

HOA (Heaviside Operational Ansatz) revisited: recent remarks on novel exact solution methodologies in wavefunction analysis

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Abstract A viable methodology for the exact analytical solution of the multiparticle Schrodinger and Dirac equations has long been considered a holy grail of theoretical chemistry. Since a benchmark work by Torres-Vega and Frederick in the 1990s, the QPSR (Quantum Phase Space Representation) has been explored as an alternate method for solving various physical systems. Recently, the present author has developed an exact analytical symbolic solution scheme for broad classes of differential equations utilizing the HOA (Heaviside Operational Ansatz). An application of the scheme to chemical systems was initially presented in Journal of Mathematical Chemistry (Toward chemical applications of Heaviside Operational Ansatz: exact solution of radial Schrodinger equation for nonrelativistic N-particle system with pairwise $1/r(I)$ radial potential in quantum phase space. Journal of Mathematical Chemistry, 2009; 45(1):129–140). It is believed that the coupling of HOA with QPSR represents not only a fundamental breakthrough in theoretical physical chemistry, but it is promising as a basis for exact solution algorithms that would have tremendous impact on the capabilities of computational chemistry/physics. The novel methods allow the exact determination of the momentum [and configuration] space wavefunction from the QPSR wavefunction by way of a Fourier transform. In this note some remarks, examples and further directions, concerning HOA as a tool to solve and provide analytical insight into solutions of dynamical systems occurring in, but not limited to Mathematical Chemistry, are also posited.

Keywords Heaviside operators · Integral transforms · Quantum dynamics · Classical dynamics: quantum phase space · Differential equations · Exact analytical solution · Quantum chemistry · Molecular Hamiltonian · Dirac · Majorana · Functional

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differential equations · Relativistic · Schrodinger equation · Generalised Hamiltonian principle · Inhomogeneous Lagrange equation · Equations of motion · Shannon entropy · Wavelet transform · Cepstral analysis · Ehrenfest's theorem

1 Introduction

A viable methodology for the exact analytical solution of the multiparticle Schrodinger and Dirac equations has long been considered a holy grail of theoretical chemistry. Since a benchmark work by Torres-Vega and Frederick [1] in the 1990s, the QPSR has been explored as an alternate method for solving various physical systems, including the harmonic oscillator [2], Morse oscillator [3], one-dimensional hydrogen atom [4], and classical Liouville dynamics under the Wigner function [5]. QPSR approaches are particularly challenging because of the complexity of phase space wave functions and the fact that the number of coordinates doubles in the phase space representation. These challenges have heretofore prevented the exact solution of the multiparticle equation in phase space. Recently, Simpao [6] has developed an exact analytical symbolic solution scheme for broad classes of differential equations utilizing the HOA. It is proposed to apply this novel methodology to QPSR problems to obtain exact solutions for real chemical systems and their dynamics. In his preliminary work, Simpao [6] has already applied this method to a number of simple systems, including the harmonic oscillator, with solutions in agreement to those obtained by Li [2–5]. He has also demonstrated the exact solution to the radial Schrodinger equation for an N-particle system with pairwise Coulomb interaction [7]. In addition to the Schrodinger equation, the HOA method is capable of treating the Dirac equation [8] as well as differential systems governing both relativistic and non-relativistic particle dynamics. Applying these methods would allow us to pursue further exploration of this methodology, starting with the exact solution of multielectron atoms and moving toward complex molecules and reaction dynamics. It is believed that the coupling of HOA with QPSR represents not only a fundamental breakthrough in theoretical physical chemistry, but it is promising as a basis for exact solution algorithms that would have tremendous impact on the capabilities of computational chemistry/physics. As the theoretical foundation for spectroscopy is the Schrodinger equation, the significance of this discovery to the enhanced analysis of spectroscopic data is obvious. For example, the analysis of the Compton line in momentum spectroscopy necessitates the consideration of the momentum wavefunction for the molecular system under study. The novel methods [6–8] allow the exact determination of the momentum [and configuration] space wavefunction from the QPSR wavefunction by way of a Fourier transform. For example, the primary focus of [7] is the pairwise $1/r_{ij}$ interaction in context of the radial equation in the nonrelativistic Schrodinger case. This application of the exact solution ansatz developed above corresponds to the problem of n-particles with pairwise Coulomb interaction; scaling the parameters and variables of the problem yields the exact solution of the QPSR Schrodinger equation for the first-principles general polyatomic molecular Hamiltonian. Upon a straightforward slight adaptation of this non-relativistic Schrodinger result, the QPSR Dirac equation addressed in [8] imme-

diately yields the relativistic counterpart for the first-principles general polyatomic molecular Hamiltonian solution. These results form the cornerstone of the exact solution to the quantum dynamics of particular chemical systems, which shall appear elsewhere. Although all of the examples of dynamical systems mentioned above are at once solved as a special case of the general integral method already published in HOA, it is illuminating for applications to write out the solutions as the integrals are evaluated explicitly for the same. The HOA result is currently being used as the primary algorithm in the development of computer programs known as ‘solver engines’ for quantum chemistry/physics and plethora applications: to be reported elsewhere.

In this note some remarks, examples and further directions, concerning HOA as a tool to solve and provide analytical insight into solutions of dynamical systems occurring in, but not limited to Mathematical Chemistry, are posited. Among these more general considerations are the development of novel exact analytical solutions of generalised Hamiltonian/Lagrangian dynamical systems in the QPSR and classical connections; also the exact analytical solutions of attendant differential/difference equations. Though some new results are presented at the end of the Recap and the Section on generalised Hamiltonian–Lagrangian nexus later in the examples, the detailed treatment of these and many others shall appear elsewhere. The foundations of the HOA scheme will be sketched and some examples given in these Remarks, that will illustrate some of the numerous and sundry analyses that can be enhanced by HOA methods. For convenience, we begin with a recap of the HOA construction following from [6].

2 Recap of HOA

Here are the basic relations; x, p, t are respectively the configuration space position, momentum and time variables. The $\hat{}$ denotes the operators, with H and Ψ denoting the Hamiltonian and wavefunction of the phase space representation [1], respectively. Also, the α, γ , are otherwise free parameters as specified in [1].

$$\begin{aligned}
 H(x, p, t) &\rightarrow \hat{H}(\hat{x}, \hat{p}, t) = \hat{H}(i\hbar\partial_p + \alpha x, -i\hbar\partial_x + \gamma p, t), \ni \alpha + \gamma = 1 \\
 x &\rightarrow \hat{x} \equiv i\hbar\partial_p + \alpha x, p \rightarrow \hat{p} \equiv -i\hbar\partial_x + \gamma p, t \rightarrow t = t \\
 (x_1, \dots, x_n) &\rightarrow (\hat{x}_1, \dots, \hat{x}_n) = (i\hbar\partial_{p_1} + \alpha_1 x_1, \dots, i\hbar\partial_{p_n} + \alpha_n x_n), \\
 &\ni \alpha_j + \gamma_j = 1, j = 1, \dots, n \\
 (p_1, \dots, p_n) &\rightarrow (\hat{p}_1, \dots, \hat{p}_n) = (-i\hbar\partial_{x_1} + \gamma_1 p_1, \dots, -i\hbar\partial_{x_n} + \gamma_n p_n) \\
 H(x_1, \dots, x_n; p_1, \dots, p_n; t) &\rightarrow \hat{H}(\hat{x}_1, \dots, \hat{x}_n; \hat{p}_1, \dots, \hat{p}_n; t) \\
 &\equiv \hat{H}(i\hbar\partial_{p_1} + \alpha_1 x_1, \dots, i\hbar\partial_{p_n} + \alpha_n x_n; -i\hbar\partial_{x_1} + \gamma_1 p_1, \dots, -i\hbar\partial_{x_n} + \gamma_n p_n; t)
 \end{aligned} \tag{1}$$

Now with the following properties of Heaviside operational methods via Laplace transforms [6]

$$\begin{aligned}
 L_{y \rightarrow z}[f(y)] &= \int_{y_0}^{\infty} f(y)e^{-yz} dy = \check{f}(z) \\
 L_{z \rightarrow y}^{-1}[\check{f}(z)] &= \frac{1}{2\pi i} \oint_{\partial} \check{f}(z)e^{yz} dz = f(y) \\
 L_{z \rightarrow y}^{-1}[\check{f}(z)] &= \frac{1}{2\pi i} \oint_{\partial} \check{f}(z)e^{yz} dz = f(y) = \check{f}(D_y)U(y) \\
 L_{z \rightarrow y}^{-1}[\check{f}_1(z)\check{f}_2(z)] &= f_1(y) * f_2(y) = \int_{y_0}^y f_1(y-u)f_2(u)du \\
 &= \check{f}_1(D_y)\check{f}_2(D_y)U(y) = \check{f}_1(D_y)f_2(y)
 \end{aligned}$$

where $U(y)$ is the Heaviside Unit Step function

$$\begin{aligned}
 &L_{(y_1, \dots, y_n) \rightarrow (z_1, \dots, z_n)}[f(y_1, \dots, y_n)] \\
 &= \int_{y_{0n}}^{\infty} \underbrace{\dots}_n \int_{y_{01}}^{\infty} f(y_1, \dots, y_n)e^{-\sum_{j=1}^n y_j z_j} dy_1 \dots dy_n = \check{f}(z_1, \dots, z_n) \\
 &L_{(z_1, \dots, z_n) \rightarrow (y_1, \dots, y_n)}^{-1}[\check{f}(z_1, \dots, z_n)] \\
 &= \left(\frac{1}{2\pi i}\right)^n \oint_{\partial^n} \check{f}(z_1, \dots, z_n)e^{\sum_{j=1}^n y_j z_j} dz_1 \dots dz_n = f(y_1, \dots, y_n) \\
 &L_{(z_1, \dots, z_n) \rightarrow (y_1, \dots, y_n)}^{-1}[\check{f}_1(z_1, \dots, z_n)\check{f}_2(z_1, \dots, z_n)] \\
 &= f_1(y_1, \dots, y_n) \underbrace{*}_{(y_1, \dots, y_n)} f_2(y_1, \dots, y_n) \\
 &= \int_{y_{0n}}^{y_n} \underbrace{\dots}_n \int_{y_{01}}^{y_1} f_1(y_1 - y'_1, \dots, y_n - y'_n)f_2(y'_1, \dots, y'_n)dy'_1 \dots dy'_n \\
 &= \check{f}_1(\partial_{y_1}, \dots, \partial_{y_n})\check{f}_2(\partial_{y_1}, \dots, \partial_{y_n})U(y_1, \dots, y_n) \\
 &= \check{f}_1(\partial_{y_1}, \dots, \partial_{y_n})f_2(y_1, \dots, y_n) \tag{2}
 \end{aligned}$$

where the zero-subscripted variables (e.g., y_0) are the arbitrarily specified lower limits of integration.

With the phase-space convolution

$$\begin{aligned}
 &f_1(x_1, \dots, x_n; p_1, \dots, p_n) \underbrace{*}_{(x_1, \dots, x_n; p_1, \dots, p_n)} f_2(x_1, \dots, x_n; p_1, \dots, p_n) \\
 &= \int_{x_{0n}}^{x_n} \underbrace{\dots}_n \int_{x_{01}}^{x_1} \int_{p_{0n}}^{p_n} \underbrace{\dots}_n \int_{p_{01}}^{p_1} f_1(x_1 - x'_1, \dots, x_n - x'_n; p_1 - p'_1, \dots, p_n - p'_n) \\
 &\quad \times f_2(x'_1, \dots, x'_n; p'_1, \dots, p'_n)dx'_1 \dots dx'_n dp'_1 \dots dp'_n \tag{3}
 \end{aligned}$$

Lower bounds of respective phase space co-ordinates: $(x_{10}, \dots, x_{n0}; p_{10}, \dots, p_{n0})$
 Also the transform relation

$$L_{z \rightarrow y}[\check{f}(az - b)] = \frac{1}{a} e^{\frac{by}{a}} f\left(\frac{y}{a}\right)$$

$$L_{(z_1, \dots, z_n) \rightarrow (y_1, \dots, y_n)}[\check{f}(a_1 z_1 - b_1, \dots, a_n z_n - b_n)] = \prod_{j=1}^n \frac{1}{a_j} e^{\frac{b_j}{a_j} y_j} f\left(\frac{y_1}{a_1}, \dots, \frac{y_n}{a_n}\right) \tag{4}$$

From (1) the wave equation becomes

$$\hat{H} \left(\begin{matrix} i\hbar \partial_{p_1} + \alpha_1 x_1, \dots, i\hbar \partial_{p_n} + \alpha_n x_n; \\ -i\hbar \partial_{x_1} + \gamma_1 p_1, \dots, -i\hbar \partial_{x_n} + \gamma_n p_n; t \end{matrix} \right) \Psi(x_1, \dots, x_n; p_1, \dots, p_n; t)$$

$$= i\hbar \partial_t \Psi(x_1, \dots, x_n; p_1, \dots, p_n; t) \tag{5}$$

Applying the convolution identity and multivariable inverse transform of (2), the phase space convolution of (3) and relation (4) yields

$$\left[L_{\left(\begin{matrix} \partial_{x_1}, \dots, \partial_{x_n} \\ \rightarrow (x_1, \dots, x_n) \end{matrix} \right)}^{-1} \left[L_{\left(\begin{matrix} \partial_{p_1}, \dots, \partial_{p_n} \\ \rightarrow (p_1, \dots, p_n) \end{matrix} \right)}^{-1} \left[\hat{H} \left(\begin{matrix} i\hbar \partial_{p_1} + \alpha_1 x_1, \dots, i\hbar \partial_{p_n} + \alpha_n x_n; \\ -i\hbar \partial_{x_1} + \gamma_1 p_1, \dots, -i\hbar \partial_{x_n} + \gamma_n p_n; t \end{matrix} \right) \right] \right] \right]$$

$$\underbrace{\Psi(x_1, \dots, x_n; p_1, \dots, p_n; t)}_{(x_1, \dots, x_n; p_1, \dots, p_n)}$$

$$\equiv \hat{H} \left(\begin{matrix} i\hbar \partial_{p_1} + \alpha_1 x_1, \dots, i\hbar \partial_{p_n} + \alpha_n x_n; \\ -i\hbar \partial_{x_1} + \gamma_1 p_1, \dots, -i\hbar \partial_{x_n} + \gamma_n p_n; t \end{matrix} \right) \Psi(x_1, \dots, x_n; p_1, \dots, p_n; t) \tag{6}$$

Applying (6)–(5) with the convolution identities in (2) and transforming

$$L_{\left(\begin{matrix} (p_1, \dots, p_n) \\ \rightarrow (\bar{p}_1, \dots, \bar{p}_n) \end{matrix} \right)} \left[L_{\left(\begin{matrix} (x_1, \dots, x_n) \\ \rightarrow (\bar{x}_1, \dots, \bar{x}_n) \end{matrix} \right)} \left[\hat{H} \left(\begin{matrix} i\hbar \partial_{p_1} + \alpha_1 x_1, \dots, i\hbar \partial_{p_n} + \alpha_n x_n; \\ -i\hbar \partial_{x_1} + \gamma_1 p_1, \dots, -i\hbar \partial_{x_n} + \gamma_n p_n; t \end{matrix} \right) \Psi(x_1, \dots, x_n; p_1, \dots, p_n; t) \right] \right]$$

$$\equiv L_{\left(\begin{matrix} (p_1, \dots, p_n) \\ \rightarrow (\bar{p}_1, \dots, \bar{p}_n) \end{matrix} \right)} \left[L_{\left(\begin{matrix} (x_1, \dots, x_n) \\ \rightarrow (\bar{x}_1, \dots, \bar{x}_n) \end{matrix} \right)} \left[L_{\left(\begin{matrix} \partial_{p_1}, \dots, \partial_{p_n} \\ \rightarrow (p_1, \dots, p_n) \end{matrix} \right)}^{-1} \left[L_{\left(\begin{matrix} \partial_{x_1}, \dots, \partial_{x_n} \\ \rightarrow (x_1, \dots, x_n) \end{matrix} \right)}^{-1} \left[\hat{H} \left(\begin{matrix} i\hbar \partial_{p_1} + \alpha_1 x_1, \dots, i\hbar \partial_{p_n} + \alpha_n x_n; \\ -i\hbar \partial_{x_1} + \gamma_1 p_1, \dots, -i\hbar \partial_{x_n} + \gamma_n p_n; t \end{matrix} \right) \right] \right] \right] \right]$$

$$\underbrace{\Psi(x_1, \dots, x_n; p_1, \dots, p_n; t)}_{(x_1, \dots, x_n; p_1, \dots, p_n)}$$

$$= i\hbar \partial_t \Psi(x_1, \dots, x_n; p_1, \dots, p_n; t)$$

$$\equiv \hat{H} \left(\begin{matrix} i\hbar \partial_{p_1} + \alpha_1 x_1, \dots, i\hbar \partial_{p_n} + \alpha_n x_n; \\ -i\hbar \partial_{x_1} + \gamma_1 p_1, \dots, -i\hbar \partial_{x_n} + \gamma_n p_n; t \end{matrix} \right) \begin{matrix} \partial_{p_1} \mapsto \bar{p}_1, \\ \dots, \partial_{p_n} \mapsto \bar{p}_n; \\ \partial_{x_1} \mapsto \bar{x}_1, \\ \dots, \partial_{x_n} \mapsto \bar{x}_n \end{matrix} \check{\Psi}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t)$$

$$= i\hbar \partial_t \check{\Psi}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t)$$

$$\equiv \hat{H} \left(\begin{matrix} i\hbar \partial_{\bar{p}_1} + \alpha_1 \bar{x}_1, \dots, i\hbar \partial_{\bar{p}_n} + \alpha_n \bar{x}_n; \\ -i\hbar \partial_{\bar{x}_1} + \gamma_1 \bar{p}_1, \dots, -i\hbar \partial_{\bar{x}_n} + \gamma_n \bar{p}_n; t \end{matrix} \right) \check{\Psi}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t) = i\hbar \partial_t \check{\Psi}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t) \tag{7}$$

Hence the wavefunction in phase space may be analytically expressed in exact quadratures, by inverse transforming the above solution $\tilde{\Psi}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t)$ of (7) as

$$\begin{aligned} & \hat{H} \left(\begin{array}{l} i\hbar\bar{p}_1 + \alpha_1 x_1, \dots, i\hbar\bar{p}_n + \alpha_n x_n; \\ -i\hbar\bar{x}_1 + \gamma_1 p_1, \dots, -i\hbar\bar{x}_n + \gamma_n p_n; t \end{array} \right) \tilde{\Psi}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t) \\ &= i\hbar \partial_t \tilde{\Psi}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t) \Psi(x_1, \dots, x_n; p_1, \dots, p_n; t) \\ &= L_{\substack{(\bar{x}_1, \dots, \bar{x}_n) \\ \rightarrow (x_1, \dots, x_n)}}^{-1} \\ & \left[L_{\substack{(\bar{p}_1, \dots, \bar{p}_n) \\ \rightarrow (p_1, \dots, p_n)}}^{-1} \left[e^{\frac{-i}{\hbar} \int_0^t \hat{H} \left(\begin{array}{l} i\hbar\bar{p}_1 + \alpha_1 x_1, \dots, i\hbar\bar{p}_n + \alpha_n x_n; \\ -i\hbar\bar{x}_1 + \gamma_1 p_1, \dots, -i\hbar\bar{x}_n + \gamma_n p_n; u \end{array} \right) du} \right] \right] \\ & \left[\times \tilde{\Psi}_0(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t = 0) \right] \end{aligned} \quad (8)$$

It is at this point that the analysis of HOA has been developed up to the time of this writing. A “New Twist” on this was recently [13 MAY 2010] discovered by Simpao: namely an alternative exact analytical quadrature expression for the quantum phase space wave function. By observing from (8) that

$$\begin{aligned} \Psi(x_1, \dots, x_n; p_1, \dots, p_n; t) &= L_{\substack{(\bar{x}_1, \dots, \bar{x}_n) \\ \rightarrow (x_1, \dots, x_n); \\ (\bar{p}_1, \dots, \bar{p}_n) \\ \rightarrow (p_1, \dots, p_n)}}^{-1} \\ & \left(\tilde{\Psi}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t) \right. \\ & \left. = \tilde{\Psi}_0(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t = 0) e^{\frac{-i}{\hbar} \int_0^t \hat{H} \left(\begin{array}{l} i\hbar\bar{p}_1 + \frac{1}{2}x_1, \dots, i\hbar\bar{p}_n + \frac{1}{2}x_n; \\ -i\hbar\bar{x}_1 + \frac{1}{2}p_1, \dots, -i\hbar\bar{x}_n + \frac{1}{2}p_n; u \end{array} \right) du} \right) \end{aligned} \quad (8a)$$

shifted Taylor series yields

$$\begin{aligned} & e^{\frac{-i}{\hbar} \int_0^t \hat{H} \left(\begin{array}{l} i\hbar\bar{p}_1 + \frac{1}{2}x_1, \dots, i\hbar\bar{p}_n + \frac{1}{2}x_n; \\ -i\hbar\bar{x}_1 + \frac{1}{2}p_1, \dots, -i\hbar\bar{x}_n + \frac{1}{2}p_n; u \end{array} \right) du} \\ &= e^{i\hbar\bar{p}_1 \partial_{\frac{1}{2}x_1} \dots i\hbar\bar{p}_n \partial_{\frac{1}{2}x_n}} e^{-i\hbar\bar{x}_1 \partial_{\frac{1}{2}p_1} \dots -i\hbar\bar{x}_n \partial_{\frac{1}{2}p_n}} \left(e^{\frac{-i}{\hbar} \int_0^t \hat{H} \left(\begin{array}{l} \frac{1}{2}x_1, \dots, \frac{1}{2}x_n; \\ \frac{1}{2}p_1, \dots, \frac{1}{2}p_n; u \end{array} \right) du} \right) \end{aligned} \quad (8b)$$

and Heaviside’s alternative to the convolution developed above yields

$$\begin{aligned}
 & e^{i\hbar\bar{p}_1\partial_{\frac{1}{2}x_1}\cdots i\hbar\bar{p}_n\partial_{\frac{1}{2}x_n}} e^{-i\hbar\bar{x}_1\partial_{\frac{1}{2}p_1}\cdots -i\hbar\bar{x}_n\partial_{\frac{1}{2}p_n}} \left(e^{-\frac{i}{\hbar}\int_0^t \hat{H}\left(\frac{1}{2}x_1, \dots, \frac{1}{2}x_n; \frac{1}{2}p_1, \dots, \frac{1}{2}p_n; u\right) du} \right) \\
 & \equiv \delta\left(\frac{1}{2}x_1 + i\hbar\bar{p}_1, \dots, \frac{1}{2}x_n + i\hbar\bar{p}_n\right) \delta\left(\frac{1}{2}p_1 - i\hbar\bar{x}_1, \dots, \frac{1}{2}p_n - i\hbar\bar{x}_n\right) \\
 & \quad \underbrace{\left(\frac{1}{2}x_1, \dots, \frac{1}{2}x_n; \frac{1}{2}p_1, \dots, \frac{1}{2}p_n\right)}_* e^{-\frac{i}{\hbar}\int_0^t \hat{H}\left(\frac{1}{2}x_1, \dots, \frac{1}{2}x_n; \frac{1}{2}p_1, \dots, \frac{1}{2}p_n; u\right) du} \tag{8c}
 \end{aligned}$$

