Toward chemical applications of Heaviside Operational Ansatz: exact solution of radial Schrodinger equation for nonrelativistic N-particle system with pairwise $\frac{1}{r_{ij}}$ radial potential in quantum phase space

Valentino A. Simpao

Abstract   This brief note presents the exact analytical solution of an example class of dynamical systems, realized by differential equations. These problems occur in quantum mechanics and their generalizations in theoretical physics, but they particularly find application to chemical systems. Addressed is the exact analytical solution of the radial Schrodinger equation for the nonrelativistic N-particle system with pairwise $\frac{1}{r_{ij}}$ radial potential dynamics in the quantum phase space representation (QPSR) (Torres-Vega, Frederick, J. Chem. Phys. **98** 3103, 1993). Applying the formal symbolic solution scheme Heaviside Operational Ansatz (heretofore, HOA) put forward in (Electron. J. Theor. Phys. **1** , 10–16, 2004), reduces solution of the radial Schrodinger equation to exact quadratures.

1 Motivation and recap of HOA result

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 [1], the quantum phase space representation (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

V. A. Simpao (✉)
Mathematical Consultant Services, 108 Hopkinsville Street, Greenville, KY 42345, USA
e-mail: mcs007@muhlon.com

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, the present author has developed an exact analytical symbolic solution scheme for broad classes of differential equations utilizing the Heaviside Operational Ansatz (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, he 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].

In this report, we take a first step toward illustrating HOA methods in application to the exact solution of quantum chemistry problems. Namely of the non-relativistic N-particle system with pairwise $\frac{1}{r_{ij}}$ radial potential interaction, variations of which appear in many areas of quantum chemistry [e.g., the chemical elements on the periodic chart] and theoretical physics generally. After a brief review of the HOA results, the radial Schrodinger equation for this N-particle scenario will be our focus in the QPSR, as the remaining angular components of the Schrodinger equation for the system Hamiltonian are factored out via the usual seperation of variables scheme for radial potentials [6–8], and their solutions are well known. The solution of the radial Schrodinger equation for the non-relativistiic N-particle system with pairwise $\frac{1}{r_{ij}}$ radial potential interaction forms the cornerstone of the exact solution to the quantum dynamics of particular chemical systems which manifest their basic non-relativistic nature at the level of nuclei and electrons. After a straightforward scaling of variables, the present N-particle results may be used to construct the exact solution of the Schrodinger equation for the general nonrelativistic molecular Hamiltonian [7,8] which obtains as a special case. Specific chemical applications of these results are the province of other works by the present author [10,11].

2 Recap of HOA

To recall the full details of HOA results, see the original work (EJTP **1**, 10–16 2004). 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),

Recalling the fundamental HOA results, we let x, p, t respectively denote the configuration space, momentum and time variables. The $^\wedge$ denotes the operators, with H and $\boldsymbol{\Psi}$ denoting the Hamiltonian and wavefunction of the phase space representation, respectively. Also the α, γ are otherwise free parameters as specified therein the original work.

Hence for a given Hamiltonian and initial-state, the configuration space solution obtains from the quantum phase space solution as

$$\hat{H}_{\text{configuration space}} \left(x_1, \ldots, x_n, -i\hbar\partial_{x_1}, \ldots, -i\hbar\partial_{x_n}, t \right)$$
$$\Psi_{\text{configuration space}} \left(x_1, \ldots, x_n, t \right)$$
$$= i\hbar\partial_t \Psi_{\text{configuration space}} \left(x_1, \ldots, x_n, t \right)$$

$$\Psi_{\text{configuration space}} \left(x_1, \ldots, x_n, t \right)$$
$$= \int_{-\infty}^{\infty} \frac{e^{\frac{ix_1 p_1}{2\hbar}}}{\sqrt{4\pi\hbar}} \cdots \int_{-\infty}^{\infty} \frac{e^{\frac{ix_n p_n}{2\hbar}}}{\sqrt{4\pi\hbar}} L^{-1}_{\left(\begin{array}{c} (\bar{x}_1, \ldots, \bar{x}_n) \\ \to (x_1, \ldots, x_n) \end{array} \right)}$$
$$\times \left[L^{-1}_{\left(\begin{array}{c} (\bar{p}_1, \ldots, \bar{p}_n) \\ \to (p_1, \ldots, p_n) \end{array} \right)} \left[\begin{array}{c} e^{\frac{-i}{\hbar} \int_0^t \hat{H} \left(\begin{array}{c} i\hbar\bar{p}_1 + \alpha_1 x_1, \ldots, i\hbar\bar{p}_n + \alpha_n x_n; \\ -i\hbar\bar{x}_1 + \gamma_1 p_1, \ldots, -i\hbar\bar{x}_n + \gamma_n p_n; u \end{array} \right) du} \\ \times \\ \breve{\Psi}_0 \left(\bar{x}_1, \ldots, \bar{x}_n; \bar{p}_1, \ldots, \bar{p}_n; t=0 \right) \end{array} \right] \right]$$
$$\times dp_1 \ldots dp_n \tag{1}$$

