A Novel Method for Generating Approximate Wavefunctions

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Abstract

Molecular Hamiltonians are constituted by momentum operators (e.g. kinetic energy and interaction with electro-magnetic radiation), local potential operators (e.g. electron-electron coulomb, electron-nucleus and electron-external field interactions) and spin operators. In general the effect of transformations that generate states from a reference state is to destroy this form.

Here it is shown how one can generate all pure states by the action of a commutative semigroup of transformations that are diagonal in the space-spin coordinate representation that *do not* destroy this form and thus maintain the physical interpretability of effective Hamiltonians.

Using such transformations we formulate an approximation theory that has physical interpretation at all orders.

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I. INTRODUCTION

The Hamiltonian operator characterizes a physical system by describing all the interactions effecting it and determines which states are consistent with these interactions. Invariably physical Hamiltonians (as distinct from model Hamiltonians) are formulated in the space-spin *coordinate* representation, which reflects the fact that the properties of natural systems are most tangibly described primarily in terms of spatial coordinates and geometric images in a local pointwise fashion, i.e. at any given instant the momentum and potential energy (including the potential energy of interaction with like particles) associated with a specific particle is expressed in terms of a single spatial coordinate. Once the Hamiltonian has been constructed one can form discrete matrix or even other continuous representations by the introduction of proper bases (constituted by vectors that belong to the Hilbert space) or generalized bases (constituted by vectors that do not belong to the Hilbert space). However in order to obtain the physical content of such representations one invariably relates it back to the coordinate representation.

Nearly all molecular quantum mechanical approximations to Hamiltonians and/or states are formulated in the context of proper bases and when transformed back to the coordinate representation produce *non local* effective Hamiltonians, which in general makes their direct physical interpretation somewhat difficult. Consequently it would be convenient if the approximations could be expressed directly in the coordinate representation, in which they do have a clear physical interpretation. An added benefit of such a formalism would be that approximations could rigorously be suggested by certain properties of the specific system under study.

The most widely used approximation for molecular systems is the Self Consistent Field (SCF) method. One of the most appealing properties of this method is that it is based on an Independent Particle State (IPS) ansatz which permits one to give a physical interpretation to all terms in the variational expression and thus producing a pictorial model of processes involving atoms and molecules. A major computational asset of this method is that it does not involve two particle transformations thus allowing the Hamiltonian to be expressed in terms of a fixed atomic orbital basis at all stages of the optimization procedure i.e. the form

of the Hamiltonian is preserved at all steps. This permits one to introduce approximations to the Hamiltonian while still maintaining the physical meaning of the various terms e.g. the coulomb operator can be approximated by ignoring interactions between distant parts of the molecule and core interactions replaced by pseudo potentials.

The optimal Independent Particle State (IPS) is found by minimizing the expectation value of Hamiltonians with respect to (wrt) the parameters characterizing these states. This expectation value can be alternatively viewed as the expectation value of the exact or a fixed approximate Hamiltonian wrt a variable IPS *or* the expectation value of an effective Hamiltonian that depends on the variational parameters wrt a fixed reference IPS. However in latter case one often loses the ability to clearly physically interpret the various terms in the effective Hamiltonian e.g. terms that refer to local atomic centers become delocalized. When one is considering correlated approximations beyond the SCF method this latter way of viewing the energy expectation value is frequently more desirable, even taking into account the loss of direct physical interpretability, as it focuses on the most effective way of computing the energy expression e.g. consider the couple cluster method.

The variation over trial states can be formulated in terms of transformations, that frequently form a commuting set, acting on a fixed reference state. Even when the set of transformations commute they invariably do not commute with their adjoints, nor with terms in the Hamiltonian and hence produce rather complicated effective Hamiltonians. There is however a way of combining the desirable features of physical interpretability and fixed Hamiltonian form by generating all pure states from a fixed independent particle reference state by transformations that

- are diagonal in the space-spin coordinate representation
- form self adjoint commuting sets
- produce effective Hamiltonians that maintain the form of the exact Hamiltonian i.e. are expressed in terms of momentum and local potentials
- maintain the physical interpretability of all terms in effective Hamiltonians
- allow one to express the energy of any state in terms of the expectation value of an effective Hamiltonian wrt a given reference state

- produce approximations that have a direct physical interpretation.

In this article we describe how pure states can be generated from a reference state by the action of abelian semigroups of operators [1], which allows one to express the expectation value of all observable in any state in terms of "dressed" observables in the reference state. Utilizing this construction and considering inclusive sequences of semigroups we develop an approximation theory. Our construction is based on the properties of generalized bases, in particular the bases formed by the generalized eigenvectors of the coordinate operator. In section II we describe the abelian semigroups associated with this bases and prove that one can generate all pure states from a reference state using these semigroups. In section III we display the effective Hamiltonian generated by the action of this semigroup on the system Hamiltonian and in section IV we develop an approximation theory based on this construction, to be followed in section VI with some examples and a summary in section VII.

II. GENERATION OF STATES

Generalized bases of Hilbert spaces have been a cornerstone of quantum mechanics since their introduction by Dirac [2], since their inception they have been given a firm mathematical foundation in the context of Distribution theory [3], Group theory [4] and Topological Vector Spaces [5]. A full discussion of their properties can be found in [6] and they are closely related to Rigged Hilbert spaces introduced by [7]. In this section we prove that an abelian semigroup formed by operators that are diagonal in the space-spin generalized eigen basis generates all pure states form a cyclic [1] reference state. It is essential to consider abelian semigroups and *not* abelian groups as the latter can only maximally generate a proper subset of states from a reference state i.e. cyclic reference states *do not* exist for these groups.

A. Resolution of the Identity

The identity operator in $\mathcal{B}\left(\mathcal{H}^N\right)$ (see Appendix A for the definition of operator spaces) can be resolved as an integral of the projectors onto the generalized eigenvectors $\left\{\left|\mathsf{z}^N\right\rangle\right\}$ of

the N-particle space-spin position operator as

$$I = \int \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N\right| d\mathsf{z}^N \tag{1}$$

where $\left|\mathsf{z}^N\right\rangle = \left|\mathsf{z}_1 \cdots \mathsf{z}_N\right\rangle$ is the antisymmetric tensor product of N one particle generalized eigenvectors $\{\left|\mathsf{z}_j\right\rangle | 1 \leq j \leq N\}$ and $\mathsf{z}_j \equiv (\mathbf{r}_j, \xi_j)$ for a spatial position $\mathbf{r}_j$ and spin vector ξ_j. The wavefunction $\Psi\left(\mathsf{z}^N\right)$ of any pure state $\left|\Psi\right\rangle \left\langle\Psi\right|$ (see Appendix B for a discussion of states) is given by

$$\Psi\left(\mathsf{z}^N\right) = \left\langle \mathsf{z}^N | \Psi\right\rangle \tag{2}$$

and the state vector $\left|\Psi\right\rangle$ has the expansion

$$\left|\Psi\right\rangle = \int \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N | \Psi\right\rangle d\mathsf{z}^N \tag{3}$$

B. Hamiltonian

The molecular spin free Hamiltonian for a system of N-electrons and M-nuclei at fixed positions $\{\mathbf{R}_j | 1 \leq j \leq M\}$ is essentially local (i.e. all the terms are point interactions or are properties of a specific point), and is defined through its tangibly physical space-spin coordinate representation in atomic units as

$$\begin{aligned} H = & \sum_{1 \leq j < k \leq M} \frac{Z_j Z_k}{\left\|\mathbf{R}_j - \mathbf{R}_k\right\|} \\ & + \int \left\{ \sum_{1 \leq j \leq N} V_{ext}\left(\mathbf{r}_j\right) + \sum_{1 \leq j < k \leq N} \frac{1}{\left\|\mathbf{r}_j - \mathbf{r}_k\right\|} - \right. \\ & \left. \sum_{\substack{1 \leq j \leq M \\ 1 \leq k \leq N}} \frac{Z_j}{\left\|\mathbf{R}_j - \mathbf{r}_k\right\|} - \sum_{1 \leq j \leq N} \left\|\mathbf{p}_j\left(\mathbf{r}_j\right)\right\|^2 \right\} \left|\mathbf{r}^N\right\rangle \left\langle \mathbf{r}^N\right| d\mathbf{r}^N \end{aligned} \tag{4}$$