Converting from the Laplace transform image variables to their Fourier counterparts

$$\begin{aligned}
 & (\bar{p}_1, \dots, \bar{p}_n) = (ip_{\omega 1}, \dots, ip_{\omega n}), (\bar{x}_1, \dots, \bar{x}_n) = (ix_{\omega 1}, \dots, ix_{\omega n}) \\
 & \tilde{\Psi}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t) = \tilde{\Psi}(ix_{\omega 1}, \dots, ix_{\omega n}; ip_{\omega 1}, \dots, ip_{\omega n}; t) \\
 & \delta\left(\frac{1}{2}x_1 + i\hbar\bar{p}_1, \dots, \frac{1}{2}x_n + i\hbar\bar{p}_n\right) \delta\left(\frac{1}{2}p_1 - i\hbar\bar{x}_1, \dots, \frac{1}{2}p_n - i\hbar\bar{x}_n\right) \\
 & \equiv \delta\left(\frac{1}{2}x_1 - \hbar p_{\omega 1}, \dots, \frac{1}{2}x_n - \hbar p_{\omega n}\right) \delta\left(\frac{1}{2}p_1 + \hbar x_{\omega 1}, \dots, \frac{1}{2}p_n + \hbar x_{\omega n}\right) \\
 & \delta\left(\frac{1}{2}x_1 - \hbar p_{\omega 1}, \dots, \frac{1}{2}x_n - \hbar p_{\omega n}\right) \delta\left(\frac{1}{2}p_1 + \hbar x_{\omega 1}, \dots, \frac{1}{2}p_n + \hbar x_{\omega n}\right) \\
 & \quad \underbrace{\left(\frac{1}{2}x_1, \dots, \frac{1}{2}x_n; \frac{1}{2}p_1, \dots, \frac{1}{2}p_n\right)}_* e^{-\frac{i}{\hbar}\int_0^t \hat{H}\left(\frac{1}{2}x_1, \dots, \frac{1}{2}x_n; \frac{1}{2}p_1, \dots, \frac{1}{2}p_n; u\right) du} \tag{8d}
 \end{aligned}$$

Now the inverse Fourier transform of this is

$$\begin{aligned}
 & F_{(x_{\omega 1}, \dots, x_{\omega n})}^{-1} \left(\delta\left(\frac{1}{2}x_1 - \hbar p_{\omega 1}, \dots, \frac{1}{2}x_n - \hbar p_{\omega n}\right) \delta\left(\frac{1}{2}p_1 + \hbar x_{\omega 1}, \dots, \frac{1}{2}p_n + \hbar x_{\omega n}\right) \right) \\
 & \quad \underbrace{\left(\frac{1}{2}x_1, \dots, \frac{1}{2}x_n; \frac{1}{2}p_1, \dots, \frac{1}{2}p_n\right)}_* e^{-\frac{i}{\hbar}\int_0^t \hat{H}\left(\frac{1}{2}x_1, \dots, \frac{1}{2}x_n; \frac{1}{2}p_1, \dots, \frac{1}{2}p_n; u\right) du}
 \end{aligned}$$

$$\begin{aligned}
 &= \left(\frac{1}{2\pi\hbar^2}\right)^n \underbrace{\left(\frac{1}{2}x_1, \dots, \frac{1}{2}x_n; \frac{1}{2}p_1, \dots, \frac{1}{2}p_n\right)}^* e^{-\frac{i}{\hbar} \int_0^t \hat{H}\left(\frac{1}{2}x_1, \dots, \frac{1}{2}x_n; \frac{1}{2}p_1, \dots, \frac{1}{2}p_n; u\right) du} \\
 &= \left(\frac{1}{2\pi\hbar^2}\right)^n \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar} \int_0^t \hat{H}\left(\frac{1}{2}x_1 - \nu \frac{1}{2}x_1, \dots, \frac{1}{2}x_n - \nu \frac{1}{2}x_n; \frac{1}{2}p_1 - \nu \frac{1}{2}p_1, \dots, \frac{1}{2}p_n - \nu \frac{1}{2}p_n; u\right) du} \\
 &\quad \times d\nu \frac{1}{2}x_1 d\nu \frac{1}{2}p_1 \dots d\nu \frac{1}{2}x_n d\nu \frac{1}{2}p_n \tag{8e}
 \end{aligned}$$

Hence

$$\begin{aligned}
 &L^{-1} \left(\begin{matrix} (\bar{x}_1, \dots, \bar{x}_n) \\ \rightarrow (x_1, \dots, x_n); \\ (\bar{p}_1, \dots, \bar{p}_n) \\ \rightarrow (p_1, \dots, p_n) \end{matrix} \right) \left(e^{-\frac{i}{\hbar} \int_0^t \hat{H}\left(i\hbar\bar{p}_1 + \frac{1}{2}x_1, \dots, i\hbar\bar{p}_n + \frac{1}{2}x_n; -i\hbar\bar{x}_1 + \frac{1}{2}p_1, \dots, -i\hbar\bar{x}_n + \frac{1}{2}p_n; u\right) du} \right) \\
 &= \left(\frac{1}{2\pi\hbar^2}\right)^n \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar} \int_0^t \hat{H}\left(\frac{1}{2}x_1 - \nu \frac{1}{2}x_1, \dots, \frac{1}{2}x_n - \nu \frac{1}{2}x_n; \frac{1}{2}p_1 - \nu \frac{1}{2}p_1, \dots, \frac{1}{2}p_n - \nu \frac{1}{2}p_n; u\right) du} \\
 &\quad \times d\nu \frac{1}{2}x_1 d\nu \frac{1}{2}p_1 \dots d\nu \frac{1}{2}x_n d\nu \frac{1}{2}p_n \tag{8f}
 \end{aligned}$$

Thus the quantum phase space wavefunction with initial condition for the dynamics may be expressed in the direct real $(x_1, \dots, x_n; p_1, \dots, p_n)$ generalised coordinates and momenta.

$$\begin{aligned}
 \Psi(x_1, \dots, x_n; p_1, \dots, p_n; t) &= \Psi_0(x_1, \dots, x_n; p_1, \dots, p_n; t = 0) \\
 &\underbrace{\left(\frac{1}{2\pi\hbar^2}\right)^n \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar} \int_0^t \hat{H}\left(\frac{1}{2}x_1 - \nu \frac{1}{2}x_1, \dots, \frac{1}{2}x_n - \nu \frac{1}{2}x_n; \frac{1}{2}p_1 - \nu \frac{1}{2}p_1, \dots, \frac{1}{2}p_n - \nu \frac{1}{2}p_n; u\right) du}}_{\left(\frac{1}{2\pi\hbar^2}\right)^n \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar} \int_0^t \hat{H}\left(\frac{1}{2}x_1 - \nu \frac{1}{2}x_1, \dots, \frac{1}{2}x_n - \nu \frac{1}{2}x_n; \frac{1}{2}p_1 - \nu \frac{1}{2}p_1, \dots, \frac{1}{2}p_n - \nu \frac{1}{2}p_n; u\right) du}} \\
 &\quad \times d\nu \frac{1}{2}x_1 d\nu \frac{1}{2}p_1 \dots d\nu \frac{1}{2}x_n d\nu \frac{1}{2}p_n \tag{8g}
 \end{aligned}$$

It is interesting to note that the canonical choice of $\alpha = \gamma = \frac{1}{2}$ thusly $\hat{H}(i\hbar\partial_p + \frac{x}{2}, -i\hbar\partial_x + \frac{p}{2}, t), \ni \alpha + \gamma = 1$, yields the result above [which shall be used throughout the present work]; the same physics is described when $\alpha \neq \gamma$ thusly $\hat{H}(i\hbar\partial_p + \alpha x, -i\hbar\partial_x + \gamma p, t), \ni \alpha + \gamma = 1$

$$\Psi(x_1, \dots, x_n; p_1, \dots, p_n; t) = \Psi_0(x_1, \dots, x_n; p_1, \dots, p_n; t = 0)$$

$$\underbrace{\left(\frac{1}{2\pi\hbar^2} \right)^n}_{*} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{\frac{-i}{\hbar} \sum_{j=1}^n \left((\gamma_j - \alpha_j) x_j p_j + \int_0^t \hat{H} \begin{pmatrix} \alpha_1 x_1 - \nu_{\alpha_1 x_1}, \\ \dots, \alpha_n x_n - \nu_{\alpha_n x_n}; \\ \gamma_1 p_1 - \nu_{\gamma_1 p_1}, \\ \dots, \gamma_n p_n - \nu_{\gamma_n p_n}; u \end{pmatrix} du \right)} \times dv_{\alpha_1 x_1} dv_{\gamma_1 p_1} \cdots dv_{\alpha_n x_n} dv_{\gamma_n p_n} \tag{8h}$$

Moreover, if the identification

$$\begin{aligned} &\Psi(x_1, \dots, x_n; p_1, \dots, p_n; t) \\ &= \Psi_0(x_1, \dots, x_n; p_1, \dots, p_n; t = 0) \underbrace{\Psi_{\text{complementary}}(x_1, \dots, x_n; p_1, \dots, p_n; t)}_{*} \\ &\Psi_{\text{complementary}}(x_1, \dots, x_n; p_1, \dots, p_n; t) \\ &= \left(\frac{1}{2\pi\hbar^2} \right)^n \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{\frac{-i}{\hbar} \int_0^t \hat{H} \begin{pmatrix} \frac{1}{2} x_1 - \nu_{\frac{1}{2} x_1}, \dots, \frac{1}{2} x_n - \nu_{\frac{1}{2} x_n}; \\ \frac{1}{2} p_1 - \nu_{\frac{1}{2} p_1}, \dots, \frac{1}{2} p_n - \nu_{\frac{1}{2} p_n}; u \end{pmatrix} du} dv_{\frac{1}{2} x_1} dv_{\frac{1}{2} p_1} \cdots dv_{\frac{1}{2} x_n} dv_{\frac{1}{2} p_n} \end{aligned} \tag{8i}$$

is made, then upon considering the form of a continuous Wavelet transform [16] as

$$X_{\text{wavelet}}(a, b) = \frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} x(z) \psi^* \left(\frac{z}{a} - \frac{b}{a} \right) dz \tag{8j}$$

and applying this to the n -dimensional phase space integrals yields

$$\begin{aligned} &\Psi_{\text{complementary}}(x_1, \dots, x_n; p_1, \dots, p_n; t) \\ &= \left(\frac{1}{2\pi\hbar^2} \right)^n \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{\frac{-i}{\hbar} \int_0^t \hat{H} \begin{pmatrix} \frac{1}{2} x_1 - \nu_{\frac{1}{2} x_1}, \dots, \frac{1}{2} x_n - \nu_{\frac{1}{2} x_n}; \\ \frac{1}{2} p_1 - \nu_{\frac{1}{2} p_1}, \dots, \frac{1}{2} p_n - \nu_{\frac{1}{2} p_n}; u \end{pmatrix} du} dv_{\frac{1}{2} x_1} dv_{\frac{1}{2} p_1} \cdots dv_{\frac{1}{2} x_n} dv_{\frac{1}{2} p_n} \\ &e^{\frac{-i}{\hbar} \int_0^t \hat{H} \begin{pmatrix} \frac{1}{2} x_1 - \nu_{\frac{1}{2} x_1}, \dots, \frac{1}{2} x_n - \nu_{\frac{1}{2} x_n}; \\ \frac{1}{2} p_1 - \nu_{\frac{1}{2} p_1}, \dots, \frac{1}{2} p_n - \nu_{\frac{1}{2} p_n}; u \end{pmatrix} du} = \psi^* \left(\left(\frac{-1}{2} x_1 + \nu_{\frac{1}{2} x_1} \right), \dots, \left(\frac{-1}{2} x_n + \nu_{\frac{1}{2} x_n} \right) \right) \\ &\left(\frac{-1}{2} p_1 + \nu_{\frac{1}{2} p_1} \right), \dots, \left(\frac{-1}{2} p_n + \nu_{\frac{1}{2} p_n} \right) \right) \\ &X_{\text{wavelet}}(a, b) = \frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} x(z) \psi^* \left(\frac{z}{a} - \frac{b}{a} \right) dz \\ &X_{\text{wavelet}} \left(\mathbf{1}; \left(\frac{x_1}{2}, \dots, \frac{x_n}{2}; \frac{p_1}{2}, \dots, \frac{p_n}{2} \right) \right) \\ &= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \mathbf{1} e^{\frac{-i}{\hbar} \int_0^t \hat{H} \begin{pmatrix} \frac{1}{2} x_1 - \nu_{\frac{1}{2} x_1}, \dots, \frac{1}{2} x_n - \nu_{\frac{1}{2} x_n}; \\ \frac{1}{2} p_1 - \nu_{\frac{1}{2} p_1}, \dots, \frac{1}{2} p_n - \nu_{\frac{1}{2} p_n}; u \end{pmatrix} du} dv_{\frac{1}{2} x_1} dv_{\frac{1}{2} p_1} \cdots dv_{\frac{1}{2} x_n} dv_{\frac{1}{2} p_n} \\ &\Psi_{\text{complementary}}(x_1, \dots, x_n; p_1, \dots, p_n; t) \\ &= \left(\frac{1}{2\pi\hbar^2} \right)^n X_{\text{wavelet}} \left(\mathbf{1}; \left(\frac{x_1}{2}, \dots, \frac{x_n}{2}; \frac{p_1}{2}, \dots, \frac{p_n}{2} \right) \right) \end{aligned} \tag{8k}$$

thus the n -dimensional phase space extension $(\mathbf{a}, \mathbf{b}) = (\mathbf{1}; (\frac{x}{2}, \frac{p}{2}))$, $x(z)$ becomes a constant $\mathbf{1}$, ψ^* the “Mother Wavelet” and t is a free parameter with respect to the continuous Wavelet transform

Similarly, if the Cepstrum [17] is generalised from the traditional Z -transform (discrete) case to the continuous case via the Laplace transform

$$\text{Cepstrum}(f(y)) = L_{s \rightarrow y}^{-1}(\log(L_{y \rightarrow s}(f(y)))) \tag{81}$$

then

$$\begin{aligned} &\text{Cepstrum}(\Psi_{\text{complimentary}}(x_1, \dots, x_n; p_1, \dots, p_n; t)) \\ &= L^{-1}_{\left(\begin{matrix} (\bar{x}_1, \dots, \bar{x}_n) \\ \rightarrow (x_1, \dots, x_n); \\ (\bar{p}_1, \dots, \bar{p}_n) \\ \rightarrow (p_1, \dots, p_n) \end{matrix}\right)} \left(\text{Log} \left(L_{\left(\begin{matrix} (x_1, \dots, x_n) \\ \rightarrow (\bar{x}_1, \dots, \bar{x}_n); \\ (p_1, \dots, p_n) \\ \rightarrow (\bar{p}_1, \dots, \bar{p}_n) \end{matrix}\right)} (\Psi_{\text{complimentary}}(x_1, \dots, x_n; p_1, \dots, p_n; t)) \right) \right) \\ &L_{\left(\begin{matrix} (x_1, \dots, x_n) \\ \rightarrow (\bar{x}_1, \dots, \bar{x}_n); \\ (p_1, \dots, p_n) \\ \rightarrow (\bar{p}_1, \dots, \bar{p}_n) \end{matrix}\right)} (\Psi_{\text{complimentary}}(x_1, \dots, x_n; p_1, \dots, p_n; t)) \\ &= \tilde{\Psi}_{\text{complimentary}}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t) \\ &\tilde{\Psi}_{\text{complimentary}}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t) = e^{-\frac{i}{\hbar} \int_0^t \hat{H} \left(\begin{matrix} i\hbar \bar{p}_1 + \frac{1}{2} x_1, \dots, i\hbar \bar{p}_n + \frac{1}{2} x_n; \\ -i\hbar \bar{x}_1 + \frac{1}{2} p_1, \dots, -i\hbar \bar{x}_n + \frac{1}{2} p_n; u \end{matrix} \right) du} \\ &\frac{-i}{\hbar} \int_0^t \hat{H} \left(\begin{matrix} \frac{1}{2} x_1 - v_{\frac{1}{2} x_1}, \dots, \frac{1}{2} x_n - v_{\frac{1}{2} x_n}; \\ \frac{1}{2} p_1 - v_{\frac{1}{2} p_1}, \dots, \frac{1}{2} p_n - v_{\frac{1}{2} p_n}; u \end{matrix} \right) du \\ &= \psi^* \left(\begin{matrix} \left(\frac{-1}{2} x_1 + v_{\frac{1}{2} x_1} \right), \dots, \left(\frac{-1}{2} x_n + v_{\frac{1}{2} x_n} \right); \\ \left(\frac{-1}{2} p_1 + v_{\frac{1}{2} p_1} \right), \dots, \left(\frac{-1}{2} p_n + v_{\frac{1}{2} p_n} \right) \end{matrix} \right) \end{aligned}$$

$X_{\text{wavelet}}(a, b) = \frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} x(z) \psi^*(\frac{z}{a} - \frac{b}{a}) dz$, thus the n -dimensional phase space extension $(\mathbf{a}, \mathbf{b}) = (\mathbf{1}; (\frac{x}{2}, \frac{p}{2}))$, $x(z)$ becomes a constant $\mathbf{1}$, ψ^* the “Mother Wavelet” and t is a free parameter with respect to the continuous Wavelet transform

$$\begin{aligned} &\text{Cepstrum}(\Psi_{\text{complimentary}}(x_1, \dots, x_n; p_1, \dots, p_n; t)) \\ &= \left(\frac{1}{2\pi \hbar^2} \right)^n \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \mathbf{1} \left(\frac{-i}{\hbar} \int_0^t \hat{H} \left(\begin{matrix} \frac{1}{2} x_1 - v_{\frac{1}{2} x_1}, \dots, \frac{1}{2} x_n - v_{\frac{1}{2} x_n}; \\ \frac{1}{2} p_1 - v_{\frac{1}{2} p_1}, \dots, \frac{1}{2} p_n - v_{\frac{1}{2} p_n}; u \end{matrix} \right) du \right) \\ &\quad \times dv_{\frac{1}{2} x_1} dv_{\frac{1}{2} p_1} \dots dv_{\frac{1}{2} x_n} dv_{\frac{1}{2} p_n} \end{aligned}$$

Also, the Shannon entropy S , which connects Information Theory to Quantum Theory via the density

$$S = - \iint_{(\mathbf{x}, \mathbf{p})} (\Psi^*(\mathbf{x}, \mathbf{p}, t)\Psi(\mathbf{x}, \mathbf{p}, t)) \text{Log}(\Psi^*(\mathbf{x}, \mathbf{p}, t)\Psi(\mathbf{x}, \mathbf{p}, t)) \mathbf{d}\mathbf{x}\mathbf{d}\mathbf{p} \quad (8m)$$

These are some future vistas for later work elsewhere.

For now, by definition, solution in one representation implies simultaneous solution in all representations. Along these lines, an interesting consequence arises: By equations (4.18) and (4.19) of [1], it is shown that the Fourier projection onto configuration \times space of the phase space wavefunction, yields the configuration space wavefunction in the standard Schrodinger configuration space representation. Symbolically

$$\begin{aligned} \hat{H}_{\text{configuration space}}(x, -i\hbar\partial_x, t)\Psi_{\text{configuration space}}(x, t) &= i\hbar\partial_t\Psi_{\text{configuration space}}(x, t) \\ \Psi_{\text{configuration space}}(x, t) &= \int_{-\infty}^{\infty} \frac{e^{\frac{ixp}{2\hbar}}}{\sqrt{4\pi\hbar}}\Psi(x, p, t)dp \\ \hat{H}_{\text{configuration space}}(x_1, \dots, x_n, -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}, t)\Psi_{\text{configuration space}}(x_1, \dots, x_n, t) \\ &= i\hbar\partial_t\Psi_{\text{configuration space}}(x_1, \dots, x_n, t) \\ \Psi_{\text{configuration space}}(x_1, \dots, x_n, t) \\ &= \int_{-\infty}^{\infty} \frac{e^{\frac{ix_1p_1}{2\hbar}}}{\sqrt{4\pi\hbar}} \dots \int_{-\infty}^{\infty} \frac{e^{\frac{ix_npn}{2\hbar}}}{\sqrt{4\pi\hbar}}\Psi(x_1, \dots, x_n; p_1, \dots, p_n; t)dp_1 \dots dp_n \end{aligned} \quad (9)$$

In other words, the configuration space wavefunction may be expressed in terms of exact quadratures containing the phase space wavefunction determined herein, Eq. (8). Hence, Quantum Dynamics is now reduced to exact quadratures, as are all the associated purely mathematical problems that are abstracted from the physical formalism.