$$\hat{H}_{\text{configuration space}} \left(\begin{array}{c} x_1, \ldots, x_n, \\ -i\hbar\partial_{x_1}, \ldots, -i\hbar\partial_{x_n}, t \end{array} \right) \begin{array}{l} (x_1, \ldots, x_n) \mapsto \left(i\hbar\partial_{p_1} + \alpha_1 x_1, \ldots, \right. \\ i\hbar\partial_{p_n} + \alpha_n x_n \big) \\ (-i\hbar\partial_{x_1}, \ldots, -i\hbar\partial_{x_n}) \mapsto \left(-i\hbar\partial_{x_1} \right. \\ \left. + \gamma_1 p_1, \ldots, -i\hbar\partial_{x_n} + \gamma_n p_n \right) \end{array}$$

where

$$\equiv \hat{H} \left(\begin{array}{c} i\hbar\partial_{p_1} + \alpha_1 x_1, \ldots, i\hbar\partial_{p_n} + \alpha_n x_n; \\ -i\hbar\partial_{x_1} + \gamma_1 p_1, \ldots, -i\hbar\partial_{x_n} + \gamma_n p_n; t \end{array} \right) \tag{2}$$

To wit, via HOA the configuration space solution becomes

$$\boldsymbol{\Psi}_{\text{configuration space}} \left(x_1, \ldots, x_n, t \right)$$
$$= \int_{-\infty}^{\infty} \frac{e^{\frac{ix_1 p_1}{2\hbar}}}{\sqrt{4\pi\hbar}} \cdots \int_{-\infty}^{\infty} \frac{e^{\frac{ix_n p_n}{2\hbar}}}{\sqrt{4\pi\hbar}} L^{-1}_{\left(\begin{array}{c} (\bar{x}_1, \ldots, \bar{x}_n; \bar{p}_1, \ldots, \bar{p}_n) \\ \to (x_1, \ldots, x_n; p_1, \ldots, p_n) \end{array} \right)}$$

$$\times \left[\begin{array}{l} e^{\frac{-i}{\hbar} \int_0^t \hat{H}_{\text{configuration space}} \left(\begin{array}{l} x_1, \ldots, x_n, \\ -i\hbar\partial_{x_1}, \ldots, -i\hbar\partial_{x_n}, u \end{array} \right) \begin{array}{l} (x_1, \ldots, x_n) \mapsto \\ (i\hbar\bar{p}_1 + \alpha_1 x_1, \ldots, i\hbar\bar{p}_n + \alpha_n x_n) \\ (-i\hbar\partial_{x_1}, \ldots, -i\hbar\partial_{x_n}) \mapsto \\ (-i\hbar\bar{x}_1 + \gamma_1 p_1, \ldots, \\ -i\hbar\bar{x}_n + \gamma_n p_n) \end{array} du} \\ \times \\ \breve{\boldsymbol{\Psi}}_{0 \text{ configuration space}} (\bar{x}_1, \ldots, \bar{x}_n; ; t = 0) \end{array} \right]$$

$$\times dp_1 \ldots dp_n \tag{3}$$

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

Given the function $\hat{H} (\hat{x}_1, \ldots, \hat{x}_n; \hat{p}_1, \ldots, \hat{p}_n, t)$

$\left[\text{respectively } \hat{H} (x_1, \ldots, x_n; -i\hbar\partial_{x_1}, \ldots, -i\hbar\partial_{x_n}, t) \right]$ replace

$(\hat{x}_1, \ldots, \hat{x}_n; \hat{p}_1, \ldots, \hat{p}_n, t)$

$\left[\text{respectively } (x_1, \ldots, x_n; -i\hbar\partial_{x_1}, \ldots, -i\hbar\partial_{x_n}, t) \right]$ with

$(i\hbar\bar{p}_1 + \alpha_1 x_1, \ldots, i\hbar\bar{p}_n + \alpha_n x_n; -i\hbar\bar{x}_1 + \gamma_1 p_1, \ldots, -i\hbar\bar{x}_n + \gamma_1 p_n, t)$
in equation (3)

The result of course is the quantum phase space (respectively configuration space) wavefunction for the quantum dynamics wave equation. Before addressing the Radial Schrodinger equation solution, just a comment on the α and γ parameters in the above formulae. From the HOA, 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 $\hat{H} (i\hbar\partial_p + \alpha x, -i\hbar\partial_x + \gamma p, t), \ni \alpha + \gamma = 1$ takes on the symmetric canonical form when $\alpha = \gamma = \frac{1}{2}$ thusly $\hat{H} (i\hbar\partial_p + \frac{x}{2}, -i\hbar\partial_x + \frac{p}{2}, t), \ni \alpha + \gamma = 1$. 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.