where nuclei j has atomic number Z_j and is at the position $\mathbf{R}_j$, $\mathbf{r}_j$ is the position of electron j that has momentum $\mathbf{p}_j\left(\mathbf{r}_j\right) = \nabla_{\mathbf{r}_j} - \mathbf{A}_{ext\,j}\left(\mathbf{r}_j\right)$, where $\mathbf{A}_{ext\,j}\left(\mathbf{r}_j\right)$ is the sum of all external vector potentials acting on particle j and $V_{ext}\left(\mathbf{r}_j\right)$ is the sum of all external scalar potentials. For future reference we denote the one and two particle potentials V_1 and V_2 as

$$\begin{aligned} V_1 &= \int \sum_{\substack{1 \leq j \leq M \\ 1 \leq k \leq N}} \left\{ -\frac{Z_j}{\left\|\mathbf{R}_j - \mathbf{r}_k\right\|} + V_{ext}\left(\mathbf{r}_k\right) \right\} \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N\right| d\mathsf{z}^N \\ V_2 &= \int \left\{ \sum_{1 \leq j < k \leq N} \frac{1}{\left\|\mathbf{r}_j - \mathbf{r}_k\right\|} \right\} \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N\right| d\mathsf{z}^N \end{aligned} \tag{5}$$

and a constant internuclear interaction term

$$H_0 = \sum_{1\leq j<k\leq M} \frac{Z_j Z_k}{\|\mathbf{R}_j - \mathbf{R}_k\|}. \tag{6}$$

. By introducing a proper basis $\{|\varphi_j\rangle\}$ for the one particle Hilbert space $\mathcal{H}^1$ one produces a matrix representation of H. If this basis is constituted by localized atomic orbitals this matrix representation still has a physically recognizable content but if the functions $\{|\varphi_j\rangle\}$ are delocalized over all centers it is hard to discern specific physical interactions and properties. In all cases the space-spin coordinate is the defining representation that determines the matrix one.

The energy $E(\Psi)$ of a state $|\Psi\rangle$ is given by the expectation value

$$E(\Psi) = \frac{\langle\Psi|H\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{7}$$

where

$$\begin{aligned}\frac{\langle\Psi|H\Psi\rangle}{\langle\Psi|\Psi\rangle} = &\sum_{1\leq j<k\leq M} \frac{Z_j Z_k}{\|\mathbf{R}_j - \mathbf{R}_k\|} + \langle\Psi|\Psi\rangle^{-1} \left\{ \int \sum_{\substack{1\leq j\leq M \\ 1\leq k\leq N}} \frac{-Z_j \Psi\left(\mathsf{z}^N\right)^* \Psi\left(\mathsf{z}^N\right)}{\|\mathbf{R}_j - \mathbf{r}_k\|} d\mathsf{z}^N \right. \\ &- \int \sum_{1\leq j\leq N}^{N} \left[\left(\nabla_{\mathbf{r}_j} - \mathbf{A}_{ext\,j}\left(\mathsf{z}^N\right)\right) \Psi\left(\mathsf{z}^N\right)^*\right] \bullet \left[\left(\nabla_{\mathbf{r}_j} - \mathbf{A}_{ext\,j}\left(\mathsf{z}^N\right)\right) \Psi\left(\mathsf{z}^N\right)\right] d\mathsf{z}^N \\ &\left. + \int \sum_{1\leq j<k\leq N} \frac{\Psi\left(\mathsf{z}^N\right)^* \Psi\left(\mathsf{z}^N\right)}{\|\mathbf{r}_j - \mathbf{r}_k\|} d\mathsf{z}^N + \int V_{ext}\left(\mathsf{z}^N\right) \Psi\left(\mathsf{z}^N\right)^* \Psi\left(\mathsf{z}^N\right) d\mathsf{z}^N \right\}\end{aligned} \tag{8}$$

the coordinates $\mathsf{z}^N \equiv \mathsf{z}_1 \cdots \mathsf{z}_N \equiv (\mathbf{r}_1, \sigma_1), \cdots, (\mathbf{r}_N, \sigma_N)$ and the normalization is

$$\langle\Psi|\Psi\rangle = \int \Psi\left(\mathsf{z}^N\right)^* \Psi\left(\mathsf{z}^N\right) d\mathsf{z}^N \tag{9}$$

C. Pure State Generation

In the coordinate representation, all pure states (unnormalized, see Appendix B) in $\mathcal{H}^N$ can be produced from a reference pure state, $|\Psi_{ref}\rangle$, that has a wavefunction

$$\left\langle \mathsf{z}^N|\Psi_{ref}\right\rangle = \varrho\left(\mathsf{z}^N\right) e^{iS\left(\mathsf{z}^N\right)} \tag{10}$$

that is non zero *a.e.*[1] by the transformations

$$|\Psi(\nu,\omega)\rangle = \breve{T}(\nu,\omega)\,|\Psi_{ref}\rangle = \breve{\nu}_N e^{i\breve{\omega}_N}\,|\Psi_{ref}\rangle \tag{11}$$

where the operators $\breve{T}(\nu,\omega), \breve{\nu}_N$ and $\breve{\omega}_N$ are diagonal in the space-spin basis $\left\{\left|\mathsf{z}^N\right\rangle\right\}$ and are given by

$$\breve{\nu}_N = \int \nu\left(\mathsf{z}^N\right)\left|\mathsf{z}^N\right\rangle\left\langle\mathsf{z}^N\right| d\mathsf{z}^N \in \mathcal{B}\left(\mathcal{H}^N\right) \tag{12a}$$

$$\breve{\omega}_N = \int \omega\left(\mathsf{z}^N\right)\left|\mathsf{z}^N\right\rangle\left\langle\mathsf{z}^N\right| d\mathsf{z}^N \in \mathcal{B}\left(\mathcal{H}^N\right) \tag{12b}$$

and form a commuting set, which we denote as $\mathcal{C}_c$. ⌈A notational aside: In this article when it is important to distinguish between an operator belonging to $\mathcal{B}\left(\mathcal{H}^N\right)$ and its integral kernel, we denote the operator by $\breve{T}$ and the integral kernel by $T\left(\mathsf{z}^N\right)$ or $T\left(\mathsf{z}^N,\mathsf{z}'^N\right)$, if it not important to distinguish between we just use T⌋.

The strong closure [3] of the space $\mathcal{C}_c$ of diagonal integral operators that map $\mathcal{H}^N \to \mathcal{H}^N$ is the space of integral operators with symmetric integral kernels $\left\{T\left(\mathsf{z}^N\right)\right\}$ that belong to the Banach space $L_\infty\left(\mathsf{Z}^N\right)$ [1], and form a semigroup which is in particular a w^*-algebra. [8]. The following extract from Thirring [8] should be noted:

> $L_\infty\left(\mathsf{Z}^N\right)$, *considered as multiplication operators on* $L_2\left(\mathsf{Z}^N\right)$ *is maximally abelian. Every function in* $L_2\left(\mathsf{Z}^N\right)$ *that is non zero a.e. is a cyclic vector. Functions that vanish on some set* $\left[\Omega^N\right]^C = \mathsf{Z}^N - \Omega^N \subset \mathsf{Z}^N$ *form invariant subspaces. Thus* $L_\infty\left(\mathsf{Z}^N\right)$ *is reducible and not a factor* [1].

One can see that $T(\nu,\omega)\left(\mathsf{z}^N\right)$ (the integral kernel of $\breve{T}(\nu,\omega)$) is a parameterization of a representation of an abelian w^*-algebra, $\mathfrak{A}$, on $L_2\left(\mathsf{Z}^N\right)$ by $L_\infty\left(\mathsf{Z}^N\right)$. This representation is reducible as $L_2\left(\mathsf{Z}^N\right)$ contains the following invariant subspaces

$$L_2\left(\Omega^N\right) = \left\{\Psi \,\middle|\, \Psi\left(\mathsf{z}^N\right) = 0 \,\text{if}\; \mathsf{z}^N \notin \Omega^N, \int_{\Omega^N} d\mathsf{z}^N \neq 0 \,\text{and}\, \Omega^N \subset \mathsf{Z}^N\right\} \tag{13}$$

The operator $\breve{T}(\nu,\omega)$ produces elements that have amplitudes that belong to $L_2\left(\Omega^N\right)$ when $\mathrm{Supp}(\nu) = \Omega^N$ [3].