To wit, via HOA the configuration space solution becomes

$$\begin{aligned} &\Psi_{\text{configuration space}}(x_1, \dots, x_n, t) \\ &= \int_{-\infty}^{\infty} \frac{e^{\frac{ix_1p_1}{2\hbar}}}{\sqrt{4\pi\hbar}} \dots \int_{-\infty}^{\infty} \frac{e^{\frac{ix_npn}{2\hbar}}}{\sqrt{4\pi\hbar}} L^{-1} \left(\begin{matrix} (\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n) \\ \rightarrow (x_1, \dots, x_n; p_1, \dots, p_n) \end{matrix} \right) \\ &\left[\begin{matrix} \frac{-i}{\hbar} \int_0^t \hat{H}_{\text{configuration space}} \left(\begin{matrix} x_1, \dots, x_n, \\ -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}, u \end{matrix} \right) (x_1, \dots, x_n) \mapsto (i\hbar\bar{p}_1 + \alpha_1x_1, \dots, i\hbar\bar{p}_n + \alpha_nx_n) \\ (-i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}) \mapsto (-i\hbar\bar{x}_1 + \gamma_1p_1, \dots, -i\hbar\bar{x}_n + \gamma_npn) \end{matrix} \right] du \\ &\times \Psi_{0\text{configuration space}}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t = 0) \\ &\times dp_1 \dots dp_n \end{aligned} \quad (10)$$

With that said, a relatively simplistic prescription results for actually using the HOA to solve the problem,

Given the function $\hat{H}(\hat{x}_1, \dots, \hat{x}_n; \hat{p}_1, \dots, \hat{p}_n, t)$ [respectively $\hat{H}(x_1, \dots, x_n; -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}, t)$] replace $(\hat{x}_1, \dots, \hat{x}_n; \hat{p}_1, \dots, \hat{p}_n, t)$ [respectively $(x_1, \dots, x_n; -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}, t)$] with $(i\hbar\bar{p}_1 + \alpha_1x_1, \dots, i\hbar\bar{p}_n + \alpha_nx_n; -i\hbar\bar{x}_1 + \gamma_1p_1, \dots, -i\hbar\bar{x}_n + \gamma_npn, t)$ in Eq. (10)

The result of course is the quantum phase space [respectively configuration space] wavefunction for the quantum dynamics wave equation. Just a comment on the α and γ parameters in the above formulae. From the HOA [1], they are otherwise arbitrary except for the condition $\alpha + \gamma = 1$. This is explained therein as a consequence of the arbitrary phase shift associated with the quantum phase space wavefunction. Further, any choice of the parameters thus constrained yields a Hamiltonian, which is dynamically equivalent [describes the same physics] as any other choice. However, it is shown therein that the Hamiltonian operator $\hat{H}(i\hbar\partial_p + \alpha x, -i\hbar\partial_x + \gamma p, t)$, $\alpha + \gamma = 1$ takes on the symmetric canonical form when $\alpha = \gamma = \frac{1}{2}$ thusly $\hat{H}(i\hbar\partial_p + \frac{x}{2}, -i\hbar\partial_x + \frac{p}{2}, t)$, $\exists \alpha + \gamma = 1$. Notwithstanding this and with an eye towards computational simplifications for particular classes of applications, it has been found that other choices than $\alpha = \gamma = \frac{1}{2}$ sometime facilitates evaluation of the integral transforms. Unless otherwise directed, the convention for α and γ shall be specified for particular cases, presently and elsewhere. For the problems herein the $\alpha = \gamma = \frac{1}{2}$ sufficeth.

To recall the full details of HOA results, see the original work [EJTP 1 (2004), 10–16]. As pointed out therein,

Notwithstanding its quantum mechanical origins, the HOA scheme takes on a life of its own and transcends the limits of quantum applications to address a wide variety of purely formal mathematical problems as well. Among other things, the result provides a formula for obtaining an exact solution to a wide variety of variable-coefficient integro-differential equations. Since the functional dependence of the Hamiltonian operator as considered is in general arbitrary upon its arguments (i.e., independent variables, derivative operator symbols [including negative powers thereof, thus the possible integral character]), then its multivariable extension can be interpreted as the most general variable coefficient partial differential operator. Moreover, it is not confined to being a scalar or even vector operator, but may be generally construed an arbitrary rank matrix operator. In all cases of course, its rank dictates the matrix rank of the wavefunction solution.

In the present case of the Schrodinger equation, we shall be dealing with a scalar Hamiltonian structure and the solution wavefunction will be of a scalar character. (elsewhere, e.g. [9], the relativistic treatment demands the Dirac equation with such a 4×4 matrix Hamiltonian structure and the solution wavefunction will then be of a 4-dimensional column vector character).

3 Some selected HOA example calculations

3.1 Example 1. 1-Dim simple harmonic oscillator

Having completed this brief recap of the HOA from [6], now consider the first example case of the 1-dim SHO (Simple Harmonic Oscillator) dynamics in quantum phase space. Here the Hamiltonian has the form

$$\hat{H}(\hat{x}_1, \dots, \hat{x}_n; \hat{p}_1, \dots, \hat{p}_n, t) = \frac{\hat{p}^2}{2m} + a\hat{x}^2 \tag{11a}$$

Hence the solution of the phase space quantum dynamics is given by Eq. (9) as

$$\begin{aligned} &\left(\frac{(-i\hbar\partial_x + \frac{p}{2})^2}{2m} + a\left(i\hbar\partial_p + \frac{x}{2}\right)^2\right)\Psi(x; p; t) = i\hbar\partial_t\Psi(x; p; t) \\ &\left(\frac{(-i\hbar\bar{x} + \frac{p}{2})^2}{2m} + a\left(i\hbar\bar{p} + \frac{x}{2}\right)^2\right)\check{\Psi}(\bar{x}; \bar{p}; t) = i\hbar\partial_t\check{\Psi}(\bar{x}; \bar{p}; t) \\ \Psi(x; p; t) &= L_{((\bar{x})\rightarrow(x))}^{-1} \left[L_{((\bar{p})\rightarrow(p))}^{-1} \left[e^{\frac{-i\left(\frac{(-i\hbar\bar{x} + \frac{p}{2})^2}{2m} + a(i\hbar\bar{p} + \frac{x}{2})^2\right)}{\hbar}} \right] \right] \times \check{\Psi}_0(\bar{x}; \bar{p}; t = 0) \end{aligned} \tag{11b}$$

This is the computational construction of the SHO quantum phase space Schrodinger wavefunction. For the case of a Dirac delta function initial condition in quantum phase space of form $\delta(x, p)$ since the Laplace transform of this initial condition is $\check{\Psi}(\bar{x}, \bar{p}, t = 0) = 1, \Psi(x, p, t = 0) = \delta(x, p)$.

Upon evaluation of (11b) with the above $\delta(x, p)$ initial condition, the quantum phase space wavefunction is

$$\Psi(x, p, t) = \sqrt{\frac{-m}{2a}} \frac{e^{i\left(\frac{p^2 + 2amx^2}{4\hbar t}\right)}}{2\pi\hbar t} \tag{11c}$$

For sake of completeness, the case of a generalized to $a(t)$, an arbitrary function, yields

$$\begin{aligned} &\left(\frac{(-i\hbar\partial_x + \frac{p}{2})^2}{2m} + a(t)\left(i\hbar\partial_p + \frac{x}{2}\right)^2\right)\Psi(x; p; t) = i\hbar\partial_t\Psi(x; p; t) \\ &\left(\frac{(-i\hbar\bar{x} + \frac{p}{2})^2}{2m} + a(t)\left(i\hbar\bar{p} + \frac{x}{2}\right)^2\right)\check{\Psi}(\bar{x}; \bar{p}; t) = i\hbar\partial_t\check{\Psi}(\bar{x}; \bar{p}; t) \end{aligned} \tag{11d}$$

$$\begin{aligned} \Psi(x; p; t) &= L_{((\bar{x})\rightarrow(x))}^{-1} \left[L_{((\bar{p})\rightarrow(p))}^{-1} \left[e^{\frac{-i\left(i\left(\frac{(-i\hbar\bar{x} + \frac{p}{2})^2}{2m} + \int_0^t a(u)du\right) + a(t)\left(i\hbar\bar{p} + \frac{x}{2}\right)^2\right)}{\hbar}} \right] \right] \times \check{\Psi}_0(\bar{x}; \bar{p}; t = 0) \\ \Psi(x, p, t) &= \underbrace{\Psi_0(x, p, t = 0)}_{x,p} \ast \sqrt{\frac{-m}{2\int_0^t a(u)du}} \frac{e^{i\left(\frac{p^2 + 2mx^2}{4\hbar t} + \frac{\int_0^t a(u)du}{\int_0^t a(u)du}\right)}}{2\pi\hbar t} \end{aligned} \tag{11e}$$

where $\underbrace{\ast}_{x,p}$ is the x, p convolution as described in the Recap earlier.

3.2 Example 2. Schrödinger Hamiltonian with SHOs having N-arbitrary masses in pairwise anisotropic interaction

Now consider the example case of the nonrelativistic Schrödinger Hamiltonian with multiple pairwise interacting anisotropic SHOs of arbitrary masses in quantum phase space. Like the 1-dim example above, the oscillator strengths below may be generalized to arbitrary functions of time $a_{x_{ij}}(t)$, $a_{y_{ij}}(t)$, $a_{z_{ij}}(t)$ in a straightforward fashion, but the calculation is here omitted. Here the Hamiltonian has the form

$$\begin{aligned} & \hat{H}_{\text{Schrödinger}}^{\text{Anisotropic SHOs}} \\ &= \sum_i \frac{1}{2m_i} \left(\left(-i\hbar\partial_{x_i} + \frac{p_{x_i}}{2} \right)^2 + \left(-i\hbar\partial_{y_i} + \frac{p_{y_i}}{2} \right)^2 + \left(-i\hbar\partial_{z_i} + \frac{p_{z_i}}{2} \right)^2 \right) \\ &+ \sum_{i < j} \left(\begin{aligned} & a_{x_{ij}} \left(\left(i\hbar\partial_{p_{x_i}} + \frac{x_i}{2} \right) - \left(i\hbar\partial_{p_{x_j}} + \frac{x_j}{2} \right) \right)^2 \\ & + a_{y_{ij}} \left(\left(i\hbar\partial_{p_{y_i}} + \frac{y_i}{2} \right) - \left(i\hbar\partial_{p_{y_j}} + \frac{y_j}{2} \right) \right)^2 \\ & + a_{z_{ij}} \left(\left(i\hbar\partial_{p_{z_i}} + \frac{z_i}{2} \right) - \left(i\hbar\partial_{p_{z_j}} + \frac{z_j}{2} \right) \right)^2 \end{aligned} \right) \end{aligned} \quad (12a)$$

$$\begin{aligned} & \hat{H}_{\text{Schrödinger}}^{\text{Anisotropic SHOs}} \left(-i\hbar\partial_{x_i} + \frac{p_{x_i}}{2}, -i\hbar\partial_{y_i} + \frac{p_{y_i}}{2}, -i\hbar\partial_{z_i} + \frac{p_{z_i}}{2}; \right. \\ & \left. i\hbar\partial_{p_{x_i}} + \frac{x_i}{2}, i\hbar\partial_{p_{y_i}} + \frac{y_i}{2}, i\hbar\partial_{p_{z_i}} + \frac{z_i}{2} \right) \\ & \times \Psi(x_i, y_i, z_i; p_{x_i}, p_{y_i}, p_{z_i}; t) = i\hbar\partial_t \Psi(x_i, y_i, z_i; p_{x_i}, p_{y_i}, p_{z_i}; t) \end{aligned}$$

$$\begin{aligned} & \hat{H}_{\text{Schrödinger}}^{\text{Anisotropic SHOs}} = \sum_i \frac{1}{2m_i} \left(\left(-i\hbar\bar{x}_i + \frac{p_{x_i}}{2} \right)^2 + \left(-i\hbar\bar{y}_i + \frac{p_{y_i}}{2} \right)^2 + \left(-i\hbar\bar{z}_i + \frac{p_{z_i}}{2} \right)^2 \right) \\ &+ \sum_{i < j} \left(\begin{aligned} & a_{x_{ij}} \left(\left(i\hbar\bar{p}_{x_i} + \frac{x_i}{2} \right) - \left(i\hbar\bar{p}_{x_j} + \frac{x_j}{2} \right) \right)^2 \\ & + a_{y_{ij}} \left(\left(i\hbar\bar{p}_{y_i} + \frac{y_i}{2} \right) - \left(i\hbar\bar{p}_{y_j} + \frac{y_j}{2} \right) \right)^2 \\ & + a_{z_{ij}} \left(\left(i\hbar\bar{p}_{z_i} + \frac{z_i}{2} \right) - \left(i\hbar\bar{p}_{z_j} + \frac{z_j}{2} \right) \right)^2 \end{aligned} \right) \end{aligned} \quad (12b)$$

$$\hat{H}_{\text{Schrödinger}}^{\text{Anisotropic SHOs}} \left(-i\hbar\bar{x}_i + \frac{p_{x_i}}{2}, -i\hbar\bar{y}_i + \frac{p_{y_i}}{2}, -i\hbar\bar{z}_i + \frac{p_{z_i}}{2}; \right. \\ \left. i\hbar\bar{p}_{x_i} + \frac{x_i}{2}, i\hbar\bar{p}_{y_i} + \frac{y_i}{2}, i\hbar\bar{p}_{z_i} + \frac{z_i}{2} \right)$$

$$\tilde{\Psi}(\bar{x}_i, \bar{y}_i, \bar{z}_i; \bar{p}_{x_i}, \bar{p}_{y_i}, \bar{p}_{z_i}; t) = i\hbar\partial_t \tilde{\Psi}(\bar{x}_i, \bar{y}_i, \bar{z}_i; \bar{p}_{x_i}, \bar{p}_{y_i}, \bar{p}_{z_i}; t)$$

$$\Psi(x_i, y_i, z_i; p_{x_i}, p_{y_i}, p_{z_i}; t)$$

$$= L^{-1} \left(\begin{aligned} & (\bar{x}_i, \bar{y}_i, \bar{z}_i; \bar{p}_{x_i}, \bar{p}_{y_i}, \bar{p}_{z_i}) \\ & \rightarrow (x_i, y_i, z_i; p_{x_i}, p_{y_i}, p_{z_i}) \end{aligned} \right) \left[\frac{e^{-i \int_0^t \hat{H}_{\text{Schrödinger}}^{\text{Anisotropic SHOs}} \left(-i\hbar\bar{x}_i + \frac{p_{x_i}}{2}, -i\hbar\bar{y}_i + \frac{p_{y_i}}{2}, -i\hbar\bar{z}_i + \frac{p_{z_i}}{2}; \right. \right. \\ \left. \left. i\hbar\bar{p}_{x_i} + \frac{x_i}{2}, i\hbar\bar{p}_{y_i} + \frac{y_i}{2}, i\hbar\bar{p}_{z_i} + \frac{z_i}{2} \right) du}{\hbar} \right] \\ \times \tilde{\Psi}_0(\bar{x}_i, \bar{y}_i, \bar{z}_i; \bar{p}_{x_i}, \bar{p}_{y_i}, \bar{p}_{z_i}; t = 0) \quad (12c)$$

3.3 Example 3. Schrödinger molecular Hamiltonian with pairwise Coulomb interaction

Now consider the example case of the nonrelativistic SMH (Schrödinger Molecular Hamiltonian) with pairwise Coulomb interaction dynamics in quantum phase space [7]. Here the Hamiltonian has the form

$$\hat{H} = \sum_A \frac{1}{2M_A} \hat{\mathbf{p}}_A^2 + \sum_i \frac{1}{2m_e} \hat{\mathbf{p}}_i^2 + \sum_{A < B} \frac{e^2}{8\pi\epsilon_0} \left(\frac{Z_A Z_B}{|\hat{r}_A - \hat{r}_B|} \right) + \sum_{i < j} \frac{e^2}{8\pi\epsilon_0} \left(\frac{1}{|\hat{r}_i - \hat{r}_j|} \right) + \sum_{A,i} \left(\frac{-Z_A e^2}{|\hat{r}_A - \hat{r}_i|} \right)$$

$\hat{H}_{\text{Schrodinger Molecular}}$

$$\times \left(\begin{aligned} & -i\hbar\partial_{x_A} + \frac{p_{x_A}}{2}, -i\hbar\partial_{y_A} + \frac{p_{y_A}}{2}, -i\hbar\partial_{z_A} + \frac{p_{z_A}}{2}, -i\hbar\partial_{x_B} + \frac{p_{x_B}}{2}, -i\hbar\partial_{y_B} + \frac{p_{y_B}}{2}, -i\hbar\partial_{z_B} + \frac{p_{z_B}}{2}, \\ & -i\hbar\partial_{x_i} + \frac{p_{x_i}}{2}, -i\hbar\partial_{y_i} + \frac{p_{y_i}}{2}, -i\hbar\partial_{z_i} + \frac{p_{z_i}}{2}, -i\hbar\partial_{x_j} + \frac{p_{x_j}}{2}, -i\hbar\partial_{y_j} + \frac{p_{y_j}}{2}, -i\hbar\partial_{z_j} + \frac{p_{z_j}}{2}; \\ & i\hbar\partial_{p_{x_A}} + \frac{x_A}{2}, i\hbar\partial_{p_{y_A}} + \frac{y_A}{2}, i\hbar\partial_{p_{z_A}} + \frac{z_A}{2}, i\hbar\partial_{p_{x_B}} + \frac{x_B}{2}, i\hbar\partial_{p_{y_B}} + \frac{y_B}{2}, i\hbar\partial_{p_{z_B}} + \frac{z_B}{2}, \\ & i\hbar\partial_{p_{x_i}} + \frac{x_i}{2}, i\hbar\partial_{p_{y_i}} + \frac{y_i}{2}, i\hbar\partial_{p_{z_i}} + \frac{z_i}{2}, i\hbar\partial_{p_{x_j}} + \frac{x_j}{2}, i\hbar\partial_{p_{y_j}} + \frac{y_j}{2}, i\hbar\partial_{p_{z_j}} + \frac{z_j}{2} \end{aligned} \right) \tag{13a}$$

$$\begin{aligned} \hat{H}_{\text{Schrodinger Molecular}} &= \sum_A \frac{1}{2M_A} \left((-i\hbar\bar{x}_A + \frac{p_{x_A}}{2})^2 + (-i\hbar\bar{y}_A + \frac{p_{y_A}}{2})^2 + (-i\hbar\bar{z}_A + \frac{p_{z_A}}{2})^2 \right) \\ &+ \sum_i \frac{1}{2m_e} \left((-i\hbar\bar{x}_i + \frac{p_{x_i}}{2})^2 + (-i\hbar\bar{y}_i + \frac{p_{y_i}}{2})^2 + (-i\hbar\bar{z}_i + \frac{p_{z_i}}{2})^2 \right) \\ &+ \sum_{A < B} \frac{e^2}{8\pi\epsilon_0} \frac{Z_A Z_B}{\left| \begin{aligned} & ((i\hbar\bar{p}_{x_A} + \frac{x_A}{2}) - (i\hbar\bar{p}_{x_B} + \frac{x_B}{2}))^2 \\ & + ((i\hbar\bar{p}_{y_A} + \frac{y_A}{2}) - (i\hbar\bar{p}_{y_B} + \frac{y_B}{2}))^2 \\ & + ((i\hbar\bar{p}_{z_A} + \frac{z_A}{2}) - (i\hbar\bar{p}_{z_B} + \frac{z_B}{2}))^2 \end{aligned} \right|} \\ &+ \sum_{i < j} \frac{e^2}{8\pi\epsilon_0} \frac{1}{\left| \begin{aligned} & ((i\hbar\bar{p}_{x_i} + \frac{x_i}{2}) - (i\hbar\bar{p}_{x_j} + \frac{x_j}{2}))^2 \\ & + ((i\hbar\bar{p}_{y_i} + \frac{y_i}{2}) - (i\hbar\bar{p}_{y_j} + \frac{y_j}{2}))^2 \\ & + ((i\hbar\bar{p}_{z_i} + \frac{z_i}{2}) - (i\hbar\bar{p}_{z_j} + \frac{z_j}{2}))^2 \end{aligned} \right|} \\ &+ \sum_{A,i} \frac{-Z_A e^2}{\left| \begin{aligned} & ((i\hbar\bar{p}_{x_A} + \frac{x_A}{2}) - (i\hbar\bar{p}_{x_i} + \frac{x_i}{2}))^2 \\ & + ((i\hbar\bar{p}_{y_A} + \frac{y_A}{2}) - (i\hbar\bar{p}_{y_i} + \frac{y_i}{2}))^2 \\ & + ((i\hbar\bar{p}_{z_A} + \frac{z_A}{2}) - (i\hbar\bar{p}_{z_i} + \frac{z_i}{2}))^2 \end{aligned} \right|} \end{aligned} \tag{13b}$$