3 HOA solution of radial Schrödinger equation for nonrelativistiic N-particle system with pairwise $\frac{1}{r_{ij}}$ radial potential Interaction

Now on to the main result with the solution of the radial Schrodinger equation for the non-relativistiic 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 [6]. Hence no particle is fixed as a center of motion. As stated earlier the angular components separate in the usual way by Refs. [6–8]. Here a_i, b_i, c_i are scaling constants, $L_i(L_i + 1)$ are the angular coupling terms and $\mathbf{r} = (r_1, \ldots, r_N) = (r_{i=1,\ldots,N})$, $\mathbf{p_r} = (p_{r_1}, \ldots, p_{r_N}) = (p_{r_{i=1,\ldots,N}})$. The resulting radial Hamiltonian yields a radial Schrodinger equation of form

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

$$
= i\hbar\partial_t \Psi_{\mathbf{r} \text{ phasespace}} (\mathbf{r}; \mathbf{p_r}; t) \tag{4}
$$

Hence via HOA from Eq. 3,

$$
\begin{aligned}
\Bigg(\sum_i &\left(\frac{\left(-i\hbar\bar{r}_i + \frac{p_{r_i}}{2}\right)^2}{2m_i} + \frac{2b_i}{\left(i\hbar\bar{p}_{r_i} + \frac{r_i}{2}\right)} \left(-i\hbar\bar{r}_i + \frac{p_{r_i}}{2}\right) + \frac{c_i L_i(L_i+1)}{\left(i\hbar\bar{p}_{r_i} + \frac{r_i}{2}\right)^2} \right) \\
&+ \sum_{i<j} a_{ij} \left(\frac{1}{\left|\left(i\hbar\bar{p}_{r_i} + \frac{r_i}{2}\right) - \left(i\hbar\bar{p}_{r_j} + \frac{r_j}{2}\right)\right|} \right) \Bigg) \\
&\times \breve{\Psi}_{\mathbf{r} \text{ phasespace}} (\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t)
\end{aligned}
$$

$$
= i\hbar\partial_t \breve{\Psi}_{\mathbf{r} \text{ phasespace}} (\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t) \tag{5}
$$

Yielding the exact analytical solution given in quadratures as

$$
\Psi_{\mathbf{r} \text{ phasespace}} (\mathbf{r}; \mathbf{p_r}; t) = L^{-1}_{\left(\substack{\bar{\mathbf{r}} \to \mathbf{r}; \\ \bar{\mathbf{p}}_{\mathbf{r}} \to \mathbf{p_r}}\right)}
$$

$$
\times \left(e^{\frac{-it}{\hbar}\left(\sum_i \left(\frac{\left(-i\hbar\bar{r}_i + \frac{p_{r_i}}{2}\right)^2}{2m_i} + \frac{2b_i}{\left(i\hbar\bar{p}_{r_i} + \frac{r_i}{2}\right)} \left(-i\hbar\bar{r}_i + \frac{p_{r_i}}{2}\right) + \frac{c_i L_i(L_i+1)}{\left(i\hbar\bar{p}_{r_i} + \frac{r_i}{2}\right)^2} \right) + \sum_{i<j} a_{ij} \left(\frac{1}{\left|\left(i\hbar\bar{p}_{r_i} + \frac{r_i}{2}\right) - \left(i\hbar\bar{p}_{r_j} + \frac{r_j}{2}\right)\right|} \right) \right)} \times \breve{\Psi}_{0\mathbf{r} \text{ phasespace}} (\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t = 0) \right) \tag{6}
$$

To evaluate (6), recall that

$$\breve{\Psi}_{\mathbf{r} \text{ phasespace}} (\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t)$$

$$= e^{\frac{-it}{\hbar} \left(\sum_i \left(\frac{\left(-i\hbar\bar{r}_i + \frac{pr_i}{2} \right)^2}{2m_i} \right) \right)} \times e^{\frac{-it}{\hbar} \left(\sum_i \left(\frac{2b_i}{\left(i\hbar\bar{p}r_i + \frac{r_i}{2} \right)} \left(-i\hbar\bar{r}_i + \frac{pr_i}{2} \right) \right) \right)}$$

$$\times e^{\frac{-it}{\hbar} \left(\sum_i \left(\frac{c_i L_i (L_i+1)}{\left(i\hbar\bar{p}r_i + \frac{r_i}{2} \right)^2} \right) \right)} \times e^{\frac{-it}{\hbar} \left(\sum_{i<j} a_{ij} \left(\frac{1}{\left| \left(i\hbar\bar{p}r_i + \frac{r_i}{2} \right) - \left(i\hbar\bar{p}r_j + \frac{r_j}{2} \right) \right|} \right) \right)}$$

$$\times \breve{\Psi}_{0\mathbf{r} \text{ phasespace}} (\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t = 0) \tag{7}$$

Upon evaluating the inverse Laplace transforms and utilizing convolution products herein symbolized as $\underbrace{*}_{\mathbf{r}}$ or $\underbrace{*}_{\mathbf{p}_{\mathbf{r}}}$ or $\underbrace{*}_{\mathbf{r}, \mathbf{p}_{\mathbf{r}}}$ [12,13].