The set of invertible diagonal operators in $\mathfrak{A}$ form a group, $\mathfrak{G}$, that also has a reducible representation on $L_\infty\left(\mathsf{Z}^N\right)$, as clearly $L_2\left(\Omega^N\right)$ are also invariant subspaces of $\mathfrak{G}$. However *it is not true* that every function in $L_2\left(\mathsf{Z}^N\right)$ that is nonzero *a.e.* is a cyclic vector for $\mathfrak{G}$ and in fact there do not exist *any* cyclic vectors for $\mathfrak{G}$ in $L_2\left(\mathsf{Z}^N\right)$ and thus one can never generate all pure states by the action of $\mathfrak{G}$ on a reference state.

We can contrast this semigroup to ones formed by proper bases of N-particle space by comparing the preceding to the discrete case by focusing on a proper basis $\{|\Phi_j\rangle\}$ of $\mathcal{H}^N$,

the abelian algebra, $\mathcal{C}_d$, generated by $\left\{ \sum_{1\leq j\leq\infty} \lambda_j \left|\Phi_j\right\rangle \left\langle\Phi_j\right| \right\}$ and a reference state $\left|\Phi_{ref}\right\rangle = \sum_{1\leq j\leq\infty} \alpha_j \left|\Phi_j\right\rangle$ that has the property that $\alpha_j \neq 0 \, \forall i$ (see Appendix C). Similarly to $\mathcal{C}_c$ the abelian algebra $\mathcal{C}_d$ can also generate all pure states from such a reference state but it *does not* have such desirable properties wrt H as $\mathcal{C}_c$ does e.g. the potential terms in H are no longer diagonal nor will $\mathcal{C}_c$ commute with these terms.

III. EFFECTIVE HAMILTONIAN

Any pure state N-particle density operator $\breve{D}^N(\nu,\omega)$, (in general unnormalized), can be generated from a cyclic reference density $\breve{\mathcal{D}}^N_{ref}$ by the transformation

$$\breve{\mathcal{D}}^N(\nu,\omega) = \hat{T}\left(\breve{\mathcal{D}}^N_{ref}\right) = \breve{T}(\nu,\omega)\,\breve{\mathcal{D}}^N_{ref}\breve{T}(\nu,\omega)^\dagger \tag{14}$$

The transformation $\hat{T}(\nu,\omega)$ is positive as it maps the set of positive operators $\mathcal{B}_{1+}\left(\mathcal{H}^N\right)$ to itself and the set of all such $\hat{T}$ correspond to the semigroup $\mathcal{C}_c$.

As the energy expectation value $E(\nu,\omega)$ can be expressed as

$$E(\nu,\omega) = \frac{Tr\left\{H\breve{\mathcal{D}}^N(\nu,\omega)\right\}}{Tr\left\{\breve{\mathcal{D}}^N(\nu,\omega)\right\}} = \frac{Tr\left\{H\breve{T}(\nu,\omega)\,\breve{\mathcal{D}}^N_{ref}\breve{T}(\nu,\omega)^\dagger\right\}}{Tr\left\{\breve{T}(\nu,\omega)\,\breve{\mathcal{D}}^N_{ref}\breve{T}(\nu,\omega)^\dagger\right\}} = \frac{Tr\left\{\breve{T}(\nu,\omega)^\dagger H\breve{T}(\nu,\omega)\,\breve{\mathcal{D}}^N_{ref}\right\}}{Tr\left\{\breve{T}(\nu,\omega)\,\breve{\mathcal{D}}^N_{ref}\breve{T}(\nu,\omega)^\dagger\right\}} \tag{15}$$

the action of the transformation $\hat{T}(\nu,\omega)$ can be incorporated into an effective Hamiltonian $H(\nu,\omega)$ defined by

$$H(\nu,\omega) = \breve{T}(\nu,\omega)^\dagger H\breve{T}(\nu,\omega) \tag{16}$$

and all expectation values can be taken wrt the IPS $\breve{\mathcal{D}}^N_{ref}$.

The Hamiltonians, H, we consider are of the form

$$H = H_0 - \mathbf{P}\bullet\mathbf{P} + V_1 + V_2 \tag{17}$$

where H_0 is a constant, $\mathbf{P}$ the total *generalized* momentum operator for the system, V_1 is the sum of all one particle potential operators and V_2 is the sum of all two particle potential operators. The *generalized* momentum is defined in terms of one particle *generalized* momentum operators as

$$\mathbf{P} = \sum_{1\leq j\leq N} \mathbf{p}_j \tag{18}$$

where

$$\mathbf{p}_j = -i\nabla_j - \mathbf{A}_j \tag{19}$$

$\mathbf{A}_j$ is the total external vector potential acting on particle j and

$$-i\nabla_j = -i\begin{pmatrix} \frac{\partial}{\partial x_j} \\ \frac{\partial}{\partial y_j} \\ \frac{\partial}{\partial z_j} \end{pmatrix}; \quad \mathbf{A}_j = \begin{pmatrix} A_{jx} \\ A_{jy} \\ A_{jz} \end{pmatrix} \tag{20}$$

The potentials $\{\mathbf{A}_j\}$, V_1 and V_2 are all diagonal in the space-spin representation. The operators $\left\{\breve{T}(\nu,\omega)\right\}$ *all commute* with these potentials, which is of course by design, so that

$$\begin{aligned} \breve{T}(\nu,\omega)^\dagger V \breve{T}(\nu,\omega) &= \breve{\nu}_N e^{-i\breve{\omega}_N} V \breve{\nu}_N e^{i\breve{\omega}_N} = (\breve{\nu}_N)^2 V \\ \breve{T}(\nu,\omega)^\dagger \mathbf{A}_j \breve{T}(\nu,\omega) &= \breve{\nu}_N e^{-i\breve{\omega}_N} \mathbf{A}_j \breve{\nu}_N e^{i\breve{\omega}_N} = (\breve{\nu}_N)^2 \mathbf{A}_j \end{aligned} \tag{21}$$

where $V = V_1 + V_2$

$$\begin{aligned} (\breve{\nu}_N)^2 V &= \int \nu\left(\mathsf{z}^N\right)^2 V\left(\mathsf{z}^N\right) \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N\right| d\mathsf{z}^N \\ (\breve{\nu}_N)^2 A_{j\kappa} &= \int \nu\left(\mathsf{z}^N\right)^2 A_{j\kappa}\left(\mathsf{z}^N\right) \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N\right| d\mathsf{z}^N; \qquad \kappa = x,y,z \end{aligned} \tag{22}$$

i.e. the potentials are scaled by the integral kernels $\left\{\nu\left(\mathsf{z}^N\right)\right\}$. It is *important* to note that while the Hamiltonian H only contains potentials describing up to two particle interactions, the integral kernels $\left\{\nu\left(\mathsf{z}^N\right)\right\}$ are in general *multiparticle* functions and thus produce multi-particle potentials $\left\{\nu\left(\mathsf{z}^N\right)^2 V\left(\mathsf{z}^N\right)\right\}$ describing up to simultaneous N-particle interactions. Furthermore the N-particle local scaling factors $\nu\left(\mathsf{z}^N\right)$ contain phase information pertaining to $1, 2, \cdots, M < N$ particle interactions and the N-particle local phase $\omega\left(\mathsf{z}^N\right)$ contains local scaling information pertaining to $1, 2, \cdots, M < N$ particle interactions as will discussed in the examples.