Hence the quantum phase space Hamiltonian is specified by the HOA and results in the quantum phase space wave function for a given initial condition via (10) as

$$\begin{aligned}
 & \Psi \begin{pmatrix} x_A, y_A, z_A, x_B, y_B, z_B, \\ x_i, y_i, z_i, x_j, y_j, z_j; \\ p_{x_A}, p_{y_A}, p_{z_A}, p_{x_B}, p_{y_B}, p_{z_B}, \\ p_{x_i}, p_{y_i}, p_{z_i}, p_{x_j}, p_{y_j}, p_{z_j}; t \end{pmatrix} \\
 &= L^{-1} \left(\begin{pmatrix} \bar{x}_A, \bar{y}_A, \bar{z}_A, \bar{x}_B, \bar{y}_B, \bar{z}_B, \\ \bar{x}_i, \bar{y}_i, \bar{z}_i, \bar{x}_j, \bar{y}_j, \bar{z}_j; \\ p_{x_A}, p_{y_A}, p_{z_A}, p_{x_B}, p_{y_B}, p_{z_B}, \\ p_{x_i}, p_{y_i}, p_{z_i}, p_{x_j}, p_{y_j}, p_{z_j} \end{pmatrix} \right) \\
 &\rightarrow \left(\begin{pmatrix} x_A, y_A, z_A, x_B, y_B, z_B, \\ x_i, y_i, z_i, x_j, y_j, z_j; \\ p_{x_A}, p_{y_A}, p_{z_A}, p_{x_B}, p_{y_B}, p_{z_B}, \\ p_{x_i}, p_{y_i}, p_{z_i}, p_{x_j}, p_{y_j}, p_{z_j} \end{pmatrix} \right) \\
 &e^{\left[\frac{-i}{\hbar} \int_0^t \hat{H} \text{Schrodinger Molecular} \begin{pmatrix} -i\hbar\bar{x}_A + \frac{p_{x_A}}{2}, -i\hbar\bar{y}_A + \frac{p_{y_A}}{2}, -i\hbar\bar{z}_A + \frac{p_{z_A}}{2}, -i\hbar\bar{x}_i + \frac{p_{x_i}}{2}, -i\hbar\bar{y}_i + \frac{p_{y_i}}{2}, -i\hbar\bar{z}_i + \frac{p_{z_i}}{2}; \\ i\hbar\bar{p}_{x_A} + \frac{x_A}{2}, i\hbar\bar{p}_{y_A} + \frac{y_A}{2}, i\hbar\bar{p}_{z_A} + \frac{z_A}{2}, i\hbar\bar{p}_{x_B} + \frac{x_B}{2}, i\hbar\bar{p}_{y_B} + \frac{y_B}{2}, i\hbar\bar{p}_{z_B} + \frac{z_B}{2}, \\ i\hbar\bar{p}_{x_i} + \frac{x_i}{2}, i\hbar\bar{p}_{y_i} + \frac{y_i}{2}, i\hbar\bar{p}_{z_i} + \frac{z_i}{2}, i\hbar\bar{p}_{x_j} + \frac{x_j}{2}, i\hbar\bar{p}_{y_j} + \frac{y_j}{2}, i\hbar\bar{p}_{z_j} + \frac{z_j}{2} \end{pmatrix} du \right] \\
 &\times \tilde{\Psi}_0(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t = 0) \tag{13c}
 \end{aligned}$$

Where the SMH is expressed as

$$\hat{H} \text{Schrodinger Molecular} \begin{pmatrix} -i\hbar\bar{x}_A + \frac{p_{x_A}}{2}, -i\hbar\bar{y}_A + \frac{p_{y_A}}{2}, -i\hbar\bar{z}_A + \frac{p_{z_A}}{2}, -i\hbar\bar{x}_B + \frac{p_{x_B}}{2}, -i\hbar\bar{y}_B + \frac{p_{y_B}}{2}, -i\hbar\bar{z}_B + \frac{p_{z_B}}{2}, \\ -i\hbar\bar{x}_i + \frac{p_{x_i}}{2}, -i\hbar\bar{y}_i + \frac{p_{y_i}}{2}, -i\hbar\bar{z}_i + \frac{p_{z_i}}{2}, -i\hbar\bar{x}_j + \frac{p_{x_j}}{2}, -i\hbar\bar{y}_j + \frac{p_{y_j}}{2}, -i\hbar\bar{z}_j + \frac{p_{z_j}}{2}; \\ i\hbar\bar{p}_{x_A} + \frac{x_A}{2}, i\hbar\bar{p}_{y_A} + \frac{y_A}{2}, i\hbar\bar{p}_{z_A} + \frac{z_A}{2}, i\hbar\bar{p}_{x_B} + \frac{x_B}{2}, i\hbar\bar{p}_{y_B} + \frac{y_B}{2}, i\hbar\bar{p}_{z_B} + \frac{z_B}{2}, \\ i\hbar\bar{p}_{x_i} + \frac{x_i}{2}, i\hbar\bar{p}_{y_i} + \frac{y_i}{2}, i\hbar\bar{p}_{z_i} + \frac{z_i}{2}, i\hbar\bar{p}_{x_j} + \frac{x_j}{2}, i\hbar\bar{p}_{y_j} + \frac{y_j}{2}, i\hbar\bar{p}_{z_j} + \frac{z_j}{2} \end{pmatrix}$$

Following from [7] for the radial component of the molecular Schrödinger equation in phase space, the HOA solution of the radial Schrödinger equation for nonrelativistic N-particle system with pairwise $\frac{1}{r_{ij}}$ radial potential interaction where $\frac{1}{r_{ij}} \equiv \frac{1}{|r_i - r_j|}$ in the QPSR. Moreover, the analysis for this multiparticle system is in the laboratory reference frame for the coordinates [7]. Hence no particle is fixed as a center of motion. As stated earlier the angular components separate in the usual way by [7]. Here a_i, b_i, c_i are scaling constants, $L_i(L_i + 1)$ are the angular coupling terms and $\mathbf{r} = (r_1, \dots, r_N) = (r_{i=1, \dots, N})$, $\mathbf{p_r} = (p_{r_1}, \dots, p_{r_N}) = (p_{r_{i=1, \dots, N}})$. The resulting radial Hamiltonian yields a radial Schrödinger equation of form

$$\begin{aligned}
 & \left(\hat{H} = \sum_i \left(\frac{(-i\hbar\partial_{r_i} + \frac{p_{r_i}}{2})^2}{2m_i} + \frac{2b_i}{(i\hbar\partial_{p_{r_i}} + \frac{r_i}{2})} \left(-i\hbar\partial_{r_i} + \frac{p_{r_i}}{2} \right) + \frac{c_i L_i(L_i + 1)}{(i\hbar\partial_{p_{r_i}} + \frac{r_i}{2})^2} \right) \right. \\
 & \left. + \sum_{i < j} a_{ij} \left(\frac{1}{|(i\hbar\partial_{p_{r_i}} + \frac{r_i}{2}) - (i\hbar\partial_{p_{r_j}} + \frac{r_j}{2})|} \right) \right) \\
 & \Psi_{\mathbf{r} \text{ phasespace}}(\mathbf{r}; \mathbf{p_r}; t) \\
 &= i\hbar\partial_t \Psi_{\mathbf{r} \text{ phasespace}}(\mathbf{r}; \mathbf{p_r}; t) \tag{13d}
 \end{aligned}$$

Hence via HOA from Eq. (10),

$$\begin{aligned} & \left(\sum_i \left(\frac{(-i\hbar\bar{r}_i + \frac{pr_i}{2})^2}{2m_i} + \frac{2b_i}{(i\hbar\bar{p}_i + \frac{r_i}{2})} \left(-i\hbar\bar{r}_i + \frac{pr_i}{2}\right) + \frac{c_i L_i(L_i+1)}{(i\hbar\bar{p}_i + \frac{r_i}{2})^2} \right) \right) \\ & + \sum_{i < j} a_{ij} \left(\frac{1}{|(i\hbar\bar{p}_i + \frac{r_i}{2}) - (i\hbar\bar{p}_j + \frac{r_j}{2})|} \right) \\ & \check{\Psi}_{\mathbf{r} \text{ phasespace}}(\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t) \\ & = i\hbar\partial_t \check{\Psi}_{\mathbf{r} \text{ phasespace}}(\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t) \end{aligned} \tag{13e}$$

Yielding the exact analytical solution given in quadratures as

$$\begin{aligned} & \Psi_{\mathbf{r} \text{ phasespace}}(\mathbf{r}; \mathbf{p}_{\mathbf{r}}; t) \\ & = L_{\left(\begin{smallmatrix} \bar{\mathbf{r}} \rightarrow \mathbf{r}; \\ \bar{\mathbf{p}}_{\mathbf{r}} \rightarrow \mathbf{p}_{\mathbf{r}} \end{smallmatrix}\right)}^{-1} \left(e^{-\frac{it}{\hbar} \left(\sum_i \left(\frac{(-i\hbar\bar{r}_i + \frac{pr_i}{2})^2}{2m_i} + \frac{2b_i}{(i\hbar\bar{p}_i + \frac{r_i}{2})} \left(-i\hbar\bar{r}_i + \frac{pr_i}{2}\right) + \frac{c_i L_i(L_i+1)}{(i\hbar\bar{p}_i + \frac{r_i}{2})^2} \right) \right)} \right. \\ & \quad \left. \times \sum_{i < j} a_{ij} \left(\frac{1}{|(i\hbar\bar{p}_i + \frac{r_i}{2}) - (i\hbar\bar{p}_j + \frac{r_j}{2})|} \right) \right) \\ & \quad \times \check{\Psi}_{0\mathbf{r} \text{ phasespace}}(\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t = 0) \end{aligned} \tag{13f}$$

To evaluate (13f), recall that

$$\begin{aligned} & \check{\Psi}_{\mathbf{r} \text{ phasespace}}(\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t) \\ & = e^{-\frac{it}{\hbar} \left(\sum_i \left(\frac{(-i\hbar\bar{r}_i + \frac{pr_i}{2})^2}{2m_i} \right) \right)} \times e^{-\frac{it}{\hbar} \left(\sum_i \left(\frac{2b_i}{(i\hbar\bar{p}_i + \frac{r_i}{2})} \left(-i\hbar\bar{r}_i + \frac{pr_i}{2}\right) \right) \right)} \\ & \quad \times e^{-\frac{it}{\hbar} \left(\sum_i \left(\frac{c_i L_i(L_i+1)}{(i\hbar\bar{p}_i + \frac{r_i}{2})^2} \right) \right)} \times e^{-\frac{it}{\hbar} \left(\sum_{i < j} a_{ij} \left(\frac{1}{|(i\hbar\bar{p}_i + \frac{r_i}{2}) - (i\hbar\bar{p}_j + \frac{r_j}{2})|} \right) \right)} \\ & \quad \times \check{\Psi}_{0\mathbf{r} \text{ phasespace}}(\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t = 0) \end{aligned} \tag{13g}$$

Upon evaluating the inverse Laplace transforms and utilizing convolution products herein symbolized as $\underbrace{*}_{\mathbf{r}}$ or $\underbrace{*}_{\mathbf{p}_{\mathbf{r}}}$ or $\underbrace{*}_{\mathbf{r}, \mathbf{p}_{\mathbf{r}}}$ [6].

$$\begin{aligned} & L_{\left(\begin{smallmatrix} \bar{\mathbf{r}} \rightarrow \mathbf{r}; \\ \bar{\mathbf{p}}_{\mathbf{r}} \rightarrow \mathbf{p}_{\mathbf{r}} \end{smallmatrix}\right)}^{-1} \check{\Psi}_{\mathbf{r} \text{ phasespace}}(\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t) \\ & = L_{(\bar{\mathbf{r}} \rightarrow \mathbf{r})}^{-1} \left(e^{-\frac{it}{\hbar} \left(\sum_i \left(\frac{(-i\hbar\bar{r}_i + \frac{pr_i}{2})^2}{2m_i} \right) \right)} \right) \underbrace{*}_{\mathbf{r}} L_{\left(\begin{smallmatrix} \bar{\mathbf{r}} \rightarrow \mathbf{r}; \\ \bar{\mathbf{p}}_{\mathbf{r}} \rightarrow \mathbf{p}_{\mathbf{r}} \end{smallmatrix}\right)}^{-1} \end{aligned}$$

$$\begin{aligned}
 & \left(e^{\frac{-it}{\hbar} \left(\sum_i \left(\frac{2b_i}{i\hbar\bar{p}_{r_i} + \frac{r_i}{2}} \left(-i\hbar\bar{r}_i + \frac{pr_i}{2} \right) \right) \right) \right) \\
 & \underbrace{*}_{\mathbf{Pr}} L_{(\bar{\mathbf{p}}_{\mathbf{r}} \rightarrow \mathbf{Pr})}^{-1} \left(e^{\frac{-it}{\hbar} \left(\sum_i \left(\frac{c_i L_i(L_i+1)}{i\hbar\bar{p}_{r_i} + \frac{r_i}{2}} \right) \right) \right) \underbrace{*}_{\mathbf{Pr}} L_{(\bar{\mathbf{p}}_{\mathbf{r}} \rightarrow \mathbf{Pr})}^{-1} \\
 & \left(e^{\frac{-it}{\hbar} \left(\sum_{i < j} a_{ij} \left(\frac{1}{\left| (i\hbar\bar{p}_{r_i} + \frac{r_i}{2}) - (i\hbar\bar{p}_{r_j} + \frac{r_j}{2}) \right|} \right) \right) \right) \\
 & \underbrace{*}_{\mathbf{r}, \mathbf{Pr}} L_{(\bar{\mathbf{r}} \rightarrow \mathbf{r}; \bar{\mathbf{p}}_{\mathbf{r}} \rightarrow \mathbf{Pr})}^{-1} \left(\tilde{\Psi}_{0\mathbf{r}} \text{ phasespace}(\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t = 0) \right) \tag{13h}
 \end{aligned}$$

Evaluating (13h) explicitly yields

$$\begin{aligned}
 & L_{(\bar{\mathbf{p}}_{\mathbf{r}} \rightarrow \mathbf{Pr})}^{-1} \left(e^{\frac{-it}{\hbar} \left(\sum_{i < j} a_{ij} \left(\frac{1}{\left| (i\hbar\bar{p}_{r_i} + \frac{r_i}{2}) - (i\hbar\bar{p}_{r_j} + \frac{r_j}{2}) \right|} \right) \right) \right) \\
 & = \underbrace{*}_{i < j} \left(\delta[p_{r_i} + p_{r_j}] \left(\frac{1}{\pi p_{r_i} \sqrt{\frac{-i\hbar}{a_{ij}t}}} e^{\frac{ip_{r_i}(r_i - r_j)}{2\hbar}} \left(\sqrt{\frac{p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] \right. \right. \right. \\
 & \quad \left. \left. \left. - \sqrt{\frac{-p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{-p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] \right) \right) \right) \\
 & \text{example } N = 3, \underbrace{f_{1,2}}_{p_{r_1}} \underbrace{*}_{p_{r_2} \cdot p_{r_3}} \underbrace{f_{1,3}}_{p_{r_1}} \underbrace{*}_{p_{r_2} \cdot p_{r_3}} \underbrace{f_{2,3}}_{p_{r_3}}, \\
 & f_{ij} = \delta[p_{r_i} + p_{r_j}] \left(\frac{1}{\pi p_{r_i} \sqrt{\frac{-i\hbar}{a_{ij}t}}} e^{\frac{ip_{r_i}(r_i - r_j)}{2\hbar}} \left(\sqrt{\frac{p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] \right. \right. \\
 & \quad \left. \left. - \sqrt{\frac{-p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{-p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] \right) \right) \tag{13i}
 \end{aligned}$$

Where $\underbrace{*}_{i < j}$ represents the convolution between the inverse transforms of the indicated terms as illustrated above in the case of $N = 3$.

$$\begin{aligned}
 &L_{\left(\begin{smallmatrix} \bar{\mathbf{r}} \rightarrow \mathbf{r}; \\ \bar{\mathbf{p}}_{\mathbf{r}} \rightarrow \mathbf{p}_{\mathbf{r}} \end{smallmatrix}\right)}^{-1} \left(e^{\frac{-it}{\hbar} \left(\sum_i \left(\frac{2b_i}{(i\hbar\bar{p}_{r_i} + \frac{r_i}{2})} \left(-i\hbar\bar{r}_i + \frac{p_{r_i}}{2} \right) \right) \right)} \right) \\
 &= \prod_i \left(\delta[p_{r_i}] \delta[r_i] + \frac{ib_i e^{\frac{2ib_i p_{r_i} t}{\hbar r_i}} (\sqrt{-ip_{r_i}} - \sqrt{ip_{r_i}}) t}{\hbar\pi r_i^2 \sqrt{|p_{r_i}|}} \right) \tag{13j}
 \end{aligned}$$

$$\begin{aligned}
 &L_{\left(\bar{\mathbf{p}}_{\mathbf{r}} \rightarrow \mathbf{p}_{\mathbf{r}}\right)}^{-1} \left(e^{\frac{-it}{\hbar} \left(\sum_i \left(\frac{c_i L_i(L_i+1)}{(i\hbar\bar{p}_{r_i} + \frac{r_i}{2})^2} \right) \right)} \right) \\
 &= \prod_i \left(\frac{-1}{24\pi\hbar^6} \left(c_i^2 L_i^2 (L_i + 1)^2 p_{r_i}^3 t^2 \left(\left(e^{\frac{ip_{r_i} r_i}{2\hbar}} - 1 \right) \text{Log} \left[\frac{-p_{r_i}}{\hbar} \right] \right. \right. \right. \\
 &\quad \left. \left. \left. + \text{Log} \left[\frac{p_{r_i}}{\hbar} \right] - \text{Log} \left[\frac{p_{r_i}}{\hbar} \right] \text{HeavisideStep}[p_{r_i}] \right) \right) \right) \tag{13k}
 \end{aligned}$$

$$L_{\left(\bar{\mathbf{r}} \rightarrow \mathbf{r}\right)}^{-1} \left(e^{\frac{-it}{\hbar} \left(\sum_i \left(\frac{(-i\hbar\bar{r}_i + \frac{p_{r_i}}{2})^2}{2m_i} \right) \right)} \right) = \prod_i \frac{e^{\frac{i(r_i^2 m_i - t r_i p_{r_i})}{2\hbar t}}}{\hbar \sqrt{\frac{2\pi i t}{\hbar m_i}}} \tag{13l}$$

Since $L_{\left(\begin{smallmatrix} \bar{\mathbf{r}} \rightarrow \mathbf{r}; \\ \bar{\mathbf{p}}_{\mathbf{r}} \rightarrow \mathbf{p}_{\mathbf{r}} \end{smallmatrix}\right)}^{-1} \left(\tilde{\Psi}_{0\mathbf{r} \text{ phasespace}}(\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t = 0) \right) = \Psi_{0\mathbf{r} \text{ phasespace}}(\mathbf{r}; \mathbf{p}_{\mathbf{r}}; t = 0)$, the evaluated inverse transforms yield the explicit solution in the QPSR

$\Psi_{\mathbf{r} \text{ phasespace}}(\mathbf{r}; \mathbf{p}_{\mathbf{r}}; t)$

$$\begin{aligned}
 &= \Psi_{0\mathbf{r} \text{ phasespace}}(\mathbf{r}; \mathbf{p}_{\mathbf{r}}; t = 0) \underbrace{*}_{\mathbf{r}, \mathbf{p}_{\mathbf{r}}} \prod_i \frac{e^{\frac{i(r_i^2 m_i - t r_i p_{r_i})}{2\hbar t}}}{\hbar \sqrt{\frac{2\pi i t}{\hbar m_i}}} \\
 &\quad \underbrace{*}_{\mathbf{r}} \prod_i \left(\delta[p_{r_i}] \delta[r_i] + \frac{ib_i e^{\frac{2ib_i p_{r_i} t}{\hbar r_i}} (\sqrt{-ip_{r_i}} - \sqrt{ip_{r_i}}) t}{\hbar\pi r_i^2 \sqrt{|p_{r_i}|}} \right) \\
 &\quad \underbrace{*}_{\mathbf{p}_{\mathbf{r}}} \prod_i \left(\frac{-1}{24\pi\hbar^6} \left(c_i^2 L_i^2 (L_i + 1)^2 p_{r_i}^3 t^2 \left(\left(e^{\frac{ip_{r_i} r_i}{2\hbar}} - 1 \right) \text{Log} \left[\frac{-p_{r_i}}{\hbar} \right] \right. \right. \right. \\
 &\quad \left. \left. \left. + \text{Log} \left[\frac{p_{r_i}}{\hbar} \right] - \text{Log} \left[\frac{p_{r_i}}{\hbar} \right] \text{HeavisideStep}[p_{r_i}] \right) \right) \right) \\
 &\quad \underbrace{*}_{\mathbf{p}_{\mathbf{r}}} \left(\underbrace{*}_{i < j} \left(\delta[p_{r_i} + p_{r_j}] \left(\frac{1}{\pi p_{r_i} \sqrt{\frac{-i\hbar}{a_{ij} t}}} e^{\frac{ip_{r_i}(r_i - r_j)}{2\hbar}} \right. \right. \right. \\
 &\quad \left. \left. \left. \left(\sqrt{\frac{p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij} t}}} \right] - \sqrt{\frac{-p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{-p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij} t}}} \right] \right) \right) \right) \right) \tag{13m}
 \end{aligned}$$

Although the above (13m) is explicitly given in the QPSR [down to the level of convolutions of explicitly calculated quantum phase space factors], an illustrative example will now be provided to help illuminate the actual application of the result for the case of three particles: $N = 3$

Now for the solution of the radial Schrodinger equation for the non-relativistic 3-particle system with pairwise $\frac{1}{r_{ij}}$ radial potential interaction where $\frac{1}{r_{ij}} \equiv \frac{1}{|r_i - r_j|}$ in the QPSR. Moreover, the analysis for this multiparticle system is in the laboratory reference frame for the coordinates [7]. Hence no particle is fixed as a center of motion. As stated earlier the angular components separate in the usual way by [7]. Here a_i, b_i, c_i are scaling constants, $L_i(L_i + 1)$ are the angular coupling terms and $\mathbf{r} = (r_1, r_2, r_3) = (r_{i=1,2,3})$, $\mathbf{p}_r = (p_{r_1}, p_{r_2}, p_{r_3}) = (p_{r_{i=1,2,3}})$. From Eq. (13d), the resulting radial Hamiltonian yields a radial Schrodinger equation of form

$$\left(\begin{aligned} & \frac{(-i\hbar\partial_{r_1} + \frac{pr_1}{2})^2}{2m_1} + \frac{(-i\hbar\partial_{r_2} + \frac{pr_2}{2})^2}{2m_2} + \frac{(-i\hbar\partial_{r_3} + \frac{pr_3}{2})^2}{2m_3} \\ & + \frac{2b_1}{(i\hbar\partial_{pr_1} + \frac{r_1}{2})} \left(-i\hbar\partial_{r_1} + \frac{pr_1}{2}\right) + \frac{2b_2}{(i\hbar\partial_{pr_2} + \frac{r_2}{2})} \left(-i\hbar\partial_{r_2} + \frac{pr_2}{2}\right) \\ & + \frac{2b_3}{(i\hbar\partial_{pr_3} + \frac{r_3}{2})} \left(-i\hbar\partial_{r_3} + \frac{pr_3}{2}\right) + \frac{c_1 L_1(L_1+1)}{(i\hbar\partial_{pr_1} + \frac{r_1}{2})^2} + \frac{c_2 L_2(L_2+1)}{(i\hbar\partial_{pr_2} + \frac{r_2}{2})^2} \\ & + \frac{c_3 L_3(L_3+1)}{(i\hbar\partial_{pr_3} + \frac{r_3}{2})^2} + a_{12} \left(\frac{1}{|(i\hbar\partial_{pr_1} + \frac{r_1}{2}) - (i\hbar\partial_{pr_2} + \frac{r_2}{2})|} \right) \\ & + a_{13} \left(\frac{1}{|(i\hbar\partial_{pr_1} + \frac{r_1}{2}) - (i\hbar\partial_{pr_3} + \frac{r_3}{2})|} \right) + a_{23} \left(\frac{1}{|(i\hbar\partial_{pr_2} + \frac{r_2}{2}) - (i\hbar\partial_{pr_3} + \frac{r_3}{2})|} \right) \end{aligned} \right) \times \Psi_{\mathbf{r} \text{ phasespace}}(r_1, r_2, r_3; p_{r_1}, p_{r_2}, p_{r_3}; t) = i\hbar\partial_t \Psi_{\mathbf{r} \text{ phasespace}}(r_1, r_2, r_3; p_{r_1}, p_{r_2}, p_{r_3}; t) \tag{13n}$$