$$L^{-1}_{\left(\substack{\bar{\mathbf{r}} \to \mathbf{r}; \\ \bar{\mathbf{p}}_{\mathbf{r}} \to \mathbf{p}_{\mathbf{r}}} \right)} \breve{\Psi}_{\mathbf{r} \text{ phasespace}} (\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t)$$

$$= L^{-1}_{(\bar{\mathbf{r}} \to \mathbf{r})} \left(e^{\frac{-it}{\hbar} \left(\sum_i \left(\frac{\left(-i\hbar\bar{r}_i + \frac{pr_i}{2} \right)^2}{2m_i} \right) \right)} \right) \underbrace{*}_{\mathbf{r}} L^{-1}_{\left(\substack{\bar{\mathbf{r}} \to \mathbf{r}; \\ \bar{\mathbf{p}}_{\mathbf{r}} \to \mathbf{p}_{\mathbf{r}}} \right)}$$

$$\times \left(e^{\frac{-it}{\hbar} \left(\sum_i \left(\frac{2b_i}{\left(i\hbar\bar{p}r_i + \frac{r_i}{2} \right)} \left(-i\hbar\bar{r}_i + \frac{pr_i}{2} \right) \right) \right)} \right)$$

$$\underbrace{*}_{\mathbf{p}_{\mathbf{r}}} L^{-1}_{(\bar{\mathbf{p}}_{\mathbf{r}} \to \mathbf{p}_{\mathbf{r}})} \left(e^{\frac{-it}{\hbar} \left(\sum_i \left(\frac{c_i L_i (L_i+1)}{\left(i\hbar\bar{p}r_i + \frac{r_i}{2} \right)^2} \right) \right)} \right) \underbrace{*}_{\mathbf{p}_{\mathbf{r}}} L^{-1}_{(\bar{\mathbf{p}}_{\mathbf{r}} \to \mathbf{p}_{\mathbf{r}})}$$

$$\times \left(e^{\frac{-it}{\hbar} \left(\sum_{i<j} a_{ij} \left(\frac{1}{\left| \left(i\hbar\bar{p}r_i + \frac{r_i}{2} \right) - \left(i\hbar\bar{p}r_j + \frac{r_j}{2} \right) \right|} \right) \right)} \right)$$

$$\underbrace{*}_{\mathbf{r}, \mathbf{p}_{\mathbf{r}}} L^{-1}_{\left(\substack{\bar{\mathbf{r}} \to \mathbf{r}; \\ \bar{\mathbf{p}}_{\mathbf{r}} \to \mathbf{p}_{\mathbf{r}}} \right)} \left(\breve{\Psi}_{0\mathbf{r} \text{ phasespace}} (\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t = 0) \right) \tag{8}$$

Evaluating (8) explicitly yields

$$L^{-1}_{(\bar{\mathbf{p}}_\mathbf{r}\to\mathbf{p}_\mathbf{r})}\left(e^{\frac{-it}{\hbar}\left(\sum_{i<j} a_{ij}\left(\frac{1}{\left|\left(i\hbar\bar{p}_{r_i}+\frac{r_i}{2}\right)-\left(i\hbar\bar{p}_{r_j}+\frac{r_j}{2}\right)\right|}\right)\right)}\right)$$

$$= \underbrace{\circledast}_{i<j}\left(\delta\left[p_{r_i}+p_{r_j}\right]\left(\frac{1}{\pi p_{r_i}\sqrt{\frac{-i\hbar}{a_{ij}t}}}e^{\frac{ip_{r_i}(r_i-r_j)}{2\hbar}}\left(\sqrt{\frac{p_{r_i}}{\hbar}}K_1\left[\frac{2\sqrt{\frac{p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}}\right]\right.\right.\right.$$

$$\left.\left.\left.-\sqrt{\frac{-p_{r_i}}{\hbar}}K_1\left[\frac{2\sqrt{\frac{-p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}}\right]\right)\right)\right)$$

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

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

$$\left.\left.-\sqrt{\frac{-p_{r_i}}{\hbar}}K_1\left[\frac{2\sqrt{\frac{-p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}}\right]\right)\right) \tag{9}$$

where $\underset{i<j}{\circledast}$ represents the convolution between the inverse transforms of the indicated terms as illustrated above in the case of N = 3.

