)} \tilde{p}^{(n)} \right) d_{nm}^{(I)}(\tilde{\mathbf{R}}) \\ &= \frac{1}{2} \sum_{n,m=1}^{F} \left( E_n(\tilde{\mathbf{R}}) - E_m(\tilde{\mathbf{R}}) \right) \left( \tilde{x}^{(n)} \tilde{x}^{(m)} + \tilde{p}^{(n)} \tilde{p}^{(m)} \right) d_{nm}^{(I)}(\tilde{\mathbf{R}}) \end{aligned} . \quad 116$$

Equation 113 then becomes

$$\begin{aligned} &\dot{P}_I(\tilde{\mathbf{R}}, \tilde{\mathbf{P}}, \tilde{\mathbf{x}}, \tilde{\mathbf{p}}) \\ &= -\sum_{k=1}^{F} \frac{\partial E_k(\tilde{\mathbf{R}})}{\partial R_I} \left( \frac{1}{2} \left( \left( \tilde{x}^{(k)} \right)^2 + \left( \tilde{p}^{(k)} \right)^2 \right) - \gamma \right) - \sum_{n,m=1}^{F} \left( E_n(\tilde{\mathbf{R}}) - E_m(\tilde{\mathbf{R}}) \right) d_{mn}^{(I)}(\tilde{\mathbf{R}}) \frac{1}{2} \left( \tilde{x}^{(n)} \tilde{x}^{(m)} + \tilde{p}^{(n)} \tilde{p}^{(m)} \right) \end{aligned}$$

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which is equivalent to the second equation of eq 76 of the main text. It indicates that the canonical momentum in the diabatic representation is covariant with *kinematic* momentum $\mathbf{P}$ rather than canonical momentum $\tilde{\mathbf{P}}$ in adiabatic representation unless all nonadiabatic coupling terms vanish. This is consistent with the spirit of the work of Cotton *et. al.* in ref [184]. Because the EOMs (eq 70 and eq 76) of the main text are identical to Hamilton's EOMs generated by eq 107, the mapping Hamiltonian (eq 79 or eq 107) is conserved during the evolution in the adiabatic representation.

### 3. The relationship between the constraint coordinate-momentum phase space and Stratonovich phase space

Stratonovich's original work[100] in 1956 maps a 2-state (spin-1/2) system onto a two-dimensional sphere. We review two kinds of further developments of the Stratonovich-Weyl mapping phase space representations for $F$-state quantum system: the first one based on the $\mathrm{SU}(2)$ structure[103, 113] and the second one based on the $\mathrm{SU}(F)$ structure[114]. We show the relationship between constrained coordinate-momentum phase space representation that we use in the Focus Article and the two kinds of Stratonovich phase space representations.

In the $\mathrm{SU}(2)$ Stratonovich phase space representation, an $F$-state system is treated as a spin-$j$ system (where $F = 2j+1$). The basis set consists of $|j, m\rangle$, the eigenstate of the square of total angular momentum

$\hat{J}^2$ and the $z$-component of angular momentum $\hat{J}_z$ with quantum numbers $j$ and $m$, respectively. The mapping kernel is

$$\hat{K}^{\mathrm{SU(2)}}_{\mathrm{ele}}(\theta,\varphi;s)=\sqrt{\frac{\pi}{2j+1}}\sum_{l=0}^{2j}(C^{jj}_{jj,l0})^{-s}\sum_{m=-l}^{l}Y^*_{lm}(\theta,\varphi)\hat{T}^j_{lm}, \quad s\in\mathbb{R} \qquad 118$$

where $\hat{T}^j_{lm}$ is the irreducible tensor operator defined as[299]

$$\hat{T}^j_{lm}=\sqrt{\frac{2l+1}{2j+1}}\sum_{m',n=-j}^{j}C^{jn}_{jm',lm}\,|j,n\rangle\langle j,m'|\,. \qquad 119$$

Here $C^{jm}_{j_1m_1,j_2m_2}=\langle jm\,|\,j_1m_1,j_2m_2\rangle$ is the well-known Clebsch-Gordan coefficient for the angular momentum coupling, and $Y_{lm}(\theta,\varphi)$ is the spherical harmonic function. The inverse kernel of $\hat{K}^{\mathrm{SU(2)}}_{\mathrm{ele}}(\theta,\varphi;s)$ is simply $\hat{K}^{\mathrm{SU(2)}}_{\mathrm{ele}}(\theta,\varphi;-s)$. We note that, although $s=1,0$, and $-1$ are traditionally associated with the $Q$, Wigner, and $P$-functions respectively and used in the literature[111, 128], parameter $s$ of eq 118 can in principle take *any* real value.