Following eq(13e)

$$\left(\begin{aligned} & \frac{(-i\hbar\bar{\partial}_{r_1} + \frac{pr_1}{2})^2}{2m_1} + \frac{(-i\hbar\bar{\partial}_{r_2} + \frac{pr_2}{2})^2}{2m_2} + \frac{(-i\hbar\bar{\partial}_{r_3} + \frac{pr_3}{2})^2}{2m_3} \\ & + \frac{2b_1}{(i\hbar\bar{p}_{r_1} + \frac{r_1}{2})} \left(-i\hbar\bar{\partial}_{r_1} + \frac{pr_1}{2}\right) + \frac{2b_2}{(i\hbar\bar{p}_{r_2} + \frac{r_2}{2})} \left(-i\hbar\bar{\partial}_{r_2} + \frac{pr_2}{2}\right) \\ & + \frac{2b_3}{(i\hbar\bar{p}_{r_3} + \frac{r_3}{2})} \left(-i\hbar\bar{\partial}_{r_3} + \frac{pr_3}{2}\right) + \frac{c_1 L_1(L_1+1)}{(i\hbar\bar{p}_{r_1} + \frac{r_1}{2})^2} + \frac{c_2 L_2(L_2+1)}{(i\hbar\bar{p}_{r_2} + \frac{r_2}{2})^2} \\ & + \frac{c_3 L_3(L_3+1)}{(i\hbar\bar{p}_{r_3} + \frac{r_3}{2})^2} + a_{12} \left(\frac{1}{|(i\hbar\bar{p}_{r_1} + \frac{r_1}{2}) - (i\hbar\bar{p}_{r_2} + \frac{r_2}{2})|} \right) \\ & + a_{13} \left(\frac{1}{|(i\hbar\bar{p}_{r_1} + \frac{r_1}{2}) - (i\hbar\bar{p}_{r_3} + \frac{r_3}{2})|} \right) + a_{23} \left(\frac{1}{|(i\hbar\bar{p}_{r_2} + \frac{r_2}{2}) - (i\hbar\bar{p}_{r_3} + \frac{r_3}{2})|} \right) \end{aligned} \right) \times \tilde{\Psi}_{\mathbf{r} \text{ phasespace}}(\bar{r}_1, \bar{r}_2, \bar{r}_3; \bar{p}_{r_1}, \bar{p}_{r_2}, \bar{p}_{r_3}; t) = i\hbar\partial_t \tilde{\Psi}_{\mathbf{r} \text{ phasespace}}(\bar{r}_1, \bar{r}_2, \bar{r}_3; \bar{p}_{r_1}, \bar{p}_{r_2}, \bar{p}_{r_3}; t) \tag{13o}$$

Proceeding as in Eq. (13f) through Eq. (13h); for $N = 3$ Eqs. (13a), (13b), (13c) and (13d) become respectively

$$L_{(\mathbf{\bar{p}}_r \rightarrow \mathbf{p}_r)}^{-1} \left(e^{\frac{-it}{\hbar} \left(\sum_{i < j} a_{ij} \left(\frac{1}{|(i\hbar \bar{p}_{r_i} + \frac{r_i}{2}) - (i\hbar \bar{p}_{r_j} + \frac{r_j}{2})|} \right) \right)} \right) \\ = \underbrace{*}_{i < j} \left(\delta[p_{r_i} + p_{r_j}] \left(\frac{1}{\pi p_{r_i} \sqrt{\frac{-i\hbar}{a_{ij}t}}} e^{\frac{ip_{r_i}(r_i - r_j)}{2\hbar}} \right. \right. \\ \left. \left. \left(\sqrt{\frac{p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] - \sqrt{\frac{-p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{-p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] \right) \right) \right)$$

example $N = 3, f_{1,2} \underbrace{*}_{p_{r_1}} f_{1,3} \underbrace{*}_{p_{r_2}, p_{r_3}} f_{2,3},$

$$f_{ij} = \delta[p_{r_i} + p_{r_j}] \left(\frac{1}{\pi p_{r_i} \sqrt{\frac{-i\hbar}{a_{ij}t}}} e^{\frac{ip_{r_i}(r_i - r_j)}{2\hbar}} \left(\sqrt{\frac{p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] \right. \right. \\ \left. \left. - \sqrt{\frac{-p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{-p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] \right) \right) \tag{13p}$$

$\Psi_{\mathbf{r}}$ phasespace $(r_1, r_2, r_3; p_{r_1} \cdot p_{r_2}, p_{r_3}; t)$

$$= \Psi_{\mathbf{r}}\text{phasespace}(r_1, r_2, r_3; p_{r_1} \cdot p_{r_2}, p_{r_3}; t = 0) \underbrace{*}_{\mathbf{r}, \mathbf{p}_r} \prod_{i=1}^3 \left(\frac{e^{\frac{i(r_i^2 m_1 - r_1 p_{r_1})}{2\hbar t}}}{\hbar \sqrt{\frac{2\pi i t}{\hbar m_1}}} \right) \\ \underbrace{*}_{\mathbf{r}} \prod_{i=1}^3 \left(\delta[p_{r_i}] \delta[r_i] + \frac{ib_i e^{\frac{2ib_i p_{r_i} t}{\hbar r_i}} (\sqrt{-ip_{r_i}} - \sqrt{ip_{r_i}}) t}{\hbar \pi r_i^2 \sqrt{|p_{r_i}|}} \right) \\ \underbrace{*}_{\mathbf{p}_r} \prod_{i=1}^3 \left(\frac{-1}{24\pi \hbar^6} \left(c_i^2 L_i^2 (L_i + 1)^2 p_{r_i}^3 t^2 \left(\left(e^{\frac{ip_{r_i} r_i}{2\hbar}} - 1 \right) \text{Log} \left[\frac{-p_{r_i}}{\hbar} \right] \right. \right. \right. \\ \left. \left. \left. + \text{Log} \left[\frac{p_{r_i}}{\hbar} \right] - \text{Log} \left[\frac{p_{r_i}}{\hbar} \right] \text{HeavisideStep}[p_{r_i}] \right) \right) \right) \\ \underbrace{*}_{\mathbf{p}_r} \left(\underbrace{*}_{i < j} \left(\delta[p_{r_i} + p_{r_j}] \left(\frac{1}{\pi p_{r_i} \sqrt{\frac{-i\hbar}{a_{ij}t}}} e^{\frac{ip_{r_i}(r_i - r_j)}{2\hbar}} \left(\sqrt{\frac{p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] \right. \right. \right. \right. \\ \left. \left. \left. - \sqrt{\frac{-p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{-p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] \right) \right) \right) \right) \tag{13q}$$

Now consider the earlier mentioned particular case of the general nonrelativistic SMH with pairwise Coulomb interaction dynamics

$$\begin{aligned} \hat{H} = & \sum_A \frac{1}{2M_A} \hat{\mathbf{P}}_A^2 + \sum_i \frac{1}{2m_e} \hat{\mathbf{P}}_i^2 + \sum_{A < B} \frac{e^2}{8\pi\epsilon_0} \left(\frac{Z_A Z_B}{|\hat{r}_A - \hat{r}_B|} \right) \\ & + \sum_{i < j} \frac{e^2}{8\pi\epsilon_0} \left(\frac{1}{|\hat{r}_i - \hat{r}_j|} \right) + \sum_{A,i} \left(\frac{-Z_A e^2}{|\hat{r}_A - \hat{r}_i|} \right) \end{aligned} \quad (13a)$$

Though we shall not pursue the details in the present note viz [7], clearly one can see that, after the angular components are separated in the usual way and with a straightforward scaling of the variables, the present N-particle result yields the solution of the radial Schrodinger equation for the general nonrelativistic molecular Hamiltonian in the QPSR which has the form

$$\begin{aligned} \hat{H}_{\text{MolecularRadial}}^{\text{Schrodinger}} = & \sum_A \frac{1}{2M_A} \\ & \left(\left(-i\hbar\partial_{r_A} + \frac{p_{r_A}}{2} \right)^2 + \frac{2}{\left(i\hbar\partial_{p_{r_A}} + \frac{r_A}{2} \right)} \left(-i\hbar\partial_{r_A} + \frac{p_{r_A}}{2} \right) + \frac{L_A(L_A + 1)}{\left(i\hbar\partial_{p_{r_A}} + \frac{r_A}{2} \right)^2} \right) \\ & + \sum_i \frac{1}{2m_e} \left(\left(-i\hbar\partial_{r_i} + \frac{p_{r_i}}{2} \right)^2 + \frac{2}{\left(i\hbar\partial_{p_{r_i}} + \frac{r_i}{2} \right)} \left(-i\hbar\partial_{r_i} + \frac{p_{r_i}}{2} \right) + \frac{L_i(L_i + 1)}{\left(i\hbar\partial_{p_{r_i}} + \frac{r_i}{2} \right)^2} \right) \\ & + \sum_{A < B} \frac{e^2}{8\pi\epsilon_0} \frac{Z_A Z_B}{\left| \left(i\hbar\partial_{p_{r_A}} + \frac{r_A}{2} \right) - \left(i\hbar\partial_{p_{r_B}} + \frac{r_B}{2} \right) \right|} \\ & + \sum_{i < j} \frac{e^2}{8\pi\epsilon_0} \frac{1}{\left| \left(i\hbar\partial_{p_{r_i}} + \frac{r_i}{2} \right) - \left(i\hbar\partial_{p_{r_j}} + \frac{r_j}{2} \right) \right|} \\ & + \sum_{A,i} \frac{-Z_A e^2}{\left| \left(i\hbar\partial_{p_{r_A}} + \frac{r_A}{2} \right) - \left(i\hbar\partial_{p_{r_i}} + \frac{r_i}{2} \right) \right|} \end{aligned} \quad (13r)$$

Hence considering the radial molecular Hamiltonian (13r) as was done in (13a) and applying HOA to (13r) as was done in (13b), the exact analytical solution of the radial Schrödinger equation for the general nonrelativistic molecular Hamiltonian in QPSR may be expressed in quadratures via the above.

3.4 Example 4. Dirac and Majorana equations with minimum-coupled electromagnetic gauge field

Following [8], first consider the related Dirac equation with minimum-coupled electromagnetic gauge field interaction

$$\mathbf{A}(x_1, x_2, x_3, t) = A_1(x_1, x_2, x_3, t)\mathbf{e}_{x_1} + A_2(x_1, x_2, x_3, t)\mathbf{e}_{x_2} + A_3(x_1, x_2, x_3, t)\mathbf{e}_{x_3}, A_0(x_1, x_2, x_3, t) \tag{14a}$$

$$\mathbf{H}_{\text{Dirac}_{4 \times 4}} \Psi_D = \left(m c^2 a_0 + \sum_{j=1}^3 (a_j (p_j - e A_j) c + e A_0) \right) \Psi_D = i \hbar \partial_t \Psi_D$$

$$\mathbf{A}(x_1, x_2, x_3, t) = A_1(x_1, x_2, x_3, t)\mathbf{e}_{x_1} + A_2(x_1, x_2, x_3, t)\mathbf{e}_{x_2} + A_3(x_1, x_2, x_3, t)\mathbf{e}_{x_3}, A_0(x_1, x_2, x_3, t)$$

$$\Psi_D \equiv \begin{pmatrix} \Psi_{D_1} \\ \Psi_{D_2} \\ \Psi_{D_3} \\ \Psi_{D_4} \end{pmatrix} : \text{4-component Dirac wavefunction}$$

$$\Psi_{D_0} \equiv \begin{pmatrix} \Psi_{D_{10}} \\ \Psi_{D_{20}} \\ \Psi_{D_{30}} \\ \Psi_{D_{40}} \end{pmatrix} : \text{4-component Dirac Initial-State}$$

$$a_0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, a_1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

$$a_2 = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}, a_3 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

Similarly for the Majorana equation minimal-coupled to the EM gauge field

$$-imc\sigma^2 \rho_M^* + (i\hbar\sigma^\mu \partial_\mu - eA_\mu)\rho_M = 0$$

$$A_\mu \equiv \begin{pmatrix} \mathbf{A}(x_1, x_2, x_3, t) = A_1(x_1, x_2, x_3, t)\mathbf{e}_{x_1} + A_2(x_1, x_2, x_3, t)\mathbf{e}_{x_2} + A_3(x_1, x_2, x_3, t)\mathbf{e}_{x_3}, \\ A_0(x_1, x_2, x_3, t) \end{pmatrix}$$

$$\rho_M = \begin{pmatrix} \rho_{M_1} \\ \rho_{M_2} \end{pmatrix} : \text{2-component Majorana wavefunction,}$$

$$\rho_{M_0} = \begin{pmatrix} \rho_{M_{10}} \\ \rho_{M_{20}} \end{pmatrix} : \text{2-component Majorana Initial-State}$$

$$\sigma^\mu : \text{usual } 2 \times 2 \text{ Pauli spin matrices } \sigma^{1,2,3}, \sigma^0 = -i\mathbf{I}_{2 \times 2} \tag{14b}$$

Now the connection between the Majorana (14b) ρ_M and Dirac (14a) Ψ_D wavefunctions subject to the Majorana self-conjugacy condition $\Psi_D = \Psi_D^C$ is thoroughly

discussed in the bibliography of [8]; only some key relationships between them are reproduced here for convenience

$$\Psi_D \equiv \begin{pmatrix} \Psi_{D1} \\ \Psi_{D2} \\ \Psi_{D3} \\ \Psi_{D4} \end{pmatrix} = \begin{pmatrix} \chi_D \\ \sigma_2 \phi_D^* \end{pmatrix}, \Psi_D^c = \begin{pmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{pmatrix} \Psi_D^{*Transpose} = \begin{pmatrix} \phi_D \\ \sigma_2 \chi_D^* \end{pmatrix},$$

$$\chi_D = \begin{pmatrix} \Psi_{D1} \\ \Psi_{D2} \end{pmatrix}, \sigma_2 \phi_D^* = \begin{pmatrix} \Psi_{D3} \\ \Psi_{D4} \end{pmatrix}, \phi_D = \begin{pmatrix} i\Psi_{D4}^* \\ -i\Psi_{D3}^* \end{pmatrix},$$

Majorana Self-Conjugacy condition $\Psi_D = \Psi_D^c$

$$\chi_D = \frac{1}{\sqrt{2}}(\rho_{M2} + i\rho_{M1}), \rho_{M2} = \frac{1}{\sqrt{2}}(\chi_D + \phi_D) = \frac{1}{\sqrt{2}} \begin{pmatrix} \Psi_{D1} + i\Psi_{D4}^* \\ \Psi_{D2} - i\Psi_{D3}^* \end{pmatrix}$$

$$\phi_D = \frac{1}{\sqrt{2}}(\rho_{M2} - i\rho_{M1}), \rho_{M1} = \frac{i}{\sqrt{2}}(\chi_D - \phi_D) = \frac{i}{\sqrt{2}} \begin{pmatrix} \Psi_{D1} - i\Psi_{D4}^* \\ \Psi_{D2} + i\Psi_{D3}^* \end{pmatrix}$$

$$\rho_M = \begin{pmatrix} \rho_{M1} \\ \rho_{M2} \end{pmatrix} \quad (14c)$$

So by way of (14c), given the related Dirac wavefunction and subject to the Majorana self-conjugacy condition $\Psi_D = \Psi_D^c$, the Majorana wavefunction ascends naturally. Moreover, by way of the HOA method, substituting the Dirac Hamiltonian of (14a) gives the quantum phase space dynamics of the Dirac system for initial conditions and EM gauge fields of general form.

$$\hat{\mathbf{H}}_{\text{Dirac}_{4 \times 4}} \begin{pmatrix} i\hbar\partial_{p_1} + \alpha_1 x_1, i\hbar\partial_{p_2} + \alpha_2 x_2, i\hbar\partial_{p_3} + \alpha_3 x_3; \\ -i\hbar\partial_{x_1} + \gamma_1 p_1, -i\hbar\partial_{x_2} + \gamma_2 p_2, -i\hbar\partial_{x_3} + \gamma_3 p_3; t \end{pmatrix}$$

$$\Psi_D(x_1, x_2, x_3; p_1, p_2, p_3; t)$$

$$= i\hbar\partial_t \Psi_D(x_1, x_2, x_3; p_1, p_2, p_3; t)$$

$$\left(m_c^2 a_0 + \sum_{j=1}^3 \begin{pmatrix} a_j(-i\hbar\partial_{x_j} + \gamma_j p_j - eA_j(i\hbar\partial_{p_1} + \alpha_1 x_1, i\hbar\partial_{p_2} + \alpha_2 x_2, i\hbar\partial_{p_3} + \alpha_3 x_3, t))^c \\ +eA_0(i\hbar\partial_{p_1} + \alpha_1 x_1, i\hbar\partial_{p_2} + \alpha_2 x_2, i\hbar\partial_{p_3} + \alpha_3 x_3; .t) \end{pmatrix} \right) \Psi_D$$

$$= i\hbar\partial_t \Psi_D$$

$$\mathbf{A}(i\hbar\partial_{p_1} + \alpha_1 x_1, i\hbar\partial_{p_2} + \alpha_2 x_2, i\hbar\partial_{p_3} + \alpha_3 x_3, t)$$

$$= A_1(i\hbar\partial_{p_1} + \alpha_1 x_1, i\hbar\partial_{p_2} + \alpha_2 x_2, i\hbar\partial_{p_3} + \alpha_3 x_3, t)\mathbf{e}_{x_1}$$

$$+ A_2(i\hbar\partial_{p_1} + \alpha_1 x_1, i\hbar\partial_{p_2} + \alpha_2 x_2, i\hbar\partial_{p_3} + \alpha_3 x_3, t)\mathbf{e}_{x_2}$$

$$+ A_3(i\hbar\partial_{p_1} + \alpha_1 x_1, i\hbar\partial_{p_2} + \alpha_2 x_2, i\hbar\partial_{p_3} + \alpha_3 x_3, t)\mathbf{e}_{x_3},$$

$$A_0(i\hbar\partial_{p_1} + \alpha_1 x_1, i\hbar\partial_{p_2} + \alpha_2 x_2, i\hbar\partial_{p_3} + \alpha_3 x_3, t)$$

$$\Psi_D \equiv \begin{pmatrix} \Psi_{D1} \\ \Psi_{D2} \\ \Psi_{D3} \\ \Psi_{D4} \end{pmatrix} : \text{4-component Dirac wavefunction} \tag{14d}$$

Hence the configuration space dynamics for the related minimal-coupled Dirac system

$$\begin{aligned} &\Psi_D \text{ configuration space } (x_1, x_2, x_3, t) \\ &= \begin{pmatrix} \Psi_{D1}(x_1, x_2, x_3, t) \\ \Psi_{D2}(x_1, x_2, x_3, t) \\ \Psi_{D3}(x_1, x_2, x_3, t) \\ \Psi_{D4}(x_1, x_2, x_3, t) \end{pmatrix}_{\text{configuration space}} \\ &= \int_{-\infty}^{\infty} \frac{e^{\frac{ix_1 p_1}{2\hbar}}}{\sqrt{4\pi\hbar}} \int_{-\infty}^{\infty} \frac{e^{\frac{ix_2 p_2}{2\hbar}}}{\sqrt{4\pi\hbar}} \int_{-\infty}^{\infty} \frac{e^{\frac{ix_3 p_3}{2\hbar}}}{\sqrt{4\pi\hbar}} L^{-1} \left(\begin{pmatrix} \bar{x}_1, \dots, \bar{x}_n; \\ \bar{p}_1, \dots, \bar{p}_n \end{pmatrix} \rightarrow \begin{pmatrix} x_1, \dots, x_n; \\ p_1, \dots, p_n \end{pmatrix} \right) \\ &e^{\left(m c^2 a_0 + \sum_{j=1}^3 a_j \begin{pmatrix} -i\hbar \bar{x}_j + \gamma_j p_j \\ -e A_j \begin{pmatrix} i\hbar \bar{p}_1 + \alpha_1 x_1, \\ i\hbar \bar{p}_2 + \alpha_2 x_2, \\ i\hbar \bar{p}_3 + \alpha_3 x_3, u \end{pmatrix} \end{pmatrix}^c \right)} du \begin{pmatrix} \tilde{\Psi}_{D01} \\ \tilde{\Psi}_{D02} \\ \tilde{\Psi}_{D03} \\ \tilde{\Psi}_{D04} \end{pmatrix} dp_1 dp_2 dp_3 \\ &\tilde{\Psi}_{D0} \left(\begin{pmatrix} \bar{x}_1, \bar{x}_2, \bar{x}_3; \\ \bar{p}_1, \bar{p}_2, \bar{p}_3; t = 0 \end{pmatrix} \right) \\ &= \begin{pmatrix} \tilde{\Psi}_{D01} \\ \tilde{\Psi}_{D02} \\ \tilde{\Psi}_{D03} \\ \tilde{\Psi}_{D04} \end{pmatrix} : \text{Transformed Initial-condition vector} \tag{14e} \end{aligned}$$

$$\begin{aligned} \rho_{M_1} &= \frac{i}{\sqrt{2}} \begin{pmatrix} \Psi_{D1}(x_1, x_2, x_3, t) - i\Psi_{D4}^*(x_1, x_2, x_3, t) \\ \Psi_{D2}(x_1, x_2, x_3, t) + i\Psi_{D3}^*(x_1, x_2, x_3, t) \end{pmatrix} \\ \rho_M \text{ configuration space} &= \begin{pmatrix} \rho_{M_1} \\ \rho_{M_2} \end{pmatrix}_{\text{configuration space}} \\ \rho_{M_0} \text{ configuration space} &= \begin{pmatrix} \rho_{M_{10}} \\ \rho_{M_{20}} \end{pmatrix}_{\text{configuration space}} \quad : \text{Majorana Initial-State} \\ \rho_{M_{20}} &= \frac{1}{\sqrt{2}} \begin{pmatrix} \Psi_{D1_0}(x_1, x_2, x_3, t) + i\Psi_{D4_0}^*(x_1, x_2, x_3, t) \\ \Psi_{D2_0}(x_1, x_2, x_3, t) - i\Psi_{D3_0}^*(x_1, x_2, x_3, t) \end{pmatrix} \\ \rho_{M_{10}} &= \frac{i}{\sqrt{2}} \begin{pmatrix} \Psi_{D1_0}(x_1, x_2, x_3, t) - i\Psi_{D4_0}^*(x_1, x_2, x_3, t) \\ \Psi_{D2_0}(x_1, x_2, x_3, t) + i\Psi_{D3_0}^*(x_1, x_2, x_3, t) \end{pmatrix} \end{aligned} \tag{14g}$$