The effect of the unitary part $\{e^{i\omega_N}\}$ of the transformations $\left\{\breve{T}(\nu,\omega)\right\}$ on the momentum operators $\{-i\nabla_j\}$ (for simplicity we consider the case where there is no external vector potential) is to produce a generalized gauge transformation i.e. producing the component operators

$$e^{-i\breve{\omega}_N}\left(-i\frac{\partial}{\partial x_j}\right)e^{i\breve{\omega}_N} = -i\frac{\partial}{\partial x_j} + \frac{\partial \breve{\omega}_N}{\partial x_j} \tag{23}$$

and 1-particle vector operators

$$e^{-i\breve{\omega}_N}\left(-i\nabla_j\right)e^{i\breve{\omega}_N} = -i\nabla_j + \nabla_j\breve{\omega}_N \tag{24}$$

(again note that $\breve{\omega}_N$ are N-particle operators). The effect of the scaling $\breve{\nu}_N$ on this is

$$\left(-i\nabla_j + \nabla_j\breve{\omega}_N\right)\breve{\nu}_N = -i\breve{\nu}_N\nabla_j - i\left(\nabla_j\breve{\nu}_N\right) + \breve{\nu}_N\left(\nabla_j\breve{\omega}_N\right) \tag{25}$$

leading to an effective kinetic energy operator (see Appendix D) which is a sum of kinetic, momentum and potential terms

$$\begin{aligned} K\left(\nu,\omega\right) = \breve{T}\left(\nu,\omega\right)^{\dagger}\left(\mathbf{P}\bullet\mathbf{P}\right)\breve{T}\left(\nu,\omega\right) = \\ -\nabla\bullet\left(\breve{\nu}^2\right)\mathbb{I}\bullet\nabla - \nabla\bullet\left(\breve{\nu}_N^2\nabla\breve{\omega}_N - i\breve{\nu}_N\nabla\breve{\nu}_N\right) \\ -\left(\breve{\nu}_N^2\nabla\breve{\omega}_N - i\breve{\nu}_N\nabla\breve{\nu}_N\right)\bullet\nabla + \left(\breve{\nu}_N\nabla\breve{\omega}_N - i\nabla\breve{\nu}_N\right)\bullet\mathbb{I}\bullet\left(\breve{\nu}_N\nabla\breve{\omega}_N - i\nabla\breve{\nu}_N\right) \end{aligned} \tag{26}$$

where $\mathbb{I}$ is $3N\times 3N$ unit matrix. Thus the effective Hamiltonian is given by

$$H\left(\nu,\omega\right) = H_0 + K\left(\nu,\omega\right) + \left(\breve{\nu}_N\right)^2 V \tag{27}$$

which displays that the effective scalar potential does not depend on the N-particle local phase factor $\exp\left\{i\omega\left(\mathsf{z}^N\right)\right\}$, but it should be noted that it *does* depend on phase relationships between the individual particles.

IV. APPROXIMATIONS

One can expand the transformation $\breve{T}\left(\nu,\omega\right)\in\mathcal{B}\left(\mathcal{H}^N\right)$ in terms of antisymmetrized tensor products of transformations [9][10] $\breve{T}_{n_j}\in\mathcal{B}\left(\mathcal{H}^{n_j}\right)$ associated with partitions $\{n_1,\ldots,n_m\}$ of N, i.e. for sets of $\{n_j|\,1\leq j\leq m\}$ where $0\leq n_j\leq N$ and $\sum\limits_{1\leq j\leq m} n_j = N$, as

$$\breve{T}\left(\nu,\omega\right) = \sum_{1\leq m\leq N}\sum_{\{n_1,\ldots,n_m\}} c_{n_1\ldots n_m}\breve{T}_{n_1}\left(\nu_{n_1},\omega_{n_1}\right)\wedge\cdots\wedge\breve{T}_{n_m}\left(\nu_{n_m},\omega_{n_m}\right) \tag{28}$$

where ν_{n_p} defines the operator $\breve{\nu}_{n_p}$ through an integral kernel $\nu_{n_p}\left(\mathsf{z}^{n_p}\right)$ with variables $\mathsf{z}^{n_p}\equiv\mathsf{z}_{q_p+1}\cdots\mathsf{z}_{q_p+n_p}$, where $q_p = n_1+\cdots+n_{p-1}$. The antisymmetrized product operator $\breve{T}_{n_1}\left(\nu_{n_1},\omega_{n_1}\right)\wedge\cdots\wedge\breve{T}_{n_m}\left(\nu_{n_m},\omega_{n_m}\right)$ is defined by

$$\begin{aligned} \breve{T}_{n_1}\left(\nu_{n_1},\omega_{n_1}\right)\wedge\cdots\wedge\breve{T}_{n_m}\left(\nu_{n_m},\omega_{n_m}\right)\left|\Phi^{n_1}_{J_{n_1}}\wedge\cdots\wedge\Phi^{n_m}_{J_{n_m}}\right\rangle \\ = \left|\breve{T}_{n_1}\left(\nu_{n_1},\omega_{n_1}\right)\Phi^{n_1}_{J_{n_1}}\wedge\cdots\wedge\breve{T}_{n_m}\left(\nu_{n_m},\omega_{n_m}\right)\Phi^{n_m}_{J_{n_m}}\right\rangle \end{aligned} \tag{29}$$

for $1 \leq J_{n_j} \leq \binom{r}{n_j}, 1 \leq j \leq m$ for a specific fixed partition $\{n_1, \ldots, n_m\}$ where $\left\{ \left| \Phi^{n_j}_{J_{n_j}} \right\rangle \middle| 1 \leq J_{n_j} \leq \binom{r}{n_j}; \{n_1, \ldots, n_m\} \right\}$ are proper bases for $\{\mathcal{H}^{n_j} | \, 1 \leq j \leq m\}$. If a factor $\breve{T}_{n_p}\left(\nu_{n_p}, \omega_{n_p}\right)$ can be expressed as a product of lower order factors e.g.

$$\breve{T}_{n_p}\left(\nu_{n_p}, \omega_{n_p}\right) = \breve{T}_{p_1}\left(\nu_{p_1}, \omega_{p_1}\right) \wedge \cdots \wedge \breve{T}_{p_m}\left(\nu_{p_m}, \omega_{p_m}\right) \tag{30}$$

where $\sum_{1 \leq j \leq m} p_j = n_p$ for a partition $\{p_1, \ldots, p_m\}$ we say it is decomposable if not, i.e. it can only be expressed as a sum of such products, we say it is indecomposable.

In general it is possible to express the expansion eq. (28) of $\breve{T}(\nu, \omega)$ in terms of *anti-symmetric* tensor products $\breve{T}_{n_1}\left(\nu_{n_1}, \omega_{n_1}\right) \wedge \cdots \wedge \breve{T}_{n_m}\left(\nu_{n_m}, \omega_{n_m}\right)$ of indecomposable operators $\left\{ \breve{T}_{n_p}\left(\nu_{n_p}, \omega_{n_p}\right) \right\}$ whose integral kernels are symmetric functions (see Appendix E) given by the *symmetric* [9][10] tensor product of the kernels of these operators as

$$T_{n_1 \cdots n_m}\left(\mathsf{z}^N\right) = T_{n_1}\left(\mathsf{z}^{n_1}\right) \vee \cdots \vee T_{n_m}\left(\mathsf{z}^{n_m}\right) \tag{31}$$

Approximations to the set of transformations $\left\{ \breve{T}(\nu, \omega) \right\}$ can be generated by placing restrictions on the expansion eq. (28) to various classes of partitions $\{n_1, \ldots, n_m\}$, the types of operators in the products and by limiting the choice of integral kernels $\nu\left(\mathsf{z}^N\right), \omega\left(\mathsf{z}^N\right)$ by expanding them in terms of fixed sets of function. For example some different types of products are produced by:

1. The partition $\{1, \ldots, 1\}$ that leads to one particle operators acting in N-particle space $\mathcal{H}^N$ whose integral kernels are formed by a product of identical one particle integral kernels

$$T\left(\mathsf{z}^N\right) = T_1^N\left(\mathsf{z}^N\right) = T_1\left(\mathsf{z}_1\right) \cdots T_1\left(\mathsf{z}_N\right) \tag{32}$$

and corresponds to a linear transformations of N-particle space $\mathcal{H}^N$ through

$$T_1 \wedge \cdots \wedge T_1 \left| \varphi_{j_1} \cdots \varphi_{j_N} \right\rangle = \left| T_1 \varphi_{j_1} \cdots T_1 \varphi_{j_N} \right\rangle; \quad 1 \leq j_1 < \cdots < j_N \leq r \tag{33}$$

where $\{|\varphi_j\rangle | \, 1 \leq j \leq r\}$ forms a complete orthonormal basis for $\mathcal{H}^1$ of dimension r.