When $F>2$, the $\mathrm{SU(2)}$ Stratonovich phase space $(\theta,\varphi)$ does *not* have a phase point-to-phase point mapping to constraint coordinate-momentum phase space, although the relation can only be constructed by virtue of the density matrix. Only when $F=2$ as in the original work of Stratonovich, there exists a phase point-to-phase point mapping to constraint coordinate-momentum phase space. The mapping kernel can be expressed in terms of the spin-coherent state,

$$\hat{K}^{\mathrm{SU(2)}}_{\mathrm{ele}}(\theta,\varphi;s)=3^{(1+s)/2}\,|\theta,\varphi\rangle\langle\theta,\varphi|+\frac{\hat{1}}{2}\left[1-3^{(1+s)/2}\right]\,. \qquad 120$$

In eq 120 spin coherent state $|\theta,\varphi\rangle$ is

$$|\theta,\varphi\rangle=\begin{pmatrix} e^{-i\varphi}\sin(\theta/2) \\ \cos(\theta/2)\end{pmatrix}, \qquad 121$$

where $(\theta,\varphi)$ are the spherical coordinate variables on the two-dimensional spherical phase space. The range of $\theta$ is $[0,\pi]$ and that for $\varphi$ is $[0,2\pi)$. When $F=2$, the explicit transformation of $(\theta,\varphi)$ to the constrained coordinate-momentum phase space $(x^{(1)},x^{(2)},p^{(1)},p^{(2)})$ is



$$\hat{K}(\theta,\phi)=\sqrt{\frac{4\pi}{2j+1}}\sum_{l=0}^{2j}\sum_{m=-l}^{l}(C^{jj}_{jj,l0})^{-s}Y^*_{lm}(\theta,\phi)\hat{T}^j_{lm}. \qquad (11)$$

Here $Y_{lm}(\theta,\phi)$ is spherical harmonics, $\hat{T}^j_{lm}$ are the irreducible tensor operators of spin $j$ [6]:

$$\hat{T}^j_{lm}=\sqrt{\frac{2l+1}{2j+1}}\sum_{m_1,m_2=-j}^{j}C^{jm_2}_{jm_1,lm}\,|j,m_2\rangle\langle j,m_1|\,. \qquad (12)$$

Eqs (11)-(12) on the right came from Note-On-Mar16-2022-BeijingTime.pdf, based on Adv. Quantum Technol., 4 (6), 2100016 (2021). doi: 10.1002/qute.202100016

$$\hat{K}(\theta,\phi)=-3^{(1+s)/2}\,|\theta,\phi\rangle\langle\theta,\phi|+\frac{\hat{1}}{2}[1+3^{(1+s)/2}]. \qquad (9)$$

Here the notation $|\theta,\phi\rangle$ refers to a spin coherent state, which has the form in nomally used basis $\{|\uparrow\rangle,|\downarrow\rangle\}$

$$|\theta,\phi\rangle=\begin{pmatrix} e^{i\phi/2}\cos(\theta/2) \\ -e^{-i\phi/2}\sin(\theta/2)\end{pmatrix}. \qquad (10)$$

Eqs (9)-(10) on the right came from Note-On-Mar16-2022-BeijingTime.pdf.

For SU(2), we adjusted the definition of coherent state eq (10) and mapping kernel eq (9) to make the definitions in Appendix 3 more self-consistent.

$$\begin{pmatrix} x^{(1)} \\ p^{(1)} \end{pmatrix} = \sqrt{2(1+2\gamma)} \begin{pmatrix}\cos\psi & -\sin\psi \\ \sin\psi & \cos\psi\end{pmatrix}\begin{pmatrix}\cos\varphi\sin(\theta/2) \\ -\sin\varphi\sin(\theta/2)\end{pmatrix}$$
$$\begin{pmatrix} x^{(2)} \\ p^{(2)} \end{pmatrix} = \sqrt{2(1+2\gamma)} \begin{pmatrix}\cos\psi & -\sin\psi \\ \sin\psi & \cos\psi\end{pmatrix}\begin{pmatrix}\cos(\theta/2) \\ 0\end{pmatrix} , \qquad 122$$

where $\psi$ is an additional global phase.

The second kind of representation is the $\mathrm{SU}(F)$ Stratonovich phase space[114], which is diffeomorphic to the quotient set $\mathrm{SU}(F)/\mathrm{U}(F-1)$, parameterized by $(2F-2)$ angle variables $(\boldsymbol{\theta},\boldsymbol{\varphi})=(\theta_1,\theta_2,\ldots,\theta_{F-1},\varphi_1,\varphi_2,\ldots,\varphi_{F-1})$. The range of each angle $\theta_i$ is $[0,\pi/2]$ and that for each angle $\varphi_i$ is $[0,2\pi)$. The $\mathrm{SU}(F)$ Stratonovich phase space of Tilma *et.al.*[114] has been used to prepare the initial condition for the Meyer-Miller mapping model of non-adiabatic dynamics in ref [197].