$$L^{-1}_{\left(\substack{\bar{\mathbf{r}}\to\mathbf{r};\\ \bar{\mathbf{p}}_\mathbf{r}\to\mathbf{p}_\mathbf{r}}\right)}\left(e^{\frac{-it}{\hbar}\left(\sum_i\left(\frac{2b_i}{\left(i\hbar\bar{p}_{r_i}+\frac{r_i}{2}\right)}\left(-i\hbar\bar{r}_i+\frac{p_{r_i}}{2}\right)\right)\right)}\right)$$

$$= \prod_i\left(\delta\left[p_{r_i}\right]\delta\left[r_i\right]+\frac{ib_ie^{\frac{2ib_ip_{r_i}t}{\hbar r_i}}\left(\sqrt{-ip_{r_i}}-\sqrt{ip_{r_i}}\right)t}{\hbar\pi r_i^2\sqrt{|p_{r_i}|}}\right) \tag{10}$$

$$L^{-1}_{(\bar{\mathbf{p}}_\mathbf{r}\to\mathbf{p}_\mathbf{r})}\left(e^{\frac{-it}{\hbar}\left(\sum_i\left(\frac{c_iL_i(L_i+1)}{\left(i\hbar\bar{p}_{r_i}+\frac{r_i}{2}\right)^2}\right)\right)}\right)$$

$$= \prod_i\left(\frac{-1}{24\pi\hbar^6}\left(C_i^2L_i^2(L_i+1)^2 p_{r_i}^3 t^2\left(\begin{array}{c}\left(e^{\frac{ip_{r_i}r_i}{2\hbar}}-1\right)Log\left[\frac{-p_{r_i}}{\hbar}\right]\\ +Log\left[\frac{p_{r_i}}{\hbar}-Log\left[\frac{p_{r_i}}{\hbar}\right]\right]\\ HeavisideStep[p_{r_i}]\end{array}\right)\right)\right) \tag{11}$$

$$L_{(\bar{\mathbf{r}} \to \mathbf{r})}^{-1}\left(e^{\frac{-it}{\hbar}\left(\sum_i\left(\frac{\left(-i\hbar\bar{r}_i+\frac{p_{r_i}}{2}\right)^2}{2m_i}\right)\right)}\right) = \prod_i \frac{e^{\frac{i\left(r_i^2 m_i - t r_i p_{r_i}\right)}{2\hbar t}}}{\hbar\sqrt{\frac{2\pi i t}{\hbar m_i}}} \tag{12}$$

Since $L_{\begin{pmatrix}\bar{\mathbf{r}} \to \mathbf{r};\\ \bar{\mathbf{p}}_{\mathbf{r}} \to \mathbf{p}_{\mathbf{r}}\end{pmatrix}}^{-1}\left(\breve{\Psi}_{0\mathbf{r}\text{ phasespace}}(\bar{\mathbf{r}}; \bar{\mathbf{p}}_{\mathbf{r}}; t{=}0)\right) = \Psi_{0\mathbf{r}\text{ phasespace}}(\mathbf{r}; \mathbf{p}_{\mathbf{r}}; t{=}0)$,

the evaluated inverse transforms yield the explicit solution in the QPSR

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

$$= \Psi_{0\mathbf{r}\text{ phasespace}}(\mathbf{r}; \mathbf{p}_{\mathbf{r}}; t=0) \underbrace{*}_{\mathbf{r},\mathbf{p}_{\mathbf{r}}} \prod_i \frac{e^{\frac{i\left(r_i^2 m_i - t r_i p_{r_i}\right)}{2\hbar t}}}{\hbar\sqrt{\frac{2\pi i t}{\hbar m_i}}}$$

$$\underbrace{*}_{\mathbf{r}} \prod_i \left(\delta\left[p_{r_i}\right]\delta\left[r_i\right] + \frac{i b_i e^{\frac{2 i b_i p_{r_i} t}{\hbar r_i}}\left(\sqrt{-i p_{r_i}} - \sqrt{i p_{r_i}}\right) t}{\hbar \pi r_i^2 \sqrt{|p_{r_i}|}}\right)$$

$$\underbrace{*}_{\mathbf{p}_{\mathbf{r}}} \prod_i \left(\frac{-1}{24 \pi \hbar^6}\left(c_i^2 L_i^2 \left(L_i^+ 1\right)^2 p_{r_i}^3 t^2\right.\right.$$

$$\times \left.\left(\left(e^{\frac{i p_{r_i} r_i}{2\hbar}} - 1\right) Log\left[\frac{-p_{r_i}}{\hbar}\right]\right.\right.$$

$$\left.\left.\left.+ Log\left[\frac{p_{r_i}}{\hbar}\right] - Log\left[\frac{p_{r_i}}{\hbar}\right] HeavisideStep\left[p_{r_i}\right]\right)\right)\right)$$

$$\underbrace{*}_{\mathbf{p}_{\mathbf{r}}}\left(\underbrace{\circledast}_{i<j}\left(\delta\left[p_{r_i}+p_{r_j}\right]\left(\frac{1}{\pi p_{r_i}\sqrt{\frac{-i\hbar}{a_{ij}t}}}e^{\frac{i p_{r_i}\left(r_i - r_j\right)}{2\hbar}}\left(\sqrt{\frac{p_{r_i}}{\hbar}} K_1\left[\frac{2\sqrt{\frac{p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}}\right]\right.\right.\right.\right.$$

$$\left.\left.\left.\left.- \sqrt{\frac{-p_{r_i}}{\hbar}} K_1\left[\frac{2\sqrt{\frac{-p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}}\right]\right)\right)\right)\right) \tag{13}$$