2. The partition $\{1, \ldots, 1\}$ that leads to N-particle operators acting in N-particle space $\mathcal{H}^N$ whose integral kernels are formed by a product of different one particle integral kernels

$$T\left(\mathsf{z}^N\right) = \sum_{\sigma \in \mathcal{S}_N} T_1\left(\mathsf{z}_{\sigma(1)}\right) \cdots T_N\left(\mathsf{z}_{\sigma(N)}\right) \tag{34}$$

These transformations correspond to

$$T_1 \wedge \cdots \wedge T_N \left|\varphi_1 \cdots \varphi_N\right\rangle = \left|T_1\varphi_1 \cdots T_N\varphi_N\right\rangle \qquad \forall \left|\varphi_j\right\rangle \in \mathcal{H}^N, 1 \leq j \leq N \tag{35}$$

which *are not induced* by linear transformations of one particle space $\mathcal{H}^1$ unless $T_1 = \cdots = T_N$. The integral kernel of this transformation can be developed using the polar decomposition $T_j\left(\mathsf{z}\right) = \nu_j\left(\mathsf{z}\right) e^{i\omega_j(\mathsf{z})}$ to give

$$\begin{aligned} T\left(\mathsf{z}^N\right) &= \sum_{\sigma\in\mathcal{S}_N} \nu_{\sigma(1)}\left(\mathsf{z}_1\right) e^{i\omega_{\sigma(1)}(\mathsf{z}_1)} \cdots \nu_{\sigma(N)}\left(\mathsf{z}_N\right) e^{i\omega_{\sigma(N)}(\mathsf{z}_N)} \\ &= \sum_{\sigma\in\mathcal{S}_N} \nu_{\sigma(1)}\left(\mathsf{z}_1\right) \cdots \nu_{\sigma(N)}\left(\mathsf{z}_N\right) e^{i\left\{\omega_{\sigma(1)}(\mathsf{z}_1)+\cdots+\omega_{\sigma(N)}(\mathsf{z}_N)\right\}} \end{aligned} \tag{36}$$

One should be careful to note that in this expansion $\nu\left(\mathsf{z}^N\right) \neq \sum_{\sigma\in\mathcal{S}_N} \nu_{\sigma(1)}\left(\mathsf{z}_1\right) \cdots \nu_{\sigma(N)}\left(\mathsf{z}_N\right)$, and $\omega\left(\mathsf{z}^N\right) \neq \sum\limits_{1\leq j\leq N} \omega_{\sigma(j)}\left(\mathsf{z}_j\right)$ but each are in fact complicated functions of $\{\nu_j, \omega_j | 1 \leq j \leq N\}$. Thus although $T\left(\mathsf{z}^N\right) = \nu\left(\mathsf{z}^N\right) e^{i\omega\left(\mathsf{z}^N\right)}$ and the norm $\left\|\left|T_1\varphi_1 \cdots T_N\varphi_N\right\rangle\right\|$ is *independent* of the N-particle phase $\omega\left(\mathsf{z}^N\right)$ it is *not* independent of the individual particle phases $\{\omega_j\left(\mathsf{z}_j\right)\}$. Another important point to note from this example is that IPSs *are not all* generated from a reference IPS by one particle diagonal operators i.e. by transformations of the form $T_1 \wedge \cdots \wedge T_1$ but they *are all* generated by N-particle transformations of the form $T_1 \wedge T_2 \wedge \cdots \wedge T_N$, (see section V for a discussion of how these diagonal N-particle operators correspond to non diagonal 1-particle operators)

3. The partition $\{2, \ldots, 2\}$ that leads to N-particle operators acting in N-particle space $\mathcal{H}^N$ whose integral kernels are formed by a product of identical two particle integral kernels (of course there must be an even number of particles in this case)

$$T\left(\mathsf{z}^N\right) = T_2^{\frac{N}{2}}\left(\mathsf{z}^N\right) = \sum_{\sigma\in\mathcal{S}_N} T_2\left(\mathsf{z}_{\sigma(1)}\mathsf{z}_{\sigma(2)}\right) \cdots T_2\left(\mathsf{z}_{\sigma(N-1)}\mathsf{z}_{\sigma(N)}\right) \tag{37}$$

through the definition

$$T_2 \wedge \cdots \wedge T_2 \left|g_1 \cdots g_{\frac{N}{2}}\right\rangle = \left|T_2 g_1 \cdots T_2 g_{\frac{N}{2}}\right\rangle \qquad \forall \left|g_j\right\rangle \in \mathcal{H}^2, 1 \leq j \leq \frac{N}{2} \tag{38}$$

Using the expansion eq. (28) one can decompose $T\left(\mathsf{z}^N\right)$ in terms of indecomposable parts indexed by $\{n_1, \ldots, n_m\}$ e.g.

$$T\left(\mathsf{z}^N\right) = \sum_{1\leq m\leq N} \sum_{\{n_1,\ldots,n_m\}} T_{n_1\ldots n_m}\left(\mathsf{z}^N\right) \tag{39}$$

and formulate approximations to the energy functional $E(\nu,\omega)$ by truncating and approximating terms in this expansion. For instance one might choose the parts indexed by $\{1,\cdots,1\}$ which contains integral kernels of the form

$$T\left(\mathsf{z}^N\right) = T_1(\mathsf{z}_1) \vee \cdots \vee T_N(\mathsf{z}_N) \tag{40}$$

which includes p-particle operator integral kernels of the form

$$T_1(\mathsf{z}_1) \vee \cdots \vee T_p(\mathsf{z}_p) \vee \delta(\mathsf{z}_{p+1}) \vee \cdots \vee \delta(\mathsf{z}_N); \quad T_j \neq T_k, 1 \leq j < k \leq p; 1 \leq p \leq N \tag{41}$$

and 1-particle operators integral kernels of the form

$$T_1(\mathsf{z}_1) \vee \cdots \vee T_1(\mathsf{z}_N). \tag{42}$$

or just restrict attention to the operator kernels of eq. (42). A higher level of approximation would include parts indexed by $\{1,\cdots,1\}$ and all or a selection from integral kernels indexed by $\{2,1,\cdots,1\},\{2,2,1,\cdots,1\},\ldots,\{2,2,\cdots,2\}$ and so on....

V. COMMUTATIVE VERSUS NONCOMMUTATIVE TRANSFORMATIONS

Example 2 of section IV showed that all IPSs can be generated by an *abelian* semigroup $\mathcal{C}_c$ of diagonal N-particle operators, $T_1 \wedge \cdots \wedge T_N$, composed of N diagonal one particle operators $\{T_j | \, 1 \leq j \leq N\}$. At the same time it is well known that all IPSs can be generated by the *non abelian* general linear group, $\mathcal{GL}(\mathcal{H}^1)$, of transformations that map $\mathcal{H}^1 \to \mathcal{H}^1$. In this section we explicitly describe a correspondence between $\mathcal{C}_c$ and $\mathcal{GL}(\mathcal{H}^1)$ by considering the equivalence of N-dimensional subspaces, $V(\varphi)$, spanned by the vectors $\{|\varphi_j\rangle | \, 1 \leq j \leq N\}$ of $\mathcal{H}^1$ to N-particle IPSs $|\varphi_1 \cdots \varphi_N\rangle$. The diagonal transformation

$$T_1 \wedge \cdots \wedge T_N |\varphi_1 \cdots \varphi_N\rangle = |T_1\varphi_1 \cdots T_N\varphi_N\rangle \tag{43}$$

can be associated with the transformation $\mathcal{T}(\varphi) : V(\varphi) \to V_T(\varphi)$ between the subspaces $V(\varphi)$ spanned by the *linearly independent* vectors $\{|\varphi_j\rangle | \, 1 \leq j \leq N\}$ and $V_T(\varphi)$ spanned by the *orthonormal* vectors $\{|\psi_j\rangle | \, 1 \leq j \leq N\}$ defined by

$$\mathcal{T}(\varphi)(|\varphi_1\rangle, \cdots, |\varphi_N\rangle) = (|\psi_1\rangle, \cdots, |\psi_N\rangle) = (|T_1\varphi_1\rangle, \cdots, |T_N\varphi_N\rangle)\, \mathbf{\Delta}(\varphi)^{-\frac{1}{2}} \tag{44}$$

where $\Delta(\varphi)_{jk} = \langle T_j\varphi_j | T_k\varphi_k\rangle$ and

$$\Delta(\varphi)(|T_1\varphi_1\rangle, \cdots, |T_N\varphi_N\rangle) = (|T_1\varphi_1\rangle, \cdots, |T_N\varphi_N\rangle)\, \mathbf{\Delta}(\varphi) \tag{45}$$

i.e.

$$|\psi_j\rangle = \sum_{1\leq k\leq N} |T_k\varphi_k\rangle \left(\mathbf{\Delta}\left(\varphi\right)^{-\frac{1}{2}}\right)_{kj}; \qquad 1\leq j\leq N \tag{46}$$