The mapping kernel of the $\mathrm{SU}(F)$ Stratonovich phase space is

$$\hat{K}_{\mathrm{ele}}^{\mathrm{SU}(F)}(\boldsymbol{\theta},\boldsymbol{\varphi};s)=(1+F)^{(1+s)/2}|\boldsymbol{\theta},\boldsymbol{\varphi}\rangle\langle\boldsymbol{\theta},\boldsymbol{\varphi}|+\frac{\hat{\mathbf{I}}}{F}\left(1-(1+F)^{(1+s)/2}\right), \quad s\in\mathbb{R} \qquad 123$$

and the inverse kernel is $\hat{K}_{\mathrm{ele}}^{\mathrm{SU}(F)}(\boldsymbol{\theta},\boldsymbol{\varphi};-s)$. The explicit form of the generalized coherent state $|\boldsymbol{\theta},\boldsymbol{\varphi}\rangle$ is[300, 301]

$$|\boldsymbol{\theta},\boldsymbol{\varphi}\rangle=\sum_{n=1}^{F}c_n|n\rangle , \qquad 124$$

where the coefficients are

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_{F-3} \\ c_{F-2} \\ c_{F-1} \\ c_F \end{pmatrix} = \begin{pmatrix} e^{i(\varphi_1+\varphi_2+\cdots+\varphi_{F-1})}\cos(\theta_1)\cos(\theta_2)\cdots\cos(\theta_{F-2})\sin(\theta_{F-1}) \\ -e^{i(-\varphi_1+\varphi_2+\cdots+\varphi_{F-1})}\sin(\theta_1)\cos(\theta_2)\cdots\cos(\theta_{F-2})\sin(\theta_{F-1}) \\ -e^{i(\varphi_3+\varphi_4+\cdots+\varphi_{F-1})}\sin(\theta_2)\cos(\theta_3)\cdots\cos(\theta_{F-2})\sin(\theta_{F-1}) \\ \vdots \\ -e^{i(\varphi_{F-3}+\varphi_{F-2}+\varphi_{F-1})}\sin(\theta_{F-4})\cos(\theta_{F-3})\cos(\theta_{F-2})\sin(\theta_{F-1}) \\ -e^{i(\varphi_{F-2}+\varphi_{F-1})}\sin(\theta_{F-3})\cos(\theta_{F-2})\sin(\theta_{F-1}) \\ -e^{i(\varphi_{F-1})}\sin(\theta_{F-2})\sin(\theta_{F-1}) \\ \cos(\theta_{F-1}) \end{pmatrix} . \qquad 125$$

As derived first in Appendix A of ref [132] in the spirit of ref [131] and then in the Supporting Information of ref [134], the mapping kernel of constraint coordinate-momentum phase space for a set of $F$ states (eq 29 of the main text) is denoted as,

$$\hat{K}_{\mathrm{ele}}(\mathbf{x},\mathbf{p};\gamma)=\sum_{m,n=1}^{F}\left[\frac{(x^{(m)}-ip^{(m)})(x^{(n)}+ip^{(n)})}{2}-\gamma\delta_{mn}\right]|n\rangle\langle m|=|\mathbf{x},\mathbf{p}\rangle\langle\mathbf{x},\mathbf{p}|-\gamma\hat{\mathbf{I}} , \qquad 126$$

$$x^{(n)} = \sqrt{2}\times(1+F)^{(1+s)/4}\mathrm{Re}\,\langle n|\psi_z\rangle ,$$
$$p^{(n)} = \sqrt{2}\times(1+F)^{(1+s)/4}\mathrm{Im}\,\langle n|\psi_z\rangle ; \qquad (31)$$

when $n=F$ the constrain of the circle is

$$(x^{(F)})^2+(p^{(F)})^2=2(1+F)^{(1+s)/2}\cos^2\theta_{F-1}. \qquad (32)$$

Eqs (31)-(32) on the right came from Note-On-Mar16-2022-BeijingTime.pdf.

There were some typos in eqs 31&32, we corrected them in Appendix 3.

$$\hat{K}(z)=(1+F)^{(1+s)/2}|\psi_z\rangle\langle\psi_z|+\frac{\hat{1}}{F}\left(1-(1+F)^{(1+s)/2}\right). \qquad (21)$$

$|\psi_z\rangle$ is a state related to phase space point $z$, it can be also considered as a parameterization of an arbitrary normalized state in $F$-state system up to a global phase [16, 17]:

$$|\psi_z\rangle = \begin{pmatrix} e^{i(\phi_1+\phi_2+\cdots+\phi_{F-1})}\cos(\theta_1)\cos(\theta_2)\cdots\cos(\theta_{F-2})\sin(\theta_{F-1}) \\ -e^{i(-\phi_1+\phi_2+\cdots+\phi_{F-1})}\sin(\theta_1)\cos(\theta_2)\cdots\cos(\theta_{F-2})\sin(\theta_{F-1}) \\ -e^{i(\phi_3+\phi_4+\cdots+\phi_{F-1})}\sin(\theta_2)\cos(\theta_3)\cdots\cos(\theta_{F-2})\sin(\theta_{F-1}) \\ \vdots \\ -e^{i(\phi_{F-3}+\phi_{F-2}+\phi_{F-1})}\sin(\theta_{F-4})\cos(\theta_{F-3})\cos(\theta_{F-2})\sin(\theta_{F-1}) \\ -e^{i(\phi_{F-2}+\phi_{F-1})}\sin(\theta_{F-3})\cos(\theta_{F-2})\sin(\theta_{F-1}) \\ -e^{i(\phi_{F-1})}\sin(\theta_{F-2})\sin(\theta_{F-1}) \\ \cos(\theta_{F-1}) \end{pmatrix} . \qquad (22)$$