Although the above (13) 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-relativistiic 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 [6]. Hence no particle is fixed as a center of motion. As stated earlier the angular components separate in the usual way by Refs. [6–8]. Here a_i, b_i, c_i are scaling constants, $L_i(L_i + 1)$ are the angular coupling terms and $\mathbf{r} = (r_1, r_2, r_3) = (r_{i=1,2,3})$, $\mathbf{p}_{\mathbf{r}} = (p_{r_1}, p_{r_2}, p_{r_3}) = (p_{r_{i=1,2,3}})$. From Eq. 4, the resulting radial Hamiltonian yields a radial Schrodinger equation of form

$$
\begin{pmatrix}
\dfrac{\left(-i\hbar\partial_{r_1}+\frac{p_{r_1}}{2}\right)^2}{2m_1} + \dfrac{\left(-i\hbar\partial_{r_2}+\frac{p_{r_2}}{2}\right)^2}{2m_2} + \dfrac{\left(-i\hbar\partial_{r_3}+\frac{p_{r_3}}{2}\right)^2}{2m_3} \\[2ex]
+\dfrac{2b_1}{\left(i\hbar\partial_{p_{r_1}}+\frac{r_1}{2}\right)}\left(-i\hbar\partial_{r_1}+\frac{p_{r_1}}{2}\right) + \dfrac{2b_2}{\left(i\hbar\partial_{p_{r_2}}+\frac{r_2}{2}\right)}\left(-i\hbar\partial_{r_2}+\frac{p_{r_2}}{2}\right) \\[2ex]
+\dfrac{2b_3}{\left(i\hbar\partial_{p_{r_3}}+\frac{r_3}{2}\right)}\left(-i\hbar\partial_{r_3}+\frac{p_{r_3}}{2}\right) + \dfrac{c_1 L_1(L_1+1)}{\left(i\hbar\partial_{p_{r_1}}+\frac{r_1}{2}\right)^2} + \dfrac{c_2 L_2(L_2+1)}{\left(i\hbar\partial_{p_{r_2}}+\frac{r_2}{2}\right)^2} \\[2ex]
+\dfrac{c_3 L_3(L_3+1)}{\left(i\hbar\partial_{p_{r_3}}+\frac{r_3}{2}\right)^2} + a_{12}\left(\dfrac{1}{\left|\left(i\hbar\partial_{p_{r_1}}+\frac{r_1}{2}\right)-\left(i\hbar\partial_{p_{r_2}}+\frac{r_2}{2}\right)\right|}\right) \\[2ex]
+a_{13}\left(\dfrac{1}{\left|\left(i\hbar\partial_{p_{r_1}}+\frac{r_1}{2}\right)-\left(i\hbar\partial_{p_{r_3}}+\frac{r_3}{2}\right)\right|}\right) + a_{23}\left(\dfrac{1}{\left|\left(i\hbar\partial_{p_{r_2}}+\frac{r_2}{2}\right)-\left(i\hbar\partial_{p_{r_3}}+\frac{r_3}{2}\right)\right|}\right)
\end{pmatrix}
$$
$$
\times \Psi_{\mathbf{r}} \text{ phasespace}\left(r_1,r_2,r_3; p_{r_1}.p_{r_2},p_{r_3};t\right)
$$
$$
= i\hbar\partial_t \Psi_{\mathbf{r}} \text{ phasespace}\left(r_1,r_2,r_3; p_{r_1}.p_{r_2},p_{r_3};t\right) \tag{14}
$$

Following Eq. 5

$$
\begin{pmatrix}
\dfrac{\left(-i\hbar\bar{r}_1+\frac{p_{r_1}}{2}\right)^2}{2m_1} + \dfrac{\left(-i\hbar\bar{r}_2+\frac{p_{r_2}}{2}\right)^2}{2m_2} + \dfrac{\left(-i\hbar\bar{r}_3+\frac{p_{r_3}}{2}\right)^2}{2m_3} \\[2ex]
+\dfrac{2b_1}{\left(i\hbar\bar{p}_{r_1}+\frac{r_1}{2}\right)}\left(-i\hbar\bar{r}_1+\frac{p_{r_1}}{2}\right) + \dfrac{2b_2}{\left(i\hbar\bar{p}_{r_2}+\frac{r_2}{2}\right)}\left(-i\hbar\bar{r}_2+\frac{p_{r_2}}{2}\right) \\[2ex]
+\dfrac{2b_3}{\left(i\hbar\bar{p}_{r_3}+\frac{r_3}{2}\right)}\left(-i\hbar\bar{r}_3+\frac{p_{r_3}}{2}\right) + \dfrac{c_1 L_1(L_1+1)}{\left(i\hbar\bar{p}_{r_1}+\frac{r_1}{2}\right)^2} + \dfrac{c_2 L_2(L_2+1)}{\left(i\hbar\bar{p}_{r_2}+\frac{r_2}{2}\right)^2} \\[2ex]
+\dfrac{c_3 L_3(L_3+1)}{\left(i\hbar\bar{p}_{r_3}+\frac{r_3}{2}\right)^2} + a_{12}\left(\dfrac{1}{\left|(i\hbar\bar{p}_{r_1}+\frac{r_1}{2})-(i\hbar\bar{p}_{r_2}+\frac{r_2}{2})\right|}\right) \\[2ex]
+a_{13}\left(\dfrac{1}{\left|(i\hbar\bar{p}_{r_1}+\frac{r_1}{2})-(i\hbar\bar{p}_{r_3}+\frac{r_3}{2})\right|}\right) + a_{23}\left(\dfrac{1}{\left|(i\hbar\bar{p}_{r_2}+\frac{r_2}{2})-(i\hbar\bar{p}_{r_3}+\frac{r_3}{2})\right|}\right)
\end{pmatrix}
$$
$$
\times \breve{\Psi}_{\mathbf{r}} \text{ phasespace}\left(\bar{r}_1,\bar{r}_2,\bar{r}_3; \bar{p}_{r_1},\bar{p}_{r_2},\bar{p}_{r_3};t\right)
$$
$$
= i\hbar\partial_t \breve{\Psi}_{\mathbf{r}} \text{ phasespace}\left(\bar{r}_1,\bar{r}_2,\bar{r}_3; \bar{p}_{r_1},\bar{p}_{r_2},\bar{p}_{r_3};t\right) \tag{15}
$$