Using eq. (45) we obtain

$$|\psi_1\cdots\psi_N\rangle = \det\left(\mathbf{\Delta}\left(\varphi\right)\right)^{-\frac{1}{2}} |T_1\varphi_1\cdots T_N\varphi_N\rangle \tag{47}$$

and

$$|T_1\varphi_1\cdots T_N\varphi_N\rangle = \det\left(\mathbf{\Delta}\left(\varphi\right)\right)^{\frac{1}{2}} |\psi_1\cdots\psi_N\rangle \tag{48}$$

Hence the action of the N-particle diagonal transformation $T_1\wedge\cdots\wedge T_N$ on the IPS $|\varphi_1\cdots\varphi_N\rangle$ produces the IPS $|T_1\varphi_1\cdots T_N\varphi_N\rangle$ that can also be generated by the action of the one particle transformation $\mathcal{R}\left(\varphi\right)$ on $|\varphi_1\cdots\varphi_N\rangle$ where $\mathcal{R}\left(\varphi\right) = \mathbf{\Delta}\left(\varphi\right)^{\frac{1}{2}}\mathcal{T}\left(\varphi\right)$ i.e.

$$\begin{aligned} T_1\wedge\cdots\wedge T_N\,|\varphi_1\cdots\varphi_N\rangle &= \mathcal{R}\left(\varphi\right)\wedge\cdots\wedge\mathcal{R}\left(\varphi\right)|\varphi_1\cdots\varphi_N\rangle \\ &= |\mathcal{R}\left(\varphi\right)\varphi_1\cdots\mathcal{R}\left(\varphi\right)\varphi_N\rangle = \left|\mathbf{\Delta}\left(\varphi\right)^{\frac{1}{2}}\mathcal{T}\left(\varphi\right)\varphi_1\cdots\mathbf{\Delta}\left(\varphi\right)^{\frac{1}{2}}\mathcal{T}\left(\varphi\right)\varphi_N\right\rangle \\ &= \det\left(\mathbf{\Delta}\left(\varphi\right)\right)^{\frac{1}{2}}|\mathcal{T}\left(\varphi\right)\varphi_1\cdots\mathcal{T}\left(\varphi\right)\varphi_N\rangle = |T_1\varphi_1\cdots T_N\varphi_N\rangle \end{aligned} \tag{49}$$

The transformations $\{T_j\}$ and $\{T_1\wedge\cdots\wedge T_N\}$ form commuting sets, are diagonal in the space-spin coordinate representation and are semigroups, while the transformations $\{\mathcal{R}\left(\varphi\right)\}$ and $\{\mathcal{R}\left(\varphi\right)\wedge\cdots\wedge\mathcal{R}\left(\varphi\right)\}$ are not in general diagonal in this representation nor do they form commuting sets, but they do form a group.

The correspondence between the N-particle transformation $T_1\wedge\cdots\wedge T_N$ and the one particle transformation $\mathcal{R}\left(\varphi\right)$ depends on the existence of the *one* dimensional representation $\det\left(\mathbf{\Delta}\right)$ of Δ in $\mathcal{H}^N$. This does *not* carry over to the analogous construction applied to transformations defined in $\mathcal{H}^2$ e.g. as in example 3 of section IV, thus one cannot obtain such a correspondence between a transformation on $\mathcal{H}^2$ and a product of diagonal transformation acting in $\mathcal{H}^N$.

It is interesting to note the form of the first order reduced density operators, $L_N^1\left(D^N\right)$ associated with the normalized states

$$D^N = \frac{|T_1\varphi_1\cdots T_N\varphi_N\rangle\langle T_1\varphi_1\cdots T_N\varphi_N|}{\langle T_1\varphi_1\cdots T_N\varphi_N|T_1\varphi_1\cdots T_N\varphi_N\rangle} \tag{50}$$

are

$$L_N^1\left(D^N\right) = \sum_{1\leq j,k\leq N} |T_j\varphi_j\rangle\left(\Delta^{-1}\right)_{jk}\langle T_k\varphi_k| = \sum_{1\leq j\leq N} |\psi_j\rangle\langle\psi_j| \tag{51}$$

which leads to vastly simplified expressions for expectation values wrt the state $|T_1\varphi_1\cdots T_N\varphi_N\rangle$ than the general ones developed in section VI. Eq. (51) covers the case $T_j = I_j\ 1 \leq j \leq N$ leading to

$$L_N^1\left(\frac{|\varphi_1\cdots\varphi_N\rangle\langle\varphi_1\cdots\varphi_N|}{\langle\varphi_1\cdots\varphi_N|\varphi_1\cdots\varphi_N\rangle}\right) = \sum_{1\leq j,k\leq N}|\varphi_j\rangle\left(\Delta^{-1}\right)_{jk}\langle\varphi_k| = \sum_{1\leq j\leq N}|\psi_j\rangle\langle\psi_j| \tag{52}$$

where $\Delta_{jk} = \langle\varphi_j|\varphi_k\rangle$.

VI. EXAMPLES

We first consider the approximation indexed by $\{1,\cdots,1\}$ and develop it in manner that can be used for higher order approximations so that we can see the general structure common to all levels of approximation. It is clear however that the resulting expressions are more complicated than the ones that would be obtained if we utilized the correspondence described in section V.

A. Approximations indexed by $\{1,\cdots,1\}$

The transformations that we consider in this case are

$$\breve{T}_1\wedge\cdots\wedge\breve{T}_N\,|\varphi_1\cdots\varphi_N\rangle = \left|\breve{T}_1\varphi_1\cdots\breve{T}_N\varphi_N\right\rangle \tag{53}$$

That have integral kernels

$$\begin{aligned} T\left(\mathsf{z}^N\right) &= T_1\left(\mathsf{z}_1\right)\vee\cdots\vee T_N\left(\mathsf{z}_N\right) = \sum_{\sigma\in\mathcal{S}_N}T_1\left(\mathsf{z}_{\sigma(1)}\right)\cdots T_N\left(\mathsf{z}_{\sigma(N)}\right) \\ &= \sum_{\sigma\in\mathcal{S}_N}T_{\sigma(1)}\left(\mathsf{z}_1\right)\cdots T_{\sigma(N)}\left(\mathsf{z}_N\right) \\ &= \sum_{\sigma\in\mathcal{S}_N}\nu_{\sigma(1)}\left(\mathsf{z}_1\right)\cdots\nu_{\sigma(N)}\left(\mathsf{z}_N\right)e^{i\left\{\omega_{\sigma(1)}(\mathsf{z}_1)+\cdots+\omega_{\sigma(N)}(\mathsf{z}_N)\right\}} \end{aligned} \tag{54}$$

where

$$\omega_{\sigma(j)}\left(\mathsf{z}_j\right) = \delta\left(\mathsf{z}_1\right)\cdots\delta\left(\mathsf{z}_{j-1}\right)\omega_{\sigma(j)}\left(\mathsf{z}_j\right)\delta\left(\mathsf{z}_{j+1}\right)\cdots\delta\left(\mathsf{z}_N\right) \tag{55}$$

and the kernels $\{\nu_j\left(\mathsf{z}_j\right)|1\leq j\leq N\}$ could be equal to each other or be delta functions as could the kernels $\{\omega_j\left(\mathsf{z}_j\right)|1\leq j\leq N\}$. The N-particle kernels ν,ω are both functions of the 1-particle kernels $\{\nu_1,\ldots,\nu_N,\omega_1,\ldots,\omega_N\}$ i.e.

$$\begin{aligned} \nu &= \nu\left(\nu_1,\ldots,\nu_N,\omega_1,\ldots,\omega_N\right) \\ \omega &= \omega\left(\nu_1,\ldots,\nu_N,\omega_1,\ldots,\omega_N\right) \end{aligned} \tag{56}$$