3.5 Example 5. Dirac molecular Hamiltonian with pairwise Coulomb–Breit interaction

Now consider the example case of the relativistic molecular Hamiltonian with pairwise (DCB) Dirac–Coulomb–Briet interaction dynamics in quantum phase space. Here the Hamiltonian has the 4×4 matrix form

$$\begin{aligned} \hat{\mathbf{H}}_{4 \times 4}^{\text{DiracCoulombBreit}} &= \sum_A \left(a_{0_A} M_A c^2 + a_{x_A} \left(-i\hbar\partial_{x_A} + \frac{p_{x_A}}{2} \right) c \right. \\ &\quad \left. + a_{y_A} \left(-i\hbar\partial_{y_A} + \frac{p_{y_A}}{2} \right) c + a_{z_A} \left(-i\hbar\partial_{z_A} + \frac{p_{z_A}}{2} \right) \right) \\ &\quad + \sum_i \left(a_{0_i} m_e c^2 + a_{x_i} \left(-i\hbar\partial_{x_i} + \frac{p_{x_i}}{2} \right) c \right. \\ &\quad \left. + a_{y_i} \left(-i\hbar\partial_{y_i} + \frac{p_{y_i}}{2} \right) c + a_{z_i} \left(-i\hbar\partial_{z_i} + \frac{p_{z_i}}{2} \right) \right) \\ &\quad + \sum_{A < B} \frac{e^2}{8\pi\epsilon_0} \frac{Z_A Z_B \left(1 + \frac{1}{2} \left((\mathbf{a}_A \cdot \mathbf{a}_B) + \frac{(\mathbf{a}_A \cdot \mathbf{r}_{AB})(\mathbf{a}_B \cdot \mathbf{r}_{AB})}{r_{AB}^2} \right) \right)}{\left| \begin{aligned} &\left((i\hbar\partial_{p_{x_A}} + \frac{x_A}{2}) - (i\hbar\partial_{p_{x_B}} + \frac{x_B}{2}) \right)^2 \\ &+ \left((i\hbar\partial_{p_{y_A}} + \frac{y_A}{2}) - (i\hbar\partial_{p_{y_B}} + \frac{y_B}{2}) \right)^2 \\ &+ \left((i\hbar\partial_{p_{z_A}} + \frac{z_A}{2}) - (i\hbar\partial_{p_{z_B}} + \frac{z_B}{2}) \right)^2 \end{aligned} \right|} \end{aligned}$$

$$\begin{aligned}
 & + \sum_{i < j} \frac{e^2}{8\pi\epsilon_0} \frac{\left(1 + \frac{1}{2} \left((\mathbf{a}_i \cdot \mathbf{a}_j) + \frac{(\mathbf{a}_i \cdot \mathbf{r}_{ij})(\mathbf{a}_j \cdot \mathbf{r}_{ij})}{r_{ij}^2} \right) \right)}{\left| \left((i\hbar\partial_{p_{x_i}} + \frac{x_i}{2}) - (i\hbar\partial_{p_{x_j}} + \frac{x_j}{2}) \right)^2 \right.} \\
 & \quad \left. + \left((i\hbar\partial_{p_{y_i}} + \frac{y_i}{2}) - (i\hbar\partial_{p_{y_j}} + \frac{y_j}{2}) \right)^2 \right.} \\
 & \quad \left. + \left((i\hbar\partial_{p_{z_i}} + \frac{z_i}{2}) - (i\hbar\partial_{p_{z_j}} + \frac{z_j}{2}) \right)^2 \right|} \\
 & + \sum_{A,i} \frac{-Z_A e^2 \left(1 + \frac{1}{2} \left((\mathbf{a}_A \cdot \mathbf{a}_i) + \frac{(\mathbf{a}_A \cdot \mathbf{r}_{Ai})(\mathbf{a}_i \cdot \mathbf{r}_{Ai})}{r_{Ai}^2} \right) \right)}{\left| \left((i\hbar\partial_{p_{x_A}} + \frac{x_A}{2}) - (i\hbar\partial_{p_{x_i}} + \frac{x_i}{2}) \right)^2 \right.} \\
 & \quad \left. + \left((i\hbar\partial_{p_{y_A}} + \frac{y_A}{2}) - (i\hbar\partial_{p_{y_i}} + \frac{y_i}{2}) \right)^2 \right.} \\
 & \quad \left. + \left((i\hbar\partial_{p_{z_A}} + \frac{z_A}{2}) - (i\hbar\partial_{p_{z_i}} + \frac{z_i}{2}) \right)^2 \right|} \tag{15a}
 \end{aligned}$$

$$\mathbf{a}_0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \mathbf{a}_x = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \mathbf{a}_y = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}, \mathbf{a}_z = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

$$\mathbf{a} = a_x \hat{\mathbf{e}}_x + a_y \hat{\mathbf{e}}_y + a_z \hat{\mathbf{e}}_z$$

$$\sum_{i < j} \frac{1}{r_{ij}} \left(1 + \frac{1}{2} \left((\mathbf{a}_i \cdot \mathbf{a}_j) + \frac{(\mathbf{a}_i \cdot \mathbf{r}_{ij})(\mathbf{a}_j \cdot \mathbf{r}_{ij})}{r_{ij}^2} \right) \right),$$

$$\begin{aligned}
 \mathbf{r}_{ij} &= \left((i\hbar\partial_{p_{x_i}} + \frac{x_i}{2}) - (i\hbar\partial_{p_{x_j}} + \frac{x_j}{2}) \right) \hat{\mathbf{e}}_x \\
 &+ \left((i\hbar\partial_{p_{y_i}} + \frac{y_i}{2}) - (i\hbar\partial_{p_{y_j}} + \frac{y_j}{2}) \right) \hat{\mathbf{e}}_y + \left((i\hbar\partial_{p_{z_i}} + \frac{z_i}{2}) - (i\hbar\partial_{p_{z_j}} + \frac{z_j}{2}) \right) \hat{\mathbf{e}}_z \\
 r_{ij} &= \left| \left((i\hbar\partial_{p_{x_i}} + \frac{x_i}{2}) - (i\hbar\partial_{p_{x_j}} + \frac{x_j}{2}) \right) \hat{\mathbf{e}}_x \right. \\
 & \left. + \left((i\hbar\partial_{p_{y_i}} + \frac{y_i}{2}) - (i\hbar\partial_{p_{y_j}} + \frac{y_j}{2}) \right) \hat{\mathbf{e}}_y + \left((i\hbar\partial_{p_{z_i}} + \frac{z_i}{2}) - (i\hbar\partial_{p_{z_j}} + \frac{z_j}{2}) \right) \hat{\mathbf{e}}_z \right| \tag{15b}
 \end{aligned}$$

Since the Hamiltonian of this system is matrix-valued $\hat{\mathbf{H}}_{4 \times 4 \text{ DiracCoulombBreit Molecular}}$, the quantum phase space wavefunction is a column vector $\Psi_{4 \times 1 \text{ column vector}}$

$$\Psi_{4 \times 1 \text{ column vector}} \begin{pmatrix} x_A, y_A, z_A, x_B, y_B, z_B, \\ x_i, y_i, z_i, x_j, y_j, z_j; \\ p_{x_A}, p_{y_A}, p_{z_A}, p_{x_B}, p_{y_B}, p_{z_B}, \\ p_{x_i}, p_{y_i}, p_{z_i}, p_{x_j}, p_{y_j}, p_{z_j}; t \end{pmatrix}$$

$$\begin{aligned}
 &= L^{-1} \left(\begin{matrix} (\bar{x}_A, \bar{y}_A, \bar{z}_A, \bar{x}_B, \bar{y}_B, \bar{z}_B, \\ \bar{x}_i, \bar{y}_i, \bar{z}_i, \bar{x}_j, \bar{y}_j, \bar{z}_j \\ \rightarrow (x_A, y_A, z_A, x_B, y_B, z_B, \\ x_i, y_i, z_i, x_j, y_j, z_j) \end{matrix} \right) \left[L^{-1} \left(\begin{matrix} (p_{x_A}, p_{y_A}, p_{z_A}, p_{x_B}, p_{y_B}, p_{z_B}, \\ p_{x_i}, p_{y_i}, p_{z_i}, p_{x_j}, p_{y_j}, p_{z_j} \\ \rightarrow (p_{x_A}, p_{y_A}, p_{z_A}, p_{x_B}, p_{y_B}, p_{z_B}, \\ p_{x_i}, p_{y_i}, p_{z_i}, p_{x_j}, p_{y_j}, p_{z_j} \end{matrix} \right) \right) \\
 &\left[\int_0^t \int_{-\infty}^{\infty} \hat{H}_{4 \times 4 \text{DiracCoulombBreit}}^{\text{Molecular}} \left(\begin{matrix} -i\hbar\bar{x}_A + \frac{p_{x_A}}{2}, -i\hbar\bar{y}_A + \frac{p_{y_A}}{2}, -i\hbar\bar{z}_A + \frac{p_{z_A}}{2}, -i\hbar\bar{x}_i + \frac{p_{x_i}}{2}, -i\hbar\bar{y}_i + \frac{p_{y_i}}{2}, \\ -i\hbar\bar{z}_i + \frac{p_{z_i}}{2}; \\ i\hbar\bar{p}_{x_A} + \frac{x_A}{2}, i\hbar\bar{p}_{y_A} + \frac{y_A}{2}, i\hbar\bar{p}_{z_A} + \frac{z_A}{2}, i\hbar\bar{p}_{x_B} + \frac{x_B}{2}, i\hbar\bar{p}_{y_B} + \frac{y_B}{2}, i\hbar\bar{p}_{z_B} \\ + \frac{z_B}{2}, \\ i\hbar\bar{p}_{x_i} + \frac{x_i}{2}, i\hbar\bar{p}_{y_i} + \frac{y_i}{2}, i\hbar\bar{p}_{z_i} + \frac{z_i}{2}, i\hbar\bar{p}_{x_j} + \frac{x_j}{2}, i\hbar\bar{p}_{y_j} + \frac{y_j}{2}, i\hbar\bar{p}_{z_j} + \frac{z_j}{2} \end{matrix} \right) du \right] \\
 &\times \underbrace{\Psi}_{4 \times 1 \text{ column vector}}(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t = 0) \tag{15c}
 \end{aligned}$$

$$\begin{aligned}
 \hat{H}_{4 \times 4 \text{DiracCoulombBreit}}^{\text{Molecular}} &= \sum_A \left(a_{0_A} M_A c^2 + a_{x_A} \left(-i\hbar\bar{x}_A + \frac{p_{x_A}}{2} \right) c \right. \\
 &+ a_{y_A} \left(-i\hbar\bar{y}_A + \frac{p_{y_A}}{2} \right) c + a_{z_A} \left(-i\hbar\bar{z}_A + \frac{p_{z_A}}{2} \right) \Big) \\
 &+ \sum_i \left(a_{0_i} m_e c^2 + a_{x_i} \left(-i\hbar\bar{x}_i + \frac{p_{x_i}}{2} \right) c + a_{y_i} \left(-i\hbar\bar{y}_i + \frac{p_{y_i}}{2} \right) c \right. \\
 &+ a_{z_i} \left(-i\hbar\bar{z}_i + \frac{p_{z_i}}{2} \right) \Big) \\
 &+ \sum_{A < B} \frac{e^2}{8\pi\epsilon_0} \frac{Z_A Z_B \left(1 + \frac{1}{2} \left((\mathbf{a}_A \cdot \mathbf{a}_B) + \frac{(\mathbf{a}_A \cdot \mathbf{r}_{AB})(\mathbf{a}_B \cdot \mathbf{r}_{AB})}{r_{AB}^2} \right) \right)}{\left| \begin{matrix} ((i\hbar\bar{p}_{x_A} + \frac{x_A}{2}) - (i\hbar\bar{p}_{x_B} + \frac{x_B}{2}))^2 \\ + ((i\hbar\bar{p}_{y_A} + \frac{y_A}{2}) - (i\hbar\bar{p}_{y_B} + \frac{y_B}{2}))^2 \\ + ((i\hbar\bar{p}_{z_A} + \frac{z_A}{2}) - (i\hbar\bar{p}_{z_B} + \frac{z_B}{2}))^2 \end{matrix} \right|} \\
 &+ \sum_{i < j} \frac{e^2}{8\pi\epsilon_0} \frac{\left(1 + \frac{1}{2} \left((\mathbf{a}_i \cdot \mathbf{a}_j) + \frac{(\mathbf{a}_i \cdot \mathbf{r}_{ij})(\mathbf{a}_j \cdot \mathbf{r}_{ij})}{r_{ij}^2} \right) \right)}{\left| \begin{matrix} ((i\hbar\bar{p}_{x_i} + \frac{x_i}{2}) - (i\hbar\bar{p}_{x_j} + \frac{x_j}{2}))^2 \\ + ((i\hbar\bar{p}_{y_i} + \frac{y_i}{2}) - (i\hbar\bar{p}_{y_j} + \frac{y_j}{2}))^2 \\ + ((i\hbar\bar{p}_{z_i} + \frac{z_i}{2}) - (i\hbar\bar{p}_{z_j} + \frac{z_j}{2}))^2 \end{matrix} \right|} \\
 &+ \sum_{A, i} \frac{-Z_A e^2 \left(1 + \frac{1}{2} \left((\mathbf{a}_A \cdot \mathbf{a}_i) + \frac{(\mathbf{a}_A \cdot \mathbf{r}_{Ai})(\mathbf{a}_i \cdot \mathbf{r}_{Ai})}{r_{Ai}^2} \right) \right)}{\left| \begin{matrix} ((i\hbar\bar{p}_{x_A} + \frac{x_A}{2}) - (i\hbar\bar{p}_{x_i} + \frac{x_i}{2}))^2 \\ + ((i\hbar\bar{p}_{y_A} + \frac{y_A}{2}) - (i\hbar\bar{p}_{y_i} + \frac{y_i}{2}))^2 \\ + ((i\hbar\bar{p}_{z_A} + \frac{z_A}{2}) - (i\hbar\bar{p}_{z_i} + \frac{z_i}{2}))^2 \end{matrix} \right|} \tag{15d}
 \end{aligned}$$

4 Comment

Though Examples 1–5 are useful applications of HOA outright for various chemical applications, so also are various combinations of these Examples. For instance,

mixing the results of Example 2 (Schrödinger Hamiltonian with SHOs having N -Arbitrary Masses in Pairwise Anisotropic Interaction) with Example 3 (Schrödinger Molecular Hamiltonian with Pairwise Coulomb Interaction) utilizing the extension to time-dependent parameters in Example 1 (1-dim Simple Harmonic Oscillator), one arrives at a QPSR description of non-relativistic molecular systems interacting with an external time-varying bath environment with anisotropic harmonic constitutive properties. Further, Example 4 (Dirac and Majorana Equations with Minimum-Coupled Electromagnetic Gauge Field) and Example 5 (Dirac Molecular Hamiltonian with Pairwise Coulomb-Breit Interaction) may be mixed to yield a QPSR description of relativistic molecular systems in external electromagnetic fields [9, 10].

Thus far, the Examples of the HOA results with usefulness in Chemical Dynamics have been based on a direct use of particular Hamiltonians to model the particular scenarios in question. We now will consider some additional Examples where the HOA results are used as a formal tool to achieve exact analytical solutions of more general formal mathematical problems of interest in Mathematical Chemistry and Beyond.

4.1 Example 6. Exact quadrature solution of linear eigenvalue problem for general class of variable coefficient differential operators

Recall from the HOA Recap in this note, that

Notwithstanding its quantum mechanical origins, the HOA scheme takes on a life of its own and transcends the limits of quantum applications to address a wide variety of purely formal mathematical problems as well. Among other things, the result provides a formula for obtaining an exact solution to a wide variety of variable-coefficient integro-differential equations. Since the functional dependence of the Hamiltonian operator as considered is in general arbitrary upon its arguments (i.e., independent variables, derivative operator symbols [including negative powers thereof, thus the possible integral character]), then its multivariable extension can be interpreted as the most general variable coefficient partial differential operator. Moreover, it is not confined to being a scalar or even vector operator, but may be generally construed an arbitrary rank matrix operator. In all cases of course, its rank dictates the matrix rank of the wavefunction solution.

Recall Eq. (10) of the Recap

$$\begin{aligned} & \hat{H}_{\text{configuration space}}(x_1, \dots, x_n, -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}, t)\Psi_{\text{configuration space}}(x_1, \dots, x_n, t) \\ &= i\hbar\partial_t\Psi_{\text{configuration space}}(x_1, \dots, x_n, t) \\ & \Psi_{\text{configuration space}}(x_1, \dots, x_n, t) \\ &= \int_{-\infty}^{\infty} \frac{e^{\frac{ix_1 p_1}{2\hbar}}}{\sqrt{4\pi\hbar}} \dots \int_{-\infty}^{\infty} \frac{e^{\frac{ix_n p_n}{2\hbar}}}{\sqrt{4\pi\hbar}} \Psi(x_1, \dots, x_n; p_1, \dots, p_n; t) dp_1 \dots dp_n \\ & \Psi_{\text{configuration space}}(x_1, \dots, x_n, t) \end{aligned}$$

$$\begin{aligned}
 &= \int_{-\infty}^{\infty} \frac{e^{-\frac{i x_1 p_1}{2\hbar}}}{\sqrt{4\pi\hbar}} \cdots \int_{-\infty}^{\infty} \frac{e^{-\frac{i x_n p_n}{2\hbar}}}{\sqrt{4\pi\hbar}} L^{-1} \left(\begin{matrix} (\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n) \\ \mapsto (x_1, \dots, x_n; p_1, \dots, p_n) \end{matrix} \right) \\
 &\left[e^{-\frac{i}{\hbar} \int_0^t \hat{H}_{\text{configuration space}} \left(\begin{matrix} x_1, \dots, x_n, \\ -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}, u \end{matrix} \right) (x_1, \dots, x_n) \mapsto (i\hbar\bar{p}_1 + \alpha_1 x_1, \dots, i\hbar\bar{p}_n + \alpha_n x_n) \right. \\
 &\left. \times \tilde{\Psi}_0_{\text{configuration space}} (\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t = 0) \right] \\
 &\times dp_1 \dots dp_n
 \end{aligned}$$

Now suppose that

$$\begin{aligned}
 &\hat{H}_{\text{configuration space}} (x_1, \dots, x_n, -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}, t) \\
 &= \hat{H}_{\text{configuration space}} (x_1, \dots, x_n, -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}) \\
 &\quad \text{scleronomic} \\
 &\hat{H}_{\text{configuration space}} (x_1, \dots, x_n, -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}) \Psi_{\text{configuration space}} (x_1, \dots, x_n, t) \\
 &\quad \text{scleronomic} \\
 &= i\hbar\partial_t \Psi_{\text{configuration space}} (x_1, \dots, x_n, t)
 \end{aligned} \tag{16a}$$

Hence Fourier transforming (16a) with respect to t

$$\begin{aligned}
 F_{t \rightarrow \omega} [f(t)] &= \int_{t_0}^{\infty} f(t) e^{-it\omega} dt \\
 F_{t \rightarrow \omega} \left[\begin{matrix} \hat{H}_{\text{configuration space}} (x_1, \dots, x_n, -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}) \Psi_{\text{configuration space}} (x_1, \dots, x_n, t) \\ \text{scleronomic} \\ = i\hbar\partial_t \Psi_{\text{configuration space}} (x_1, \dots, x_n, t) \end{matrix} \right] \\
 &= \hat{H}_{\text{configuration space}} (x_1, \dots, x_n, -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}) \Psi_{\text{configuration space}} (x_1, \dots, x_n, \omega) \\
 &\quad \text{scleronomic} \qquad \qquad \qquad \omega \text{ eigenvalue} \\
 &= \hbar\omega \Psi_{\text{configuration space}} (x_1, \dots, x_n, \omega) \\
 &\quad \omega \text{ eigenvalue}
 \end{aligned} \tag{16b}$$