Eqs (21)-(22) on the right came from Note-On-Mar16-2022-BeijingTime.pdf, which were originally from J. Phys. A Math. Theor. 45, 015302 (2012). doi: 10.1088/1751-8113/45/1/015302.

$$\hat{K}(z)=\sum_{m,n=1}^{F}\left[\frac{(x^{(m)}-ip^{(m)})(x^{(n)}+ip^{(n)})}{2}-\gamma\delta_{mn}\right]|n\rangle\langle m|=|\tilde{\psi}_z\rangle\langle\tilde{\psi}_z|-\gamma\hat{1}. \qquad (25)$$

Eq (25) on the right came from Note-On-Mar16-2022-BeijingTime.pdf.

where the non-normalized state $|\mathbf{x},\mathbf{p}\rangle$ is

$$\sum_{n=1}^{F}\frac{x^{(n)}+ip^{(n)}}{\sqrt{2}}|n\rangle. \quad (127)$$

$$|\tilde{\psi}_z\rangle = \sum_{n=1}^{F}\frac{x^{(n)}+ip^{(n)}}{\sqrt{2}}|n\rangle\,. \quad (26)$$

Eq (26) on the right came from Note-On-Mar16-2022-BeijingTime.pdf.

The $\mathrm{U}(F)$ constraint coordinate-momentum phase space of the $(2F-1)$-dimensional sphere is diffeomorphic to $\mathrm{U}(F)/\mathrm{U}(F-1)$. (The difference between $\mathrm{U}(F)$ and $\mathrm{SU}(F)\times\mathrm{U}(1)$ is excluded by the division over $\mathrm{U}(F-1)$.) Comparison of $\hat{K}_{\mathrm{ele}}^{\mathrm{SU}(F)}(\boldsymbol{\theta},\boldsymbol{\varphi};s)$ to $\hat{K}_{\mathrm{ele}}(\mathbf{x},\mathbf{p};\gamma)$ implies that the two kernels are closely related. The correspondence between parameters $s$ and $\gamma$ reads

$$1+F\gamma=(1+F)^{(1+s)/2}\ . \quad (128)$$

$$2(1+F\gamma)=(1+F)^{(1+s)/2}. \quad (33)$$

Eq (33) on the right came from Note-On-Mar16-2022-BeijingTime.pdf, although there was a typo in eq (33), which was corrected in Appendix 3. We also noted the same equation in the previous document Note-on-August26-2021-BeijingTime.pdf (on page 4 of it), where the result was correct, where \alpha in Note-on-August26-2021-BeijingTime.pdf is (1+s)/2 in eq (33).

$$\gamma_\alpha \equiv \frac{(1+F)^\alpha-1}{F}\in\left(-\frac{1}{F},+\infty\right),\ \text{when}\ \alpha\in\mathbb{R}.$$

It is evident (from eq 128, the relation between constraint coordinate-momentum phase space and the $\mathrm{SU}(F)$ Stratonovich phase space) that parameter $s$ can be any real number in eq 123, *not* limited to $s=1,0$, or $-1$, where the corresponding value of parameter $\gamma$ of constraint coordinate-momentum phase space is $\gamma=1,\left(\sqrt{1+F}-1\right)/F$, or $0$. This has been clearly mentioned in refs [57, 58, 134].

Any normalized pure state of the $F$-dimensional Hilbert space uniquely corresponds to a state on constraint coordinate-momentum phase space, $|\mathbf{x},\mathbf{p}\rangle$, which is equivalent to $\exp[i\psi]|\boldsymbol{\theta},\boldsymbol{\varphi}\rangle$ with $\psi$ as the global phase. That is, the correspondence between $(\boldsymbol{\theta},\boldsymbol{\varphi})$ and $(\mathbf{x},\mathbf{p})$ is

$$\begin{pmatrix}x^{(n)}\\ p^{(n)}\end{pmatrix}=\sqrt{2(1+F\gamma)}\begin{pmatrix}\cos\psi & -\sin\psi\\ \sin\psi & \cos\psi\end{pmatrix}\begin{pmatrix}\mathrm{Re}\langle n|\boldsymbol{\theta},\boldsymbol{\varphi}\rangle\\ \mathrm{Im}\langle n|\boldsymbol{\theta},\boldsymbol{\varphi}\rangle\end{pmatrix}\ . \quad (129)$$

$$x^{(n)} = \sqrt{2}\times(1+F)^{(1+s)/4}\mathrm{Re}\,\langle n|\psi_z\rangle\,,$$
$$p^{(n)} = \sqrt{2}\times(1+F)^{(1+s)/4}\mathrm{Im}\,\langle n|\psi_z\rangle\,; \quad (31)$$

when $n=F$ the constrain of the circle is

$$(x^{(F)})^2+(p^{(F)})^2=2(1+F)^{(1+s)/2}\cos^2\theta_{F-1}. \quad (32)$$

Eqs (31)-(32) on the right came from Note-On-Mar16-2022-BeijingTime.pdf.