The first term we need to evaluate is the normalization

$$\begin{aligned} Tr\left\{\breve{\mathcal{D}}^{N}\left(\nu,\omega\right)\right\} &= \left\langle \breve{T}\left(\nu,\omega\right)\varphi_1\cdots\varphi_N\right| \breve{T}\left(\nu,\omega\right)\varphi_1\cdots\varphi_N\Big\rangle \\ &= \sum_{\sigma,\sigma'\in\mathcal{S}_N}\left\langle \breve{T}_{\sigma(1)}\cdots\breve{T}_{\sigma(N)}\varphi_1\cdots\varphi_N\left|\breve{T}_{\sigma'(1)}\cdots\breve{T}_{\sigma'(N)}\varphi_1\cdots\varphi_N\right\rangle\right. \\ &= \sum_{\sigma,\sigma'\in\mathcal{S}_N}\left\langle \breve{T}_{\sigma(1)}\varphi_1\cdots\breve{T}_{\sigma(N)}\varphi_N\left|\breve{T}_{\sigma'(1)}\varphi_1\cdots\breve{T}_{\sigma'(N)}\varphi_N\right\rangle\right. \\ &= \left\langle \varphi_1\cdots\varphi_N\right| \breve{S}_{eff}\left(\nu,\omega\right)\varphi_1\cdots\varphi_N\Big\rangle \equiv \mathcal{S}\left(\nu,\omega\right) \end{aligned} \tag{57}$$

where $|\varphi_1\cdots\varphi_N\rangle$ is a fixed IPS. The effect of the multiparticle potential $T_{\sigma(1)}\cdots T_{\sigma(N)}$ on an IPS is to produce a new IPS so that we obtain the inner product between two different IPSs leading to the normalization

$$\mathcal{S}\left(\nu,\omega\right)=\sum_{\sigma,\sigma'\in\mathcal{S}_N}\det\left\{\mathbf{S}_{\sigma\sigma'}\right\} \tag{58}$$

where

$$\begin{aligned} \left(\mathbf{S}_{\sigma\sigma'}\right)_{jk} &= \left\langle \nu_{\sigma(j)}e^{i\omega_{\sigma(j)}}\varphi_j\right| \nu_{\sigma'(k)}e^{i\omega_{\sigma'(k)}}\varphi_k\Big\rangle = \\ &\int\varphi_j\left(\mathsf{z}\right)^*\varphi_k\left(\mathsf{z}\right)e^{i\left(\omega_{\sigma'(k)}(\mathsf{z})-\omega_{\sigma(j)}(\mathsf{z})\right)}\nu_{\sigma(j)}\left(\mathsf{z}\right)\nu_{\sigma'(k)}\left(\mathsf{z}\right)d\mathsf{z} \end{aligned} \tag{59}$$

The second term produced by the effective Hamiltonian is the expectation value $\mathcal{K}\left(\nu,\omega\right)$ wrt the IPS $|\varphi_1\cdots\varphi_N\rangle$

$$\mathcal{K}\left(\nu,\omega\right)=\mathcal{S}\left(\nu,\omega\right)^{-1}\left\langle \varphi_1\cdots\varphi_N\right| K\left(\nu,\omega\right)\varphi_1\cdots\varphi_N\rangle \tag{60}$$

of the effective kinetic energy operator $K\left(\nu,\omega\right)$ given by

$$\begin{aligned} \mathcal{K}\left(\nu,\omega\right)=\mathcal{S}\left(\nu,\omega\right)^{-1}\sum_{\sigma,\sigma'\in\mathcal{S}_N}&\left\{\left\langle \nu_{\sigma(1)}e^{i\omega_{\sigma(1)}}\varphi_1\cdots e^{i\omega_{\sigma(N)}}\nu_{\sigma(N)}\varphi_N\right.\right. \\ &\left.\left.\left(-\sum_{1\leq j\leq N}\nabla_j^2\right)e^{i\omega_{\sigma'(1)}}\nu_{\sigma'(1)}\varphi_1\cdots e^{i\omega_{\sigma'(N)}}\nu_{\sigma\prime(N)}\varphi_N\right\rangle\right\} \end{aligned} \tag{61}$$

which can be evaluated by utilizing the expressions described in Appendix F that have been developed by [11] to give

$$\mathcal{K}\left(\nu,\omega\right)=\sum_{\sigma,\sigma'\in\mathcal{S}_N}\mathrm{Tr}\left\{\mathbf{K}_{\sigma\sigma'}\,\mathrm{adj}\left(\mathbf{S}_{\sigma\sigma'}\right)\right\} \tag{62}$$

where

$$\left(\mathbf{K}_{\sigma\sigma'}\right)_{jk}=-\int\left\{\nabla\varphi_j\left(\mathsf{z}\right)^*\bullet\nabla\varphi_k\left(\mathsf{z}\right)\nu_{\sigma(j)}\left(\mathsf{z}\right)\nu_{\sigma'(k)}\left(\mathsf{z}\right)e^{i\left\{\omega_{\sigma'(k)}(\mathsf{z})-\omega_{\sigma(j)}(\mathsf{z})\right\}}\right\}d\mathsf{z} \tag{63}$$

The expectation value of the one particle potential term

$$\mathcal{V}_1(\nu,\omega) = \mathcal{S}(\nu,\omega)^{-1}\nu_{\sigma(1)}\left\langle e^{i\omega_{\sigma(1)}}\varphi_1\cdots e^{i\omega_{\sigma(N)}}\nu_{\sigma(N)}\varphi_N\right| \times \\ V_1 e^{i\omega_{\sigma'(1)}}\nu_{\sigma'(1)}\varphi_1\cdots e^{i\omega_{\sigma'(N)}}\nu_{\sigma\prime(N)}\varphi_N\Big\rangle \tag{64}$$

can be evaluated to give

$$\mathcal{V}_1(\nu,\omega) = \mathcal{S}(\nu,\omega)^{-1}\sum_{\sigma,\sigma'\in\mathcal{S}_N}\mathrm{Tr}\left\{\mathbf{V}_{1\sigma\sigma'}\,\mathrm{adj}\left(\mathbf{S}_{\sigma\sigma'}\right)\right\} \tag{65}$$

where $V_1\left(\mathsf{z}^N\right) = \sum_{1\le j\le N} V_1\left(\mathsf{z}_j\right)$ and

$$\left(\mathbf{V}_{1\sigma\sigma'}\right)_{jk} = \int\left\{V_1\left(\mathsf{z}_1\right)\varphi_j\left(\mathsf{z}_1\right)^*\varphi_k\left(\mathsf{z}_1\right)\nu_{\sigma(j)}\left(\mathsf{z}_1\right)\nu_{\sigma'(k)}\left(\mathsf{z}_1\right)e^{i\left\{\omega_{\sigma'(k)}(\mathsf{z})-\omega_{\sigma(j)}(\mathsf{z})\right\}}\right\}d\mathsf{z}_1 \tag{66}$$

The expectation value $\mathcal{V}_2(\nu)$ of the coulomb potential term is given by

$$\mathcal{V}_2(\nu,\omega) = \mathcal{S}(\nu,\omega)^{-1}\left\langle\nu_{\sigma(1)}e^{i\omega_{\sigma(1)}}\varphi_1\cdots e^{i\omega_{\sigma(N)}}\nu_{\sigma(N)}\varphi_N\left|V_2\right.e^{i\omega_{\sigma'(1)}}\nu_{\sigma'(1)}\varphi_1\cdots e^{i\omega_{\sigma'(N)}}\nu_{\sigma\prime(N)}\varphi_N\right\rangle \tag{67}$$

which can be evaluated using the expressions in Appendix F as

$$\mathcal{S}(\nu,\omega)^{-1}\sum_{\sigma,\sigma'\in\mathcal{S}_N} Tr\left\{\mathbf{G}_{\sigma,\sigma'}\,\mathrm{adj}^{(2)}\left(\mathbf{S}_{\sigma\sigma'}\right)\right\} \tag{68}$$

where

$$\left(\mathbf{G}_{\sigma,\sigma'}\right)_{jklm} = \int\Big\{\nu_{\sigma(j)}\left(\mathsf{z}_1\right)\varphi_j\left(\mathsf{z}_1\right)^*\nu_{\sigma(k)}\left(\mathsf{z}_1\right)\varphi_k\left(\mathsf{z}_1\right)^*\nu_l\left(\mathsf{z}_2\right)\varphi_{\sigma'(l)}\left(\mathsf{z}_2\right)\nu_m\left(\mathsf{z}_2\right)\varphi_{\sigma'(m)}\left(\mathsf{z}_2\right) \\ \times\frac{e^{i\left\{\omega_{\sigma'(l)}(\mathsf{z}_2)+\omega_{\sigma'(m)}(\mathsf{z}_2)-\omega_{\sigma(j)}(\mathsf{z}_1)-\omega_{\sigma(k)}(\mathsf{z}_1)\right\}}}{\|\mathbf{r}_1-\mathbf{r}_2\|} \\ -\nu_{\sigma(j)}\left(\mathsf{z}_2\right)\varphi_j\left(\mathsf{z}_2\right)^*\nu_{\sigma(k)}\left(\mathsf{z}_2\right)\varphi_k\left(\mathsf{z}_2\right)^*\nu_l\left(\mathsf{z}_1\right)\varphi_{\sigma'(l)}\left(\mathsf{z}_1\right)\nu_m\left(\mathsf{z}_1\right)\varphi_{\sigma'(m)}\left(\mathsf{z}_1\right) \\ \times\frac{e^{i\left\{\omega_{\sigma'(l)}(\mathsf{z}_1)+\omega_{\sigma'(m)}(\mathsf{z}_1)-\omega_{\sigma(j)}(\mathsf{z}_2)-\omega_{\sigma(k)}(\mathsf{z}_2)\right\}}}{\|\mathbf{r}_1-\mathbf{r}_2\|}\Big\}d\mathsf{z}_1d\mathsf{z}_2 \tag{69}$$