So

$$\begin{aligned}
 &\hat{H}_{\text{configuration space}} (x_1, \dots, x_n, -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n}) \Psi_{\text{configuration space}} (x_1, \dots, x_n, \omega) \\
 &\quad \text{scleronomic} \qquad \qquad \qquad \omega \text{ eigenvalue} \\
 &= \hbar\omega \Psi_{\text{configuration space}} (x_1, \dots, x_n, \omega) \\
 &\quad \omega \text{ eigenvalue} \\
 &\ni F_{t \rightarrow \omega} \left(\tilde{\Psi}_0_{\text{configuration space}} \left(\begin{matrix} \bar{x}_1, \dots, \bar{x}_n; \\ \bar{p}_1, \dots, \bar{p}_n; t = 0 \end{matrix} \right) \right. \\
 &\left. e^{-\frac{i}{\hbar} t \hat{H}_{\text{configuration space}} \left(\begin{matrix} x_1, \dots, x_n, \\ -i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n} \end{matrix} \right) \left(\begin{matrix} (x_1, \dots, x_n) \\ \mapsto (i\hbar\bar{p}_1 + \alpha_1 x_1, \dots, i\hbar\bar{p}_n + \alpha_n x_n) \\ \left(-i\hbar\partial_{x_1}, \dots, -i\hbar\partial_{x_n} \right) \\ \mapsto (-i\hbar\bar{x}_1 + \gamma_1 p_1, \dots, -i\hbar\bar{x}_n + \gamma_n p_n) \end{matrix} \right)} \right)
 \end{aligned}$$

$$\begin{aligned}
 &= \check{\Psi}_0 \text{ configuration space} \left(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t = 0 \right) \\
 &\times \delta \left(\omega - \frac{1}{\hbar} \hat{H}_{\text{configuration space}} \left(x_1, \dots, x_n, -i\hbar \partial_{x_1}, \dots, -i\hbar \partial_{x_n} \right) \begin{pmatrix} (x_1, \dots, x_n) \\ \mapsto (i\hbar \bar{p}_1 + \alpha_1 x_1, \dots, i\hbar \bar{p}_n + \alpha_n x_n) \\ (-i\hbar \partial_{x_1}, \dots, -i\hbar \partial_{x_n}) \\ \mapsto (-i\hbar \bar{x}_1 + \gamma_1 p_1, \dots, -i\hbar \bar{x}_n + \gamma_n p_n) \end{pmatrix} \right) \quad (16c)
 \end{aligned}$$

Hence

$$\begin{aligned}
 &F_{t \rightarrow \omega} \left(\Psi_{\text{configuration space}}(x_1, \dots, x_n, t) = \int_{-\infty}^{\infty} \frac{e^{\frac{i x_1 p_1}{2\hbar}}}{\sqrt{4\pi\hbar}} \dots \int_{-\infty}^{\infty} \frac{e^{\frac{i x_n p_n}{2\hbar}}}{\sqrt{4\pi\hbar}} L^{-1} \begin{pmatrix} (\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n) \\ \mapsto (x_1, \dots, x_n; p_1, \dots, p_n) \end{pmatrix} \right) \\
 &\left[e \begin{pmatrix} \frac{-i}{\hbar} t \hat{H}_{\text{configuration space}} \left(x_1, \dots, x_n, -i\hbar \partial_{x_1}, \dots, -i\hbar \partial_{x_n} \right) \begin{pmatrix} (x_1, \dots, x_n) \\ \mapsto (i\hbar \bar{p}_1 + \alpha_1 x_1, \dots, i\hbar \bar{p}_n + \alpha_n x_n) \\ (-i\hbar \partial_{x_1}, \dots, -i\hbar \partial_{x_n}) \\ \mapsto (-i\hbar \bar{x}_1 + \gamma_1 p_1, \dots, -i\hbar \bar{x}_n + \gamma_n p_n) \end{pmatrix} \\ \times \check{\Psi}_0 \text{ configuration space} \left(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t = 0 \right) \end{pmatrix} dp_1 \dots dp_n \right] \\
 &\Psi_{\text{configuration space}}(x_1, \dots, x_n, \omega) \\
 &\omega \text{ eigenvalue} \\
 &= \int_{-\infty}^{\infty} \frac{e^{\frac{i x_1 p_1}{2\hbar}}}{\sqrt{4\pi\hbar}} \dots \int_{-\infty}^{\infty} \frac{e^{\frac{i x_n p_n}{2\hbar}}}{\sqrt{4\pi\hbar}} L^{-1} \begin{pmatrix} (\bar{x}_1, \dots, \bar{x}_n) \\ \bar{p}_1, \dots, \bar{p}_n \\ \mapsto (x_1, \dots, x_n) \\ \mapsto (p_1, \dots, p_n) \end{pmatrix} \\
 &\left[\sqrt{2\pi} \delta \left(\omega - \frac{1}{\hbar} \hat{H}_{\text{configuration space}} \left(x_1, \dots, x_n, -i\hbar \partial_{x_1}, \dots, -i\hbar \partial_{x_n} \right) \begin{pmatrix} (x_1, \dots, x_n) \\ \mapsto (i\hbar \bar{p}_1 + \alpha_1 x_1, \dots, i\hbar \bar{p}_n + \alpha_n x_n) \\ (-i\hbar \partial_{x_1}, \dots, -i\hbar \partial_{x_n}) \\ \mapsto (-i\hbar \bar{x}_1 + \gamma_1 p_1, \dots, -i\hbar \bar{x}_n + \gamma_n p_n) \end{pmatrix} \right) \right. \\
 &\left. \times \check{\Psi}_0 \text{ configuration space} \left(\bar{x}_1, \dots, \bar{x}_n; \bar{p}_1, \dots, \bar{p}_n; t = 0 \right) \right] \\
 &\times dp_1 \dots dp_n \quad (16d)
 \end{aligned}$$

To facilitate the evaluation of (16e) the identity for Dirac Delta functions is useful

$$\delta(g(u)) = \sum_{j=1}^n \frac{\delta(u - u_j)}{|(D_u g(u))|_{u=u_j}}, \ni g(u_j) = 0, (D_u g(u))|_{u=u_j} \neq 0$$

Which completes the construction of the result.

To illustrate this, consider the Example 1 (1-dim SHO) with constant strength a . Applying the formalism above in (16d) to the term from (11d) yields

$$\begin{aligned} & \left(\frac{(-i\hbar\partial_x)^2}{2m} + ax^2 \right) \Psi_{\text{configuration space}}(x, t) = i\hbar\partial_t \Psi_{\text{configuration space}}(x, t) \\ & F_{t \rightarrow \omega} \left(\Psi_{\text{configuration space}}(x, t) = \int_{-\infty}^{\infty} \frac{e^{\frac{ixp}{2\hbar}}}{\sqrt{4\pi\hbar}} L_{\left(\begin{smallmatrix} (\bar{x}; \bar{p}) \\ \rightarrow (x; p) \end{smallmatrix}\right)}^{-1} \left[\tilde{\Psi}_0(\bar{x}, \bar{p}, t=0) e^{\frac{-i}{\hbar} t \left(\frac{(-i\hbar\partial_x)^2}{2m} + ax^2 \right)} \begin{matrix} (x) \\ \mapsto (i\hbar\bar{p} + \alpha x) \\ (-i\hbar\partial_x) \\ \mapsto (-i\hbar\bar{x} + \gamma p) \end{matrix} \right] dp \right) \\ & \Psi_{\text{configuration space}}(x, \omega) \\ & \omega \text{ eigenvalue} \\ & = \int_{-\infty}^{\infty} \frac{e^{\frac{ixp}{2\hbar}}}{\sqrt{4\pi\hbar}} L_{\left(\begin{smallmatrix} (\bar{x}; \bar{p}) \\ \rightarrow (x; p) \end{smallmatrix}\right)}^{-1} \left[\sqrt{2\pi} \tilde{\Psi}_0(\bar{x}, \bar{p}, t=0) \delta \left(\omega - \frac{1}{\hbar} \left(\frac{(-i\hbar\bar{x} + \frac{p}{2})^2}{2m} + a \left(i\hbar\bar{p} + \frac{x}{2} \right)^2 \right) \right) \right] dp \\ & \left(\frac{(-i\hbar\partial_x)^2}{2m} + ax^2 - \hbar\omega \right) \Psi_{\text{configuration space}}(x, \omega) = 0 \end{aligned} \tag{16e}$$

Just to point out, if the potential term of the SHO above ax^2 is replaced with a potential term of arbitrary functional profile as $V(x)$ then (16e) generalizes to

$$\begin{aligned} & \left(\frac{(-i\hbar\partial_x)^2}{2m} + V(x) \right) \Psi_{\text{configuration space}}(x, t) = i\hbar\partial_t \Psi_{\text{configuration space}}(x, t) \\ & F_{t \rightarrow \omega} \left(\Psi_{\text{configuration space}}(x, t) = \int_{-\infty}^{\infty} \frac{e^{\frac{ixp}{2\hbar}}}{\sqrt{4\pi\hbar}} L_{\left(\begin{smallmatrix} (\bar{x}; \bar{p}) \\ \rightarrow (x; p) \end{smallmatrix}\right)}^{-1} \left[\tilde{\Psi}_0(\bar{x}, \bar{p}, t=0) e^{\frac{-i}{\hbar} t \left(\frac{(-i\hbar\partial_x)^2}{2m} + V(x) \right)} \begin{matrix} (x) \\ \mapsto (i\hbar\bar{p} + \alpha x) \\ (-i\hbar\partial_x) \\ \mapsto (-i\hbar\bar{x} + \gamma p) \end{matrix} \right] dp \right) \\ & \Psi_{\text{configuration space}}(x, \omega) \\ & \omega \text{ eigenvalue} \\ & = \int_{-\infty}^{\infty} \frac{e^{\frac{ixp}{2\hbar}}}{\sqrt{4\pi\hbar}} L_{\left(\begin{smallmatrix} (\bar{x}; \bar{p}) \\ \rightarrow (x; p) \end{smallmatrix}\right)}^{-1} \left[\sqrt{2\pi} \tilde{\Psi}_0(\bar{x}, \bar{p}, t=0) \right. \\ & \left. \delta \left(\omega - \frac{1}{\hbar} \left(\frac{(-i\hbar\bar{x} + \frac{p}{2})^2}{2m} + V \left(i\hbar\bar{p} + \frac{x}{2} \right) \right) \right) \right] dp \\ & \left(\frac{(-i\hbar\partial_x)^2}{2m} + V(x) - \hbar\omega \right) \Psi_{\text{configuration space}}(x, \omega) = 0 \end{aligned} \tag{16f}$$

It is worth re-emphasizing that the result (16d) of course is immediately applicable to non-seperable Hamiltonians in general, such as Example 3 (SMH with Pairwise Coulomb Interaction), yielding the solution of the radial Molecular Schrodinger eigenvalue equation and many others.

4.2 Example 7. Exact quadrature solution of general class of variable-coefficient differential equations

In view of the arbitrary functional form of the Hamiltonian and its connection with a Lagrangian [11–13] for the given problem,

$$H(x_1, \dots, x_n; p_1, \dots, p_n; t) = \sum_{j=1}^n p_j \dot{x}_j - L(x_1, \dots, x_n; \dot{x}_1, \dots, \dot{x}_n; t)$$

$$p_j = \partial_{\dot{x}_j} L(x_1, \dots, x_n; \dot{x}_1, \dots, \dot{x}_n; t) \quad (17a)$$

Consider now the equations of motion for the case of an external force $F(x_1, \dots, x_n; \dot{x}_1, \dots, \dot{x}_n; t)$ (viz the GHP (Generalised Hamilton Principle) given as

$$(-D_t) \partial_{\dot{x}_j} L(x_1, \dots, x_n; \dot{x}_1, \dots, \dot{x}_n; t) + \partial_{x_j} L(x_1, \dots, x_n; \dot{x}_1, \dots, \dot{x}_n; t) = F(x_1, \dots, x_n; \dot{x}_1, \dots, \dot{x}_n; t) \quad (17b)$$

It follows that (17b) extends naturally to accommodate higher-order derivatives for several variables, though the notation becomes cumbersome [12, 13]. As such we will below only construct the results for the case of one dependent variable x as

$$\sum_{j=1}^n (-D_t)^j \partial_{(D_t)^j x} L(x; \dot{x}; \ddot{x}; \dots; D_t^n x; t) + \partial_x L(x; \dot{x}; \ddot{x}; \dots; D_t^n x; t) = F(x; \dot{x}; \ddot{x}; \dots; D_t^n x; t)$$

for example $n = 4$ yields

$$\left(D_t^4 \partial_{D_t^4 x} - D_t^3 \partial_{D_t^3 x} + D_t^2 \partial_{D_t^2 x} - (D_t) \partial_{D_t x} + \partial_x \right) \times L \left(x; \dot{x}; \ddot{x}; \ddot{\ddot{x}}; \left(\frac{dx}{dt} \right)^4; t \right) = F \left(x; \dot{x}; \ddot{x}; \ddot{\ddot{x}}; \left(\frac{dx}{dt} \right)^4; t \right) \quad (17c)$$

In turn, these order- n derivative Lagrangians are reducible to first-order derivative systems by way of variable substitutions [12, 13]. In this note, the properties in (17b) and (17c) are pointed out explicitly, as they form the essential basis for applying to HOA scheme to any system that can be put in the Hamiltonian form: from higher-order Lagrangian systems of discrete particles to continuous fields [11–15]; they all admit to HOA solution as they are all ultimately transformable to the Hamiltonian formulation of dynamics. So, without loss of generality, we consider the case of (17b) in one dependent variable x

$$(-D_t)\partial_{\dot{x}}L(x; \dot{x}; t) + \partial_xL(x; \dot{x}; t) = F(x; \dot{x}; t) \tag{17d}$$

Now to illustrate HOA in the context of this Generalised Hamiltonian–Lagrangian connection, take the Lagrangian $L(x; \dot{x}; t) = \frac{m(\dot{x}^2)}{2} - a(t)x^2$ and no external term $F(x; \dot{x}; t) = 0$ from the GHP, yielding from (17d)

$$\begin{aligned} (-D_t)\partial_{\dot{x}}\left(\frac{m(\dot{x}^2)}{2} - a(t)x^2\right) + \partial_x\left(\frac{m(\dot{x}^2)}{2} - a(t)x^2\right) &= 0 \\ \frac{m\ddot{x}}{2} + a(t)x &= 0 \end{aligned} \tag{17e}$$

which is the equation of motion for the classical SHO Lagrangian with arbitrary time-dependent strength $a(t)$ therein. By way of (17a), the Hamiltonian that corresponds to the system in (17e) is $H = \frac{p^2}{2m} + a(t)x^2$: this is clearly the Hamiltonian for Example 1 herein: the quantum version of this system. Following Example 1, the QPSR of this system is given by

$$\begin{aligned} &\left(\frac{(-i\hbar\partial_x + \frac{p}{2})^2}{2m} + a(t)\left(i\hbar\partial_p + \frac{x}{2}\right)^2\right)\Psi(x; p; t) = i\hbar\partial_t\Psi(x; p; t) \\ &\left(\frac{(-i\hbar\bar{x} + \frac{p}{2})^2}{2m} + a(t)\left(i\hbar\bar{p} + \frac{x}{2}\right)^2\right)\check{\Psi}(\bar{x}; \bar{p}; t) = i\hbar\partial_t\check{\Psi}(\bar{x}; \bar{p}; t) \\ \Psi(x; p; t) &= L_{((\bar{x})\rightarrow(x))}^{-1} \left[L_{((\bar{p})\rightarrow(p))}^{-1} \left[\begin{aligned} &e^{-\frac{i\left(t\left(\frac{-i\hbar\bar{x} + \frac{p}{2}}{2m}\right)^2 + \int_0^t a(u)du\left(i\hbar\bar{p} + \frac{x}{2}\right)^2\right)}{\hbar} \\ &\times \check{\Psi}_0(\bar{x}; \bar{p}; t = 0) \end{aligned} \right] \right] \tag{11d} \end{aligned}$$

With the configuration space wavefunction via QPSR wavefunction for this system given as

$$\begin{aligned} \Psi_{\text{configuration space}}(x, t) &= \int_{-\infty}^{\infty} \frac{e^{\frac{ixp}{\hbar}}}{\sqrt{4\pi\hbar}} \\ &\left[\underbrace{\Psi_0(x, p, t = 0)}_{x,p} \ast \sqrt{\frac{-m}{2\int_0^t a(u)du}} e^{i\left(\frac{p^2 + 2mx^2}{4\hbar t} \int_0^t a(u)du\right)} \right] dp \tag{11e} \end{aligned}$$

Now it follows by way of Ehrenfest’s Theorem that the expectation value of the position [also momentum] operator follows its classical counterpart’s equations of motion in any framework (e.g., Hamiltonian, Lagrangian, etc). Following the Recap herein, applying the configuration position operator $\hat{x} \equiv x$ to the system wavefunction (11e) to yield the expectation value of the position operator as

$$\begin{aligned} \langle x(t) \rangle &= \int_{\text{Configuration Space}} (\Psi_{\text{configuration space}}^*(x, t)(x) \Psi_{\text{configuration space}}(x, t)) dx \\ &= \int_{-\infty}^{\infty} \frac{e^{\frac{ixp}{2\hbar}}}{\sqrt{4\pi\hbar}} \left[\Psi_0(x, p, t = 0) \underbrace{*}_{x,p} \sqrt{\frac{-m}{2 \int_0^t a(u) du}} \frac{e^{i\left(\frac{p^2+2mx^2 \int_0^t a(u) du}{4\hbar t \int_0^t a(u) du}\right)}}{2\pi\hbar t} \right] dp \end{aligned} \quad (17f)$$

So

$$\begin{aligned} \langle x(t) \rangle &= \int_{\text{Configuration Space}} |\Psi_{\text{configuration space}}(x, t)|^2 x dx \\ &= \left| \int_{-\infty}^{\infty} \frac{e^{\frac{ixp}{2\hbar}}}{\sqrt{4\pi\hbar}} \left[\Psi_0(x, p, t = 0) \underbrace{*}_{x,p} \sqrt{\frac{-m}{2 \int_0^t a(u) du}} \frac{e^{i\left(\frac{p^2+2mx^2 \int_0^t a(u) du}{4\hbar t \int_0^t a(u) du}\right)}}{2\pi\hbar t} \right] dp \right|^2 \end{aligned} \quad (17g)$$

The upshot of Eq. (17g) is that $\langle x(t) \rangle$ follows the same equation of motion (17e). Therefore

$$\begin{aligned} \frac{m \ddot{\langle x(t) \rangle}}{2} + a(t) \langle x(t) \rangle &= 0 \\ \langle x(t) \rangle &= \int_{\text{Configuration Space}} \left| \int_{-\infty}^{\infty} \frac{e^{\frac{ixp}{2\hbar}}}{\sqrt{4\pi\hbar}} \left[\Psi_0(x, p, t = 0) \underbrace{*}_{x,p} \sqrt{\frac{-m}{2 \int_0^t a(u) du}} \frac{e^{i\left(\frac{p^2+2mx^2 \int_0^t a(u) du}{4\hbar t \int_0^t a(u) du}\right)}}{2\pi\hbar t} \right] dp \right|^2 x dx \end{aligned} \quad (17h)$$

Thus Example 7 above provides an exact analytical quadrature solution to the given related classical equations of motion as well. By way of the Hamiltonian-Lagrangian correspondence, though the variables are different, (17h) provides an exact analytical quadrature solution of the purely mathematical problem of the exact analytical quadrature solution to the second-order linear ordinary differential equation with arbitrary variable coefficient in its canonical homogeneous form

$$\ddot{y}(t) + b(t)y(t) = 0$$

a problem which should require no introduction.

Finally, consider now the Lagrangian $L(x; \dot{x}; t) = \frac{5(\dot{x}^2)}{4} + \frac{x^{\frac{5}{2}}}{t^{\frac{1}{2}}}$ and no external term $F(x; \dot{x}; t) = 0$ from the GHP, yielding from (17d)

$$(-D_t)\partial_{\dot{x}}\left(\frac{5(\dot{x}^2)}{4} + \frac{x^{\frac{5}{2}}}{t^{\frac{1}{2}}}\right) + \partial_x\left(\frac{5(\dot{x}^2)}{4} + \frac{x^{\frac{5}{2}}}{t^{\frac{1}{2}}}\right) = 0$$

$$\ddot{x} = \frac{x^{\frac{3}{2}}}{t^{\frac{1}{2}}} \tag{17i}$$

following HOA yields

$$\left(\frac{(-i\hbar\partial_x + \frac{p}{2})^2}{2(5/2)} - \frac{1}{t^{\frac{1}{2}}}\left(i\hbar\partial_p + \frac{x}{2}\right)^{\frac{5}{2}}\right)\Psi(x; p; t) = i\hbar\partial_t\Psi(x; p; t), \ni m = \frac{5}{2}$$

$$\left(\frac{(-i\hbar\bar{x} + \frac{p}{2})^2}{5} - \frac{1}{t^{\frac{1}{2}}}\left(i\hbar\bar{p} + \frac{x}{2}\right)^{\frac{5}{2}}\right)\tilde{\Psi}(\bar{x}; \bar{p}; t) = i\hbar\partial_t\tilde{\Psi}(\bar{x}; \bar{p}; t)$$

$$\Psi(x; p; t) = L_{((\bar{x}) \rightarrow (x))}^{-1} \left[L_{((\bar{p}) \rightarrow (p))}^{-1} \left[\tilde{\Psi}_0(\bar{x}; \bar{p}; t = 0) e^{-i\left(\frac{(-i\hbar\bar{x} + \frac{p}{2})^2}{5} - 2t^{\frac{1}{2}}(i\hbar\bar{p} + \frac{x}{2})^{\frac{5}{2}}\right)} \right] \right] \tag{17j}$$

By way of the prescription of (17f) through (17h), we arrive at

$$\langle x(t) \rangle = \int_{\text{Configuration Space}} |\Psi_{\text{configuration space}}(x, t)|^2 x dx$$

$$= \left| \int_{-\infty}^{\infty} \frac{e^{\frac{ixp}{\hbar}}}{\sqrt{4\pi\hbar}} L_{((\bar{x}; \bar{p}) \rightarrow (x; p))}^{-1} \left[\tilde{\Psi}_0(\bar{x}, \bar{p}, t = 0) e^{-i\left(\frac{(-i\hbar\bar{x} + \frac{p}{2})^2}{5} - 2t^{\frac{1}{2}}(i\hbar\bar{p} + \frac{x}{2})^{\frac{5}{2}}\right)} \right] dp \right|^2$$

$$\langle x(t) \rangle = \frac{\langle x(t) \rangle^{\frac{3}{2}}}{t^{\frac{1}{2}}} \tag{17k}$$

Hence (17k) is an exact quadrature solution of the Thomas–Fermi equation.