There were typos in eqs (31)&(32), we corrected them in Appendix 3.

Under the transformation, eq 129, mapping functions $A_C(\boldsymbol{\theta},\boldsymbol{\varphi};s)=\mathrm{Tr}\left[\hat{A}\,\hat{K}_{\mathrm{ele}}^{\mathrm{SU}(F)}(\boldsymbol{\theta},\boldsymbol{\varphi};s)\right]$ and $A_C(\mathbf{x},\mathbf{p};\gamma)=\mathrm{Tr}\left[\hat{A}\,\hat{K}_{\mathrm{ele}}(\mathbf{x},\mathbf{p};\gamma)\right]$ of an operator $\hat{A}$ share the same value. The global phase, $\psi$, which is missing in the $\mathrm{SU}(F)$ Stratonovich phase space, however, is important for the expression of quantum dynamics.

When we consider quantum dynamics in a finite $F$-dimensional Hilbert space, if the Hamiltonian operator includes linear components beyond the identity operator and generator operators of phase space group, it is impossible to derive trajectory-based exact dynamics. The $\mathrm{SU}(2)$ group involves the identity operator and angular momentum operators as generators on $\mathbb{S}^2$ sphere. It produces trajectory-based exact dynamics only for two-state systems, but fails to do so for all $F>2$ cases. It is claimed that trajectory-based dynamics is a good approximation for the large spin limit ( $F \to \infty$ ) though [109, 111, 302]. Except for the $F = 2$ case, the expression of quantum dynamics on the $\mathrm{SU}(2)$ Stratonovich phase space has no direct relation to the trajectory-based exact dynamics on constrained coordinate-momentum phase space.

The $\mathrm{SU}(F)$ Stratonovich phase space, however, produces trajectory-based exact dynamics for the finite $F$-dimensional Hilbert space. This is because that the evolution generated by any Hamiltonian of the $F$-dimensional Hilbert space is the action of some group element of $\mathrm{SU}(F)$.[303] The inherent symplectic structure of Stratonovich phase space indicates that the trajectory-based exact dynamics can be produced by the corresponding mapping Hamiltonian function $H_C = \mathrm{Tr}[\hat{H}\hat{K}_{\mathrm{ele}}^{\mathrm{SU}(F)}(\theta,\varphi;s)]$, i.e.,

$$\begin{cases} \dot{\theta}_i = -\sum_{j=1}^{F-1} \frac{A_{ji}}{(1+F)^{(1+s)/2}} \frac{\partial H_C}{\partial \varphi_j} \\ \dot{\varphi}_i = +\sum_{j=1}^{F-1} \frac{A_{ij}}{(1+F)^{(1+s)/2}} \frac{\partial H_C}{\partial \theta_j} \end{cases} \qquad 130$$

The elements, $\{A_{ij}\}$, of the $(F-1)\times(F-1)$ matrix, $\mathbf{A}$, are

$$A_{ij} = \begin{cases} \frac{1}{2}\csc(2\theta_1)\csc^2\theta_{F-1}\prod_{k=2}^{F-2}\sec^2\theta_k, & i=j=1; \\ -\frac{1}{2}\cot(2\theta_1)\csc^2\theta_{F-1}\prod_{k=2}^{F-2}\sec^2\theta_k, & (i-1)=j=1; \\ \csc(2\theta_i)\csc^2\theta_{F-1}\prod_{k=i+1}^{F-2}\sec^2\theta_k, & 2\le i=j\le F-2; \\ -\frac{1}{2}\cot(\theta_i)\csc^2\theta_{F-1}\prod_{k=i+1}^{F-2}\sec^2\theta_k, & 2\le(i-1)=j\le F-2; \\ -\csc(2\theta_{F-1}), & i=j=(F-1). \end{cases} \qquad 131$$

$$\dot{z}^k = \sigma^{kl}\partial_l f_{\hat{H}}(z), \qquad (45)$$

$$\sigma^{ij} = (1+F)^{-\frac{1+s}{2}}\begin{pmatrix} 0 & -\boldsymbol{A}^{\mathrm{T}} \\ \boldsymbol{A} & 0 \end{pmatrix}, \qquad (66)$$

$$\boldsymbol{A}^{ij} = \begin{cases} \frac{1}{2}\csc(2\theta_1)\csc^2\theta_{F-1}\prod_{k=2}^{F-2}\sec^2\theta_k, & i=j=1; \\ -\frac{1}{2}\cot(2\theta_1)\csc^2\theta_{F-1}\prod_{k=2}^{F-2}\sec^2\theta_k, & (i-1)=j=1; \\ \csc(2\theta_i)\csc^2\theta_{F-1}\prod_{k=i+1}^{F-2}\sec^2\theta_k, & 2\le i=j\le F-2; \\ -\frac{1}{2}\cot(\theta_i)\csc^2\theta_{F-1}\prod_{k=i+1}^{F-2}\sec^2\theta_k, & 2\le(i-1)=j\le F-2; \\ -\csc(2\theta_{F-1}), & i=j=(F-1). \end{cases} \qquad (67)$$