Proceeding as in Eq. 6 through Eq. 8; for N = 3 Eqs. 9–12 become respectively

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

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

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

$$\left. \left. - \sqrt{\frac{-p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{-p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] \right) \right)$$

$\Psi_{\mathbf{r} \text{ phasespace}} \left(r_1, r_2, r_3; p_{r_1}.p_{r_2}, p_{r_3}; t \right)$

$$= \Psi_{\mathbf{r} \text{ phasespace}} \left(r_1, r_2, r_3; p_{r_1}.p_{r_2}, p_{r_3}; t = 0 \right) \underbrace{*}_{\mathbf{r}, \mathbf{p_r}} \prod_{i=1}^{3} \left(\frac{e^{\frac{i\left(r_1^2 m_1 - tr_1 p_{r_1}\right)}{2\hbar t}}}{\hbar \sqrt{\frac{2\pi i t}{\hbar m_1}}} \right)$$

$$\underbrace{*}_{\mathbf{r}} \prod_{i=1}^{3} \left(\delta\left[p_{r_i}\right] \delta\left[r_i\right] + \frac{ib_i e^{\frac{2ib_i p_{r_i} t}{\hbar r_i}} \left(\sqrt{-ip_{r_i}} - \sqrt{ip_{r_i}}\right) t}{\hbar \pi r_i^2 \sqrt{|p_{r_i}|}} \right)$$

$$\underbrace{*}_{\mathbf{p_r}} \prod_{i=1}^{3} \left(\frac{-1}{24\pi \hbar^6} \left(c_i^2 L_i^2 (L_i + 1)^2 p_{r_i}^3 t^2 \right. \right.$$

$$\times \left. \left. \left(\begin{array}{c} \left(e^{\frac{ip_{r_i} r_i}{2\hbar}} - 1 \right) Log\left[\frac{-p_{r_i}}{\hbar}\right] \\ + Log\left[\frac{p_{r_i}}{\hbar}\right] - Log\left[\frac{p_{r_i}}{\hbar}\right] HeavisideStep\left[p_{r_i}\right] \end{array} \right) \right) \right)$$

$$\underbrace{*}_{\mathbf{p_r}} \left(\underset{i<j}{\overset{3}{\circledast}} \left(\delta\left[p_{r_i} + p_{r_j}\right] \left(\frac{1}{\pi p_{r_i} \sqrt{\frac{-i\hbar}{a_{ij}t}}} e^{\frac{ip_{r_i}(r_i - r_j)}{2\hbar}} \right. \right. \right.$$

$$\times \left. \left. \left. \left(\sqrt{\frac{p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] - \sqrt{\frac{-p_{r_i}}{\hbar}} K_1 \left[\frac{2\sqrt{\frac{-p_{r_i}}{\hbar}}}{\sqrt{\frac{-i\hbar}{a_{ij}t}}} \right] \right) \right) \right) \right)$$ (16)

Now consider the earlier mentioned particular case of the general nonrelativistic Schrödinger molecular Hamiltonian with pairwise Coulomb interaction dynamics

$$\hat{H} = \sum_A \frac{1}{2M_A} \hat{\mathbf{P}}_A^2 + \sum_i \frac{1}{2m_e} \hat{\mathbf{P}}_i^2 + \sum_{A<B} \frac{e^2}{8\pi \varepsilon_0} \left(\frac{Z_A Z_B}{|\hat{r}_A - \hat{r}_B|} \right)$$

$$+ \sum_{i<j} \frac{e^2}{8\pi \varepsilon_0} \left(\frac{1}{|\hat{r}_i - \hat{r}_j|} \right) + \sum_{A,i} \left(\frac{-Z_A e^2}{|\hat{r}_A - \hat{r}_i|} \right)$$ (17)