Returning now to the case of a generalised Lagrange equation with the inhomogeneous term

$$(-D_t)\partial_{\dot{x}}L(x; \dot{x}; t) + \partial_xL(x; \dot{x}; t) = F(x; \dot{x}; t) \tag{17d}$$

Let us suppose that $F(x; \dot{x}; t)$ is specified from the GHP and Lagrange equation with inhomogeneous term $F(x(t); \dot{x}(t); t)$ where we recall that the arguments of this inhomogeneous term are explicitly time-dependent [i.e., rheonomic]

$$(-D_t)\partial_{\dot{x}(t)}L(x(t); \dot{x}(t); t) + \partial_{x(t)}L(x(t); \dot{x}(t); t) = F(x(t); \dot{x}(t); t) \quad (17l)$$

Letting $L(x(t); \dot{x}(t); t)$ and $F(x(t); \dot{x}(t); t)$ be scalar functions of their arguments $(x(t); \dot{x}(t); t)$, Utilising a Laplace transform

$$\begin{aligned} & L_{x(t) \rightarrow \bar{x}(t)} L(x(t); \dot{x}(t); t) \\ & \quad \dot{x}(t) \rightarrow \bar{\dot{x}}(t) \\ & \equiv \int_{\dot{x}(t)_0}^{\infty} \int_{x(t)_0}^{\infty} (f(x(t); \dot{x}(t); t)) e^{-\bar{x}(t)x(t) - \bar{\dot{x}}(t)\dot{x}(t)} d\dot{x}(t) dx(t) \\ & L_{x(t) \rightarrow \bar{x}(t)}^{-1} (\bar{f}(\bar{x}(t); \bar{\dot{x}}(t); t)) \\ & \quad \dot{x}(t) \rightarrow \bar{\dot{x}}(t) \\ & \equiv \left(\frac{1}{2\pi i} \right)^2 \oint_{\partial_{\bar{x}(t)}} \oint_{\partial_{\bar{\dot{x}}(t)}} (\bar{f}(\bar{x}(t); \bar{\dot{x}}(t); t)) e^{\bar{x}(t)x(t) + \bar{\dot{x}}(t)\dot{x}(t)} d\bar{\dot{x}}(t) d\bar{x}(t) \quad (17m) \end{aligned}$$

on the Lagrange equation, thus

$$\begin{aligned} & (-D_t)\partial_{\dot{x}(t)}L(x(t); \dot{x}(t); t) + \partial_{x(t)}L(x(t); \dot{x}(t); t) = F(x(t); \dot{x}(t); t) \\ & L_{x(t) \rightarrow \bar{x}(t)} L(x(t); \dot{x}(t); t) + \partial_{x(t)}L(x(t); \dot{x}(t); t) = F(x(t); \dot{x}(t); t) \\ & \quad \dot{x}(t) \rightarrow \bar{\dot{x}}(t) \\ & -D_t(\bar{\dot{x}}(t)\bar{L}(\bar{x}(t); \bar{\dot{x}}(t); t)) + \bar{x}(t)\bar{L}(\bar{x}(t); \bar{\dot{x}}(t); t) = \bar{F}(\bar{x}(t); \bar{\dot{x}}(t); t) \\ & (-D_t\bar{\dot{x}}(t))\bar{L}(\bar{x}(t); \bar{\dot{x}}(t); t) + \bar{\dot{x}}(t)(-D_t\bar{L}(\bar{x}(t); \bar{\dot{x}}(t); t)) \\ & \quad + \bar{x}(t)\bar{L}(\bar{x}(t); \bar{\dot{x}}(t); t) = \bar{F}(\bar{x}(t); \bar{\dot{x}}(t); t) \\ & (-\bar{\dot{x}}(t)D_t + \bar{x}(t) - D_t\bar{\dot{x}}(t))\bar{L}(\bar{x}(t); \bar{\dot{x}}(t); t) = \bar{F}(\bar{x}(t); \bar{\dot{x}}(t); t) \\ & \left(D_t + \left(\frac{D_t\bar{\dot{x}}(t)}{\bar{\dot{x}}(t)} - \frac{\bar{x}(t)}{\bar{\dot{x}}(t)} \right) \right) \bar{L}(\bar{x}(t); \bar{\dot{x}}(t); t) = \frac{\bar{F}(\bar{x}(t); \bar{\dot{x}}(t); t)}{\bar{\dot{x}}(t)} \\ & \bar{L}(\bar{x}(t); \bar{\dot{x}}(t); t) = \frac{1}{\bar{\dot{x}}(t)} e^{\int \frac{\bar{\dot{x}}(t)}{\bar{\dot{x}}(t)} dt} \int e^{-\int \frac{\bar{\dot{x}}(t)}{\bar{\dot{x}}(t)} dt} \bar{F}(\bar{x}(t); \bar{\dot{x}}(t); t) dt \\ & L_{\bar{x}(t) \rightarrow x(t)}^{-1} \left(\bar{L}(\bar{x}(t); \bar{\dot{x}}(t); t) = \frac{1}{\bar{\dot{x}}(t)} e^{\int \frac{\bar{\dot{x}}(t)}{\bar{\dot{x}}(t)} dt} \int e^{-\int \frac{\bar{\dot{x}}(t)}{\bar{\dot{x}}(t)} dt} \bar{F}(\bar{x}(t); \bar{\dot{x}}(t); t) dt \right) \\ & L(x(t); \dot{x}(t); t) = L_{\bar{x}(t) \rightarrow x(t)}^{-1} \left(\frac{1}{\bar{\dot{x}}(t)} e^{\int \frac{\bar{\dot{x}}(t)}{\bar{\dot{x}}(t)} dt} \int e^{-\int \frac{\bar{\dot{x}}(t)}{\bar{\dot{x}}(t)} dt} \bar{F}(\bar{x}(t); \bar{\dot{x}}(t); t) dt \right) \quad (17n) \end{aligned}$$

Letting $L(x(t); \dot{x}(t); t)$ and $F(x(t); \dot{x}(t); t)$ be scalar functions of their arguments $(x(t); \dot{x}(t); t)$, Now suppose $x(t), \dot{x}(t)$ are considered not simply as scalar functions of their argument t , but are generalised to be vector functions of the scalar variable t as $(\mathbf{x}(t); \dot{\mathbf{x}}(t); t)$ so that $L(\mathbf{x}(t); \dot{\mathbf{x}}(t); t)$ and $F(\mathbf{x}(t); \dot{\mathbf{x}}(t); t)$.

As a result, all of the above construction for $L(x(t); \dot{x}(t); t)$ and $F(x(t); \dot{x}(t); t)$ are generalised to $L(\mathbf{x}(t); \dot{\mathbf{x}}(t); t)$ and $F(\mathbf{x}(t); \dot{\mathbf{x}}(t); t)$ thus

$$\begin{aligned}
 &(-D_t)\partial_{\dot{\mathbf{x}}(t)}L(\mathbf{x}(t); \dot{\mathbf{x}}(t); t) + \partial_{\mathbf{x}(t)}L(\mathbf{x}(t); \dot{\mathbf{x}}(t); t) = F(\mathbf{x}(t); \dot{\mathbf{x}}(t); t) \\
 &L_{\substack{\mathbf{x}(t) \rightarrow \bar{\mathbf{x}}(t) \\ \dot{\mathbf{x}}(t) \rightarrow \bar{\dot{\mathbf{x}}}(t)}}((-D_t)\partial_{\dot{\mathbf{x}}(t)}L(\mathbf{x}(t); \dot{\mathbf{x}}(t); t) + \partial_{\mathbf{x}(t)}L(\mathbf{x}(t); \dot{\mathbf{x}}(t); t) = F(\mathbf{x}(t); \dot{\mathbf{x}}(t); t)) \\
 &-D_t(\bar{\dot{\mathbf{x}}}(t)\bar{L}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t) + \bar{\mathbf{x}}(t)\bar{L}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t) = \bar{F}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t) \\
 &(-D_t\bar{\dot{\mathbf{x}}}(t))\bar{L}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t) + \bar{\dot{\mathbf{x}}}(t)(-D_t\bar{L}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t)) \\
 &\quad + \bar{\mathbf{x}}(t)\bar{L}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t) = \bar{F}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t) \\
 &(-\bar{\dot{\mathbf{x}}}(t)D_t + \bar{\mathbf{x}}(t) - D_t\bar{\dot{\mathbf{x}}}(t))\bar{L}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t) = \bar{F}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t) \\
 &\left(D_t + \left(\frac{D_t\bar{\dot{\mathbf{x}}}(t)}{\bar{\dot{\mathbf{x}}}(t)} - \frac{\bar{\mathbf{x}}(t)}{\bar{\dot{\mathbf{x}}}(t)}\right)\right)\bar{L}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t) = \frac{\bar{F}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t)}{\bar{\dot{\mathbf{x}}}(t)} \\
 &\bar{L}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t) = \frac{1}{\bar{\dot{\mathbf{x}}}(t)}e^{\int \frac{\bar{\dot{\mathbf{x}}}(t)}{\bar{\dot{\mathbf{x}}}(t)}dt} \int e^{-\int \frac{\bar{\dot{\mathbf{x}}}(t)}{\bar{\dot{\mathbf{x}}}(t)}dt} \bar{F}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t)dt \\
 &L_{\substack{\bar{\mathbf{x}}(t) \rightarrow \mathbf{x}(t) \\ \bar{\dot{\mathbf{x}}}(t) \rightarrow \dot{\mathbf{x}}(t)}}^{-1}\left(\bar{L}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t) = \frac{1}{\bar{\dot{\mathbf{x}}}(t)}e^{\int \frac{\bar{\dot{\mathbf{x}}}(t)}{\bar{\dot{\mathbf{x}}}(t)}dt} \int e^{-\int \frac{\bar{\dot{\mathbf{x}}}(t)}{\bar{\dot{\mathbf{x}}}(t)}dt} \bar{F}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t)dt\right) \\
 &L(\mathbf{x}(t); \dot{\mathbf{x}}(t); t) = L_{\substack{\bar{\mathbf{x}}(t) \rightarrow \mathbf{x}(t) \\ \bar{\dot{\mathbf{x}}}(t) \rightarrow \dot{\mathbf{x}}(t)}}^{-1}\left(\frac{1}{\bar{\dot{\mathbf{x}}}(t)}e^{\int \frac{\bar{\dot{\mathbf{x}}}(t)}{\bar{\dot{\mathbf{x}}}(t)}dt} \int e^{-\int \frac{\bar{\dot{\mathbf{x}}}(t)}{\bar{\dot{\mathbf{x}}}(t)}dt} \bar{F}(\bar{\mathbf{x}}(t); \bar{\dot{\mathbf{x}}}(t); t)dt\right) \quad (17o)
 \end{aligned}$$

Along these lines, the component scalar variables of the vector variables, may naturally be expressed as projections of the vector variables via suitable matrix coefficients thus

$$\begin{aligned}
 &(-D_t)\partial_{\dot{\mathbf{x}}(t)}L(\mathbf{x}(t); \dot{\mathbf{x}}(t); t) + \partial_{\mathbf{x}(t)}L(\mathbf{x}(t); \dot{\mathbf{x}}(t); t) = F(\mathbf{x}(t); \dot{\mathbf{x}}(t); t) \\
 &(\mathbf{x}(t); \dot{\mathbf{x}}(t); t), \\
 &\mathbf{x}(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ \cdot \\ \cdot \\ x_n(t) \end{bmatrix}, \begin{bmatrix} 1 & & & & \\ & 0 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & 0 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \\ \cdot \\ \cdot \\ x_n(t) \end{bmatrix} = x_1(t), \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & 0 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \\ \cdot \\ \cdot \\ x_n(t) \end{bmatrix} \\
 &= x_2(t), \begin{bmatrix} 0 & & & & \\ & 0 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & 1 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \\ \cdot \\ \cdot \\ x_n(t) \end{bmatrix} = x_n(t) \\
 &\dot{\mathbf{x}}(t) = \begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \cdot \\ \cdot \\ \dot{x}_n(t) \end{bmatrix}, \begin{bmatrix} 1 & & & & \\ & 0 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & 0 \end{bmatrix} \begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \cdot \\ \cdot \\ \dot{x}_n(t) \end{bmatrix} = \dot{x}_1(t), \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & 0 \end{bmatrix} \begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \cdot \\ \cdot \\ \dot{x}_n(t) \end{bmatrix}
 \end{aligned}$$

$$= \dot{x}_2(t), \begin{bmatrix} 0 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix} \begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \vdots \\ \dot{x}_n(t) \end{bmatrix} = \dot{x}_n(t) \tag{17p}$$

So the usual system of equations in several dependent variables in (17b) may be re-cast as a single vector variable equation as above since

$$(\mathbf{x}(t); \dot{\mathbf{x}}(t); t) = \left(\begin{bmatrix} x_1(t) \\ x_2(t) \\ \vdots \\ x_n(t) \end{bmatrix}; \begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \vdots \\ \dot{x}_n(t) \end{bmatrix}; t \right)$$

While these vector variable extensions in the Lagrangian are useful in various multi-dimensional scenarios, there is another that will be mentioned here as well. Suppose we consider the Lagrange system for explicit components of an n -dimensional vector

$$\left(\begin{array}{l} ((-D_t)\partial_{\dot{x}_j(t)} + \partial_{x_j(t)})L(x_1(t), x_2(t), \dots, x_n(t); \dot{x}_1(t), \dot{x}_2(t), \dots, \dot{x}_n(t); t) \\ -F_j(x_1(t), x_2(t), \dots, x_n(t); \dot{x}_1(t), \dot{x}_2(t), \dots, \dot{x}_n(t); t) \end{array} \right) \mathbf{e}_j, \\ \vartheta j = 1, \dots, n$$

Letting $\mathbf{e}_j, \vartheta j = 1, \dots, n$ be the n -dimensional unit vector (17q)

Upon taking the interior product of the Lagrangian components vector with the unit vector yields the n -dimensional equation for the system from which an L satisfying these relations to the F_j 's may be determined thus

$$\sum_j \left(\begin{array}{l} ((-D_t)\partial_{\dot{x}_j(t)} + \partial_{x_j(t)})L(x_1(t), x_2(t), \dots, x_n(t); \dot{x}_1(t), \dot{x}_2(t), \dots, \dot{x}_n(t); t) \\ -F_j(x_1(t), x_2(t), \dots, x_n(t); \dot{x}_1(t), \dot{x}_2(t), \dots, \dot{x}_n(t); t) \end{array} \right) = 0$$

$L_{x_j(t)} \rightarrow \bar{x}_j(t)$
 $\dot{x}_j(t) \rightarrow \bar{\dot{x}}_j(t)$

$$\left(\sum_j \left(\begin{array}{l} ((-D_t)\partial_{\dot{x}_j(t)} + \partial_{x_j(t)})L(x_1(t), x_2(t), \dots, x_n(t); \dot{x}_1(t), \dot{x}_2(t), \dots, \dot{x}_n(t); t) \\ -F_j(x_1(t), x_2(t), \dots, x_n(t); \dot{x}_1(t), \dot{x}_2(t), \dots, \dot{x}_n(t); t) \end{array} \right) \right) = 0$$

$$\sum_j \left(\begin{array}{l} -D_t(\bar{x}_j(t)\bar{L}(\bar{x}_1(t), \bar{x}_2(t), \dots, \bar{x}_n(t); \bar{\dot{x}}_1(t), \bar{\dot{x}}_2(t), \dots, \bar{\dot{x}}_n(t); t)) \\ +\bar{x}_j(t)\bar{L}(\bar{x}_1(t), \bar{x}_2(t), \dots, \bar{x}_n(t); \bar{\dot{x}}_1(t), \bar{\dot{x}}_2(t), \dots, \bar{\dot{x}}_n(t); t) \\ -\bar{F}_j(\bar{x}_1(t), \bar{x}_2(t), \dots, \bar{x}_n(t); \bar{\dot{x}}_1(t), \bar{\dot{x}}_2(t), \dots, \bar{\dot{x}}_n(t); t) \end{array} \right) = 0$$

$$\sum_j \left(\begin{array}{l} (-\bar{\dot{x}}_j(t)D_t + \bar{x}_j(t) - D_t\bar{x}_j(t))\bar{L}(\bar{x}_1(t), \bar{x}_2(t), \dots, \bar{x}_n(t); \bar{\dot{x}}_1(t), \bar{\dot{x}}_2(t), \dots, \bar{\dot{x}}_n(t); t) \\ -\bar{F}_j(\bar{x}_1(t), \bar{x}_2(t), \dots, \bar{x}_n(t); \bar{\dot{x}}_1(t), \bar{\dot{x}}_2(t), \dots, \bar{\dot{x}}_n(t); t) \end{array} \right) = 0$$

$$\bar{L}(\bar{x}_1(t), \bar{x}_2(t), \dots, \bar{x}_n(t); \bar{\dot{x}}_1(t), \bar{\dot{x}}_2(t), \dots, \bar{\dot{x}}_n(t); t)$$

$$= e^{-\int \frac{\sum_j \bar{x}_j(t) - D_t\bar{x}_j(t)}{\sum_j -\bar{\dot{x}}_j(t)} dt} \tag{17r}$$

$$\times \int \left(e^{\int \frac{\sum_j \bar{x}_j(t) - D_t\bar{x}_j(t)}{\sum_j -\bar{\dot{x}}_j(t)} dt} \sum_j \bar{F}_j(\bar{x}_1(t), \bar{x}_2(t), \dots, \bar{x}_n(t); \bar{\dot{x}}_1(t), \bar{\dot{x}}_2(t), \dots, \bar{\dot{x}}_n(t); t) \right) dt$$

$$\begin{aligned}
 &L(x_1(t), x_2(t), \dots, x_n(t); \dot{x}_1(t), \dot{x}_2(t), \dots, \dot{x}_n(t); t) \\
 &= L_{x_j(t) \rightarrow \bar{x}_j(t)}^{-1} \left(e^{-\int \frac{\sum_j \bar{x}_j(t) - D_t \bar{x}_j(t)}{\sum_j -\dot{\bar{x}}_j(t)} dt} \int \left(e^{\int \frac{\sum_j \bar{x}_j(t) - D_t \bar{x}_j(t)}{\sum_j -\dot{\bar{x}}_j(t)} dt} \right. \right. \\
 &\quad \left. \left. \times \sum_j \bar{F}_j(\bar{x}_1(t), \bar{x}_2(t), \dots, \bar{x}_n(t); \dot{\bar{x}}_1(t), \dot{\bar{x}}_2(t), \dots, \dot{\bar{x}}_n(t); t) \right) dt \right) \quad (17s)
 \end{aligned}$$

So the point of (171–17r) is to determine the Lagrangian L for the given inhomogeneous term F ; and using the results developed herein earlier, from (17a) on, to determine the corresponding Hamiltonian of the system and via HOA and Ehrenfest’s Theorem, the solution of the equations defined by $F = 0$: said equations are arbitrary functions of the arguments in F .

At this point, we note some perhaps subtle aspects of the connection between the configuration and QPSR wavefunction formulations discussed in the “Recap of HOA” Section earlier in the present report [i.e. viz, Eqs. (9) and (10)]:

shifted Taylor series yields

$$\begin{aligned}
 &e^{-i\hbar f(x_1, \dots, x_n, t) \partial_{x_j}} \Psi_{\text{Configuration Space}}(x_1, \dots, x_n, t) \\
 &= \Psi_{\text{Configuration Space}}(x_1, \dots, (x_j - i\hbar f(x_1, \dots, x_n, t)), \dots, x_n, t)
 \end{aligned}$$

Hence the Hamiltonian in the configuration space formalism may be used to generate “shifted” systems of FDE (Functional Differential Equation)s, simultaneously containing discrete difference and continuous differential sectors in the same hybrid dynamics.

Also, the Shannon entropy S [i.e. viz, Eq. (8m) herein]:, which connects Information Theory to Quantum Theory via the density

$$S = - \iint_{(\mathbf{x}, \mathbf{p})} (\Psi^*(\mathbf{x}, \mathbf{p}, t) \Psi(\mathbf{x}, \mathbf{p}, t)) \text{Log}(\Psi^*(\mathbf{x}, \mathbf{p}, t) \Psi(\mathbf{x}, \mathbf{p}, t)) d\mathbf{x} d\mathbf{p}$$

provides a direct avenue for plethora applications (e.g., Refs. [19,20]).

These are some future vistas for later work elsewhere, but they warrant mention here.

Notwithstanding their intrinsic interest, the few Examples 1–7 herein these Recent Remarks do not even begin to touch the immense vista of problems that may be solved exactly via HOA methods. Indeed, the HOA may be modified to accommodate auxiliary conditions besides initial-value problems. Moreover, the integral and differential operators in the HOA may be generalized to discrete sum/finite difference operators and sundry other extensions. Since classical and quantum dynamical systems admit to Hamiltonian/Lagrangian formulation, then indeed the various other formulations [e.g., Density Functional Theory, Path Integral Formalism, Stochastic Formalisms, etc], as well as derived abstracted mathematical problems (e.g., [14, 15]) may all benefit by HOA treatments. Quoting from [6, 18], “By definition, solution in one representation implies simultaneous solution in all representations [the Physics is the same regardless

of ‘pictures’]. Hence, Quantum Dynamics is now reduced to exact quadratures, as are all the associated purely mathematical problems that are abstracted from the physical formalism.” MT21:42.

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