Eqs (45),(66)-(67) on the right came from Note-On-Mar16-2022-BeijingTime.pdf, where eq 130 of Appendix 3 on the right was the combination of eqs (45)&(66) on the right.

The explicit expression of the EOMs of eq 130 is, however, much complicated. In addition, because trigonometric functions are involved in eq 131, singularities are inevitable in the EOMs on the $\mathrm{SU}(F)$ Stratonovich phase space for $F > 2$. This makes the expression of quantum dynamics on the $\mathrm{SU}(F)$ Stratonovich phase space numerically unfavorable. In comparison, on (weighted) constrained coordinate-momentum phase space, Hamilton's EOMs are simply linear in derivatives with coefficients independent of phase variables, as well as exact.

The relation of eq 129 implies that there exists a one-to-one correspondence between exact trajectory-base dynamics on the $\mathrm{SU}(F)$ Stratonovich phase space and that on constraint coordinate-momentum phase space.

Eqs (53),(54) on the right came from Note-On-Mar16-2022-BeijingTime.pdf.

Eqs 132-135 of Appendix 3 is the combination of eqs (53),(54) on the right and the equations of motion (eqs 130&131 of Appendix 3 listed on the left of the previous page).

The addition of the global phase, $\psi$ , is critical to obtain the one-to-one correspondence. The EOM of $\psi$ reads

$$\dot{\psi} = \left[ -\frac{\partial}{\partial \lambda} + \frac{\tan\theta_{F-1}}{2\lambda}\frac{\partial}{\partial \theta_{F-1}} \right] H_C^{(\lambda)}(\boldsymbol{\theta},\boldsymbol{\varphi};s) \Big|_{\lambda=(1+F)^{\frac{1+s}{2}}} , \quad 132$$

where the extended mapping Hamiltonian function is defined by

$$H_C^{(\lambda)}(\boldsymbol{\theta},\boldsymbol{\varphi};s) = \mathrm{Tr}\left[ \hat{K}_{\mathrm{ele}}^{\mathrm{SU}(F),(\lambda)}(\boldsymbol{\theta},\boldsymbol{\varphi};s)\hat{H} \right] \quad 133$$

for the extended $\mathrm{SU}(F)$ Stratonovich mapping 'kernel'

$$\hat{K}_{\mathrm{ele}}^{\mathrm{SU}(F),(\lambda)}(\boldsymbol{\theta},\boldsymbol{\varphi};s) = \lambda |\boldsymbol{\theta},\boldsymbol{\varphi}\rangle\langle\boldsymbol{\theta},\boldsymbol{\varphi}| + \frac{\hat{I}}{F}\left( 1-(1+F)^{\frac{1+s}{2}} \right) . \quad 134$$

In eq 134 $\lambda$ is treated as an 'invariant' variable. The evolution of state $\sqrt{\lambda}e^{i\psi}|\boldsymbol{\theta},\boldsymbol{\varphi}\rangle \equiv |\mathbf{x},\mathbf{p}\rangle$ generates

$$\begin{cases} \dot{\lambda} = \dfrac{\partial}{\partial \psi} H_C^{(\lambda)}(\boldsymbol{\theta},\boldsymbol{\varphi};s) = 0 \\ \dot{\psi} = \left[ -\dfrac{\partial}{\partial \lambda} + \dfrac{\tan\theta_{F-1}}{2\lambda}\dfrac{\partial}{\partial \theta_{F-1}} \right] H_C^{(\lambda)}(\boldsymbol{\theta},\boldsymbol{\varphi};s) \\ \dot{\theta}_i = -\displaystyle\sum_{j=1}^{F-1} \dfrac{A_{ji}}{\lambda}\dfrac{\partial}{\partial \varphi_j} H_C^{(\lambda)}(\boldsymbol{\theta},\boldsymbol{\varphi};s) - \delta_{i,F-1}\dfrac{\tan\theta_{F-1}}{2\lambda}\dfrac{\partial}{\partial \psi} H_C^{(\lambda)}(\boldsymbol{\theta},\boldsymbol{\varphi};s) \\ \dot{\varphi}_i = +\displaystyle\sum_{j=1}^{F-1} \dfrac{A_{ij}}{\lambda}\dfrac{\partial}{\partial \theta_j} H_C^{(\lambda)}(\boldsymbol{\theta},\boldsymbol{\varphi};s) \end{cases} . \quad 135$$