Though we shall not pursue the details in the present note [10,11], clearly one can see that, after the angular components are separated in the usual way [6–8] 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

$$
\begin{aligned}
\hat{H}_{\substack{\text{Schrodinger}\\ \text{MolecularRadial}}} \\
= \sum_A \frac{1}{2M_A} &\left(\left(-i\hbar\partial_{r_A} + \frac{p_{r_A}}{2} \right)^2 \right. \\
&\left. + \frac{2}{\left(i\hbar\partial_{p_{r_A}} + \frac{r_A}{2} \right)} \left(-i\hbar\partial_{r_A} + \frac{p_{r_A}}{2} \right) + \frac{L_A(L_A+1)}{\left(i\hbar\partial_{p_{r_A}} + \frac{r_A}{2} \right)^2} \right) \\
+ \sum_i \frac{1}{2m_e} &\left(\left(-i\hbar\partial_{r_i} + \frac{p_{r_i}}{2} \right)^2 + \frac{2}{\left(i\hbar\partial_{p_{r_i}} + \frac{r_i}{2} \right)} \left(-i\hbar\partial_{r_i} + \frac{p_{r_i}}{2} \right) + \frac{L_i(L_i+1)}{\left(i\hbar\partial_{p_{r_i}} + \frac{r_i}{2} \right)^2} \right) \\
+ \sum_{A<B} \frac{e^2}{8\pi\varepsilon_0} &\frac{Z_A Z_B}{\left| \left(i\hbar\partial_{p_{r_A}} + \frac{r_A}{2} \right) - \left(i\hbar\partial_{p_{r_B}} + \frac{r_B}{2} \right) \right|} + \sum_{i<j} \frac{e^2}{8\pi\varepsilon_0} \frac{1}{\left| \left(i\hbar\partial_{p_{r_i}} + \frac{r_i}{2} \right) - \left(i\hbar\partial_{p_{r_j}} + \frac{r_j}{2} \right) \right|} \\
+ \sum_{A,i} &\frac{-Z_A e^2}{\left| \left(i\hbar\partial_{p_{r_A}} + \frac{r_A}{2} \right) - \left(i\hbar\partial_{p_{r_i}} + \frac{r_i}{2} \right) \right|}
\end{aligned}
\tag{18}
$$

Hence considering the radial molecular Hamiltonian (17) as was done in (4) and applying HOA to (17) as was done in (5), the exact analytical solution of the radial Schrodinger equation for the general nonrelativistic molecular Hamiltonian in QPSR may be expressed in quadratures via (6–13).

4 Closing remarks

Herein is demonstrated the exact solution to the radial Schrodinger equation for an N-particle system with pairwise Coulomb interaction. In addition to the Schrodinger Equation, upon a straightforward slight adaptation of this non-relativistic Schrodinger result, the QPSR Dirac equation addressed in [9] immediately yields the relativistic counterpart for the first-principles general polyatomic molecular Hamiltonian solution, as well as for other 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 particular 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 [13] in momentum spectroscopy necessitates the consideration of the momentum wavefunction for the molecular system under study. The novel methods addressed herein allow the exact determination of the momentum[and configuration] space wavefunction from the QPSR wavefunction by way of a Fourier transform, as seen in the Sect. 2 in this report.

References

1. Go. Torres-Vega, J.H. Frederick, J. Chem. Phys. **98**, 3103 (1993)
2. Q.S. Li, J. Lu, J. Chem. Phys. **113**(11), 4565–4571 (2000)
3. X.-G. Hu, Q.S. Li, J. Phys. A Math. Gen. **32**(1), 139–146 (1999)
4. Q.S. Li, J. Lu, Chem. Phys. Lett. **336**(1,2), 118–122 (2001)
5. Q.S. Li, G.M. Wei, L.Q. Lu, Phys. Rev. A Atom. Mol. Opt. Phys. **70**(2), 022105/1–022105/5 (2004)
6. A. Yariv, *Theory and Applications of Quantum Mechanics* (Wiley and Sons, NY, 1982)
7. R.E. Moss, *Advanced Molecular Quantum Mechanics* (Wiley and Sons, NY, 1973)
8. I. Lindgren, in *Lecture Notes in Chemistry, vol. 52: Many-Body Methods in Quantum Chemistry*, ed. by U. Kaldor (Springer, Berlin, 1989), pp. 293–306
9. V.A. Simpao, Majorana special issue. Electron. J. Theor. Phys. **3**(10), 239 (2006)
10. V.A. Simpao, Exact analysis of He atom via Heaviside operational Ansatz (in preparation)
11. V.A. Simpao, Exact analysis of H Dimer via Heaviside operational Ansatz (in preparation)
12. G.E. Roberts, H. Kaufmann, *Table of Laplace Transforms* (W.B. Saunders, 1966)
13. I. Sneddon, *The Use of Integral Transforms* (McGraw-Hill, 1972)