It is straightforward to show that under the bijection,

$$\begin{pmatrix} x^{(n)} \\ p^{(n)} \end{pmatrix} = \sqrt{2\lambda} \begin{pmatrix} \cos\psi & -\sin\psi \\ \sin\psi & \cos\psi \end{pmatrix} \begin{pmatrix} \mathrm{Re}\langle n|\boldsymbol{\theta},\boldsymbol{\varphi}\rangle \\ \mathrm{Im}\langle n|\boldsymbol{\theta},\boldsymbol{\varphi}\rangle \end{pmatrix} , \quad 136$$

between variables $(\lambda,\psi,\boldsymbol{\theta},\boldsymbol{\varphi})$ and $(\mathbf{x},\mathbf{p})$, eq 135 leads to the EOMS of phase variables of (weighted) constraint phase space

$$\dot{x}^{(n)} = +\frac{\partial H_C}{\partial p^{(n)}} \qquad \dot{p}^{(n)} = -\frac{\partial H_C}{\partial x^{(n)}} \quad 137$$



$$\begin{pmatrix} \dot{\lambda} \\ \dot{\varphi} \\ \dot{\tilde{z}}^k \end{pmatrix} = \begin{pmatrix} 0 & 1 & \\ -1 & 0 & \\ & & \sigma^{kl} \end{pmatrix} \begin{pmatrix} \partial_\lambda \\ \partial_\varphi \\ \partial_l \end{pmatrix} f_{\hat{H}}(\lambda,\tilde{z}). \quad (54)$$

$$\hat{K}(\lambda,\tilde{z}) = \lambda|\psi_{\tilde{z}}\rangle\langle\psi_{\tilde{z}}| + \mu\hat{1}. \quad (53)$$

Eqs (70-74) on the right came from Note-On-Mar16-2022-BeijingTime.pdf, which demonstrated the variable transform between the SU(F)/U(F-1) Stratonovich phase space and the constrained coordinate-momentum phase space. The variable transform must include the evolving global phase \psi and the additional variable \lambda.

$$\dot{\xi}^k = \frac{\partial\xi^k}{\partial\zeta^l}\dot{\zeta}^l \quad (70)$$

and

$$\tilde{\partial}_k \equiv \frac{\partial}{\partial\xi^k} = \frac{\partial\zeta^l}{\partial\xi^k}\frac{\partial}{\partial\zeta^l} \equiv \frac{\partial\zeta^l}{\partial\xi^k}\partial_l. \quad (71)$$

Noting the symplectic matrix in eq.(54) $\omega^{kl}$, eq.(54) becomes

$$\dot{\xi}^k = \frac{\partial\zeta^k}{\partial\xi^i}\frac{\partial\zeta^l}{\partial\xi^j}\omega^{ij}\tilde{\partial}_l f_{\hat{H}}(\xi) = \tilde{\omega}^{kl}\tilde{\partial}_l f_{\hat{H}}(\xi). \quad (72)$$

The explicit form of $\xi$ is $\xi = (x^{(1)}, p^{(1)}, \ldots, x^{(F)}, p^{(F)})$. The coordinate transform from $\zeta$ to $\xi$ is defined such that the state $|\tilde{\psi_z}\rangle$ in eq.(26) equals to the state $\sqrt{\lambda}e^{-i\varphi}|\psi_z\rangle$, where $|\psi_z\rangle$ is defined in eq.(22). The result of the matrix $\omega^{kl}$ is

$$\omega^{kl} = \begin{pmatrix} 0 & 1 & & & \\ -1 & 0 & & & \\ & & \ddots & & \\ & & & 0 & 1 \\ & & & -1 & 0 \end{pmatrix}, \quad (73)$$

which gives the pleasing equation of motion

$$\dot{x}^{(n)} = +\frac{\partial}{\partial p^{(n)}} f_{\hat{H}}(x,p), \qquad \dot{p}^{(n)} = -\frac{\partial}{\partial x^{(n)}} f_{\hat{H}}(x,p). \quad (74)$$

( see the last page )

$$\dot{x}^{(n)} = \sum_{i=1}^{2F} \frac{\partial x^{(n)}}{\partial z_i} \dot{z}_i$$
$$\dot{p}^{(n)} = \sum_{i=1}^{2F} \frac{\partial p^{(n)}}{\partial z_i} \dot{z}_i \qquad 138$$

and

$$\frac{\partial H_C}{\partial z_i} = \sum_{n=1}^{F} \frac{\partial x^{(n)}}{\partial z_i} \frac{\partial H_C}{\partial x^{(n)}} + \sum_{n=1}^{F} \frac{\partial p^{(n)}}{\partial z_i} \frac{\partial H_C}{\partial p^{(n)}} , \qquad 139$$

where $\{z_i\}$ denote variables $\{\lambda, \psi, \boldsymbol{\theta}, \boldsymbol{\varphi}\}$.

### 4. Marginal distribution functions on symmetrically weighted coordinate-momentum phase space

As demonstrated in Figure 5, the marginal distribution functions on symmetrically weighted constraint coordinate-momentum phase space demonstrate a hollow structure. Equation 50 leads to the marginal functions on symmetrically weighted coordinate-momentum phase space

$$\begin{aligned}
\mathcal{K}_{\uparrow\uparrow}(x^{(1)},x^{(2)}) &= \frac{1-2\Delta^2+2\Delta}{4\Delta}\frac{1+(x^{(1)})^2/2-(x^{(2)})^2/2}{2\pi(1+2\Delta)}\bigg|_{(x^{(1)})^2+(x^{(2)})^2\le 2(1+2\Delta)} \\
&\quad -\frac{1-2\Delta^2-2\Delta}{4\Delta}\frac{1+(x^{(1)})^2/2-(x^{(2)})^2/2}{2\pi(1-2\Delta)}\bigg|_{(x^{(1)})^2+(x^{(2)})^2\le 2(1-2\Delta)} \\
\mathcal{K}_{\uparrow\downarrow}(x^{(1)},x^{(2)}) = \mathcal{K}_{\downarrow\uparrow}(x^{(1)},x^{(2)}) &= \frac{1-2\Delta^2+2\Delta}{4\Delta}\frac{x^{(1)}x^{(2)}}{2\pi(1+2\Delta)}\bigg|_{(x^{(1)})^2+(x^{(2)})^2\le 2(1+2\Delta)} \\
&\quad -\frac{1-2\Delta^2-2\Delta}{4\Delta}\frac{x^{(1)}x^{(2)}}{2\pi(1-2\Delta)}\bigg|_{(x^{(1)})^2+(x^{(2)})^2\le 2(1-2\Delta)} \\
\mathcal{K}_{\downarrow\downarrow}(x^{(1)},x^{(2)}) &= \frac{1-2\Delta^2+2\Delta}{4\Delta}\frac{1-(x^{(1)})^2/2+(x^{(2)})^2/2}{2\pi(1+2\Delta)}\bigg|_{(x^{(1)})^2+(x^{(2)})^2\le 2(1+2\Delta)} \\
&\quad -\frac{1-2\Delta^2-2\Delta}{4\Delta}\frac{1-(x^{(1)})^2/2+(x^{(2)})^2/2}{2\pi(1-2\Delta)}\bigg|_{(x^{(1)})^2+(x^{(2)})^2\le 2(1-2\Delta)}
\end{aligned} \qquad 140$$

As $\Delta \to 0^+$, $\mathcal{K}_{nm}(x^{(1)},x^{(2)})$ approaches zero in region $(x^{(1)})^2+(x^{(2)})^2 \le 2(1-F\Delta)$, yielding the hollow structure.



## Additional Note

In Note-On-Mar16-2022-BeijingTime.pdf, we derived the equations of motion of the trajectory based on the inherent symplectic structure of phase space. It came from the fact that the orbital on the co-adjoint representation of any Lie group is a symplectic manifold. Trajectory-based dynamics is exact when the Hamiltonian belongs to the Lie algebra of the related Lie group of the phase space manifold (in terms of the covariant relation of Stratonovich-Weyl (SW) correspondence, see e.g., C. Brif and A. Mann. Phase-space formulation of quantum mechanics and quantum-state reconstruction for physical systems with Lie-group symmetries. Phys. Rev. A 59, 971–987 (1999). doi: 10.1103/physreva.59.971. ref 107 of CMS-842.R1_Proof_hi.pdf and ref 4 of Note-On-Mar16-2022-BeijingTime.pdf).

The theory was reviewed in Section 3 of Note-On-Mar16-2022-BeijingTime.pdf. Consider the SU(F)/U(F-1) Stratonovich phase space, which is a symplectic manifold, as discussed in detail in Bona's book in 2020, Chapter 2 (P. Bóna. Classical Systems in Quantum Mechanics. (Springer International Publishing, 2020). doi: 10.1007/978-3-030-45070-0. Ref 303 of CMS-842.R1_Proof_hi.pdf and ref 5 of Note-On-Mar16-2022-BeijingTime.pdf ). In order to obtain the explicit form of the symplectic structure, we employed the method introduced by Provost in 1980 (J. P. Provost and G. Vallee. “Riemannian structure on manifolds of quantum states”. Commun. Math. Phys. 76, 289–301 (1980). doi: 10.1007/bf02193559. Ref 14 of Note-On-Mar16-2022-BeijingTime.pdf). With Provost’s method, we straightforwardly achieved the explicit form of EOMs of trajectory-based dynamics from the parameterization method of the coherent state by Tilma (J. Phys. Math. Theor. 45, 015302 (2012), doi: 10.1088/1751-8113/45/1/015302.). Unfortunately, it is well known from differential geometry (differential manifold) that there exists no global non-singular frame on most manifolds, including the SU(F)/U(F-1) Stratonovich phase space. That is, it is evitable to meet singularities for trajectory-based dynamics on the SU(F)/U(F-1) Stratonovich phase space.