The value of the energy functional $E(\nu,\omega)$ is then the sum

$$E(\nu,\omega) = H_0 + \mathcal{K}(\nu,\omega) + \mathcal{V}_1(\nu,\omega) + \mathcal{V}_2(\nu,\omega) \tag{70}$$

where the kernels $\{\nu,\omega\}$ are expressed in terms of $\{\nu_1,\ldots,\nu_N,\omega_1,\ldots,\omega_N\}$ which in turn can be expanded in terms of a fixed subset of s functions $\{f_1,\ldots,f_s\}$ and the coefficients of these expansions then become the variational parameters of the problem.

B. Approximations indexed by $\{2, \cdots, 2\}$

The transformations that we consider in this case are

$$\breve{T}_1 \wedge \cdots \wedge \breve{T}_{\frac{N}{2}} \left|\varphi_1 \cdots \varphi_N\right\rangle = \sum_{\sigma \in \mathcal{S}_N} \left|\breve{T}_1 \left(\varphi_{\sigma(1)} \varphi_{\sigma(2)}\right) \cdots \breve{T}_{\frac{N}{2}} \left(\varphi_{\sigma(N-1)} \varphi_{\sigma(N)}\right)\right\rangle \tag{71}$$

where the amplitudes of $\left|T_j \left(\varphi_{\sigma(2j-1)} \varphi_{\sigma(2j)}\right)\right\rangle$ are given by

$$\left\langle \mathsf{z}_{2j-1}, \mathsf{z}_{2j} \left| T_j \left(\varphi_{\sigma(2j-1)} \varphi_{\sigma(2j)}\right)\right.\right\rangle = \int T_j \left(\mathsf{z}_{2j-1}, \mathsf{z}_{2j}\right) \varphi_{\sigma(2j-1)} \left(\mathsf{z}_{2j-1}\right) \varphi_{\sigma(2j)} \left(\mathsf{z}_{2j}\right) d\mathsf{z}_{2j-1} d\mathsf{z}_{2j} \tag{72}$$

and the integral kernels of $\breve{T}_1 \wedge \cdots \wedge \breve{T}_{\frac{N}{2}}$ are

$$\begin{aligned} T\left(\mathsf{z}^N\right) &= T_1 \left(\mathsf{z}_1, \mathsf{z}_2\right) \vee \cdots \vee T_{\frac{N}{2}} \left(\mathsf{z}_{N-1}, \mathsf{z}_N\right) = \sum_{\sigma \in \mathcal{S}_N} T_1 \left(\mathsf{z}_{\sigma(1)}, \mathsf{z}_{\sigma(2)}\right) \cdots T_{\frac{N}{2}} \left(\mathsf{z}_{\sigma(N-1)}, \mathsf{z}_{\sigma(N)}\right) \\ &= \sum_{\sigma \in \mathcal{S}_N} \nu_1 \left(\mathsf{z}_{\sigma(1)}, \mathsf{z}_{\sigma(2)}\right) \cdots \nu_{\frac{N}{2}} \left(\mathsf{z}_{\sigma(N-1)}, \mathsf{z}_{\sigma(2N)}\right) e^{\,i\ \omega_1\left(\mathsf{z}_{\sigma(1)}, \mathsf{z}_{\sigma(2)}\right) + \cdots + \omega_{\frac{N}{2}}\left(\mathsf{z}_{\sigma(N-1)}, \mathsf{z}_{\sigma(N)}\right)} \end{aligned} \tag{73}$$

where

$$\omega_j \left(\mathsf{z}_{\sigma(2j-1)}, \mathsf{z}_{\sigma(2j)}\right) = \delta\left(\mathsf{z}_1\right) \cdots \omega_j \left(\mathsf{z}_{\sigma(2j-1)}, \mathsf{z}_{\sigma(2j)}\right) \cdots \delta\left(\mathsf{z}_N\right) \tag{74}$$

In this case we must treat the effective overlap operator $S\left(\nu, \omega\right)$ as a full N-particle operator

$$\begin{aligned} S\left(\nu, \omega\right) = \int \Bigg\{ & \sum_{\sigma, \sigma' \in \mathcal{S}_N} T_1 \left(\mathsf{z}_{\sigma(1)}, \mathsf{z}_{\sigma(2)}\right)^* \cdots T_{\frac{N}{2}} \left(\mathsf{z}_{\sigma(N-1)}, \mathsf{z}_{\sigma(N)}\right)^* \\ & T_1 \left(\mathsf{z}_{\sigma'(1)}, \mathsf{z}_{\sigma'(2)}\right) \cdots T_{\frac{N}{2}} \left(\mathsf{z}_{\sigma'(N-1)}, \mathsf{z}_{\sigma'(N)}\right) \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N\right| \Bigg\} d\mathsf{z}^N \end{aligned} \tag{75}$$

and take the expectation value of this operator wrt the IPS $\left|\varphi_1 \cdots \varphi_N\right\rangle$ producing

$$\begin{aligned} & \mathcal{S}\left(\nu, \omega\right) = \left\langle \varphi_1 \cdots \varphi_N \right| S\left(\nu, \omega\right) \varphi_1 \cdots \varphi_N \rangle = \\ & \sum_{\sigma, \sigma', \sigma'' \in \mathcal{S}_N} \int \Bigg\{ \varphi_1 \left(\mathsf{z}_1\right)^* \cdots \varphi_N \left(\mathsf{z}_N\right)^* \left(-1\right)^{\pi(\sigma'')} \varphi_1 \left(\mathsf{z}_{\sigma''(1)}\right) \cdots \varphi_N \left(\mathsf{z}_{\sigma''(N)}\right) \\ & \qquad \times \prod_{1 \leq k \leq \frac{N}{2}} \nu_k \left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \nu_k \left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) \\ & \times e^{\,i\ \omega_1\left(\mathsf{z}_{\sigma'(1)}, \mathsf{z}_{\sigma'(2)}\right) - \omega_1\left(\mathsf{z}_{\sigma(1)}, \mathsf{z}_{\sigma(2)}\right) + \cdots + \omega_{\frac{N}{2}}\left(\mathsf{z}_{\sigma'(N-1)}, \mathsf{z}_{\sigma'(N)}\right) - \omega_{\frac{N}{2}}\left(\mathsf{z}_{\sigma(N-1)}, \mathsf{z}_{\sigma(N)}\right)} \Bigg\} d\mathsf{z}^N \end{aligned} \tag{76}$$

The effective kinetic energy is the expectation value $\mathcal{K}\left(\nu, \omega\right)$

$$\mathcal{K}\left(\nu, \omega\right) = \mathcal{S}\left(\nu, \omega\right)^{-1} \left\langle \varphi_1 \cdots \varphi_N \right| K\left(\nu, \omega\right) \varphi_1 \cdots \varphi_N \rangle \tag{77}$$

of the effective kinetic energy operator $K(\nu,\omega)$ given by

$$K(\nu,\omega) = \underbrace{-\nabla \bullet \left(\nu^2\right) \mathbb{I} \bullet \nabla}_{I} - \underbrace{\nabla \bullet \left(\nu^2 \nabla\omega - i\nu\nabla\nu\right)}_{II}$$
$$- \underbrace{\left(\nu^2\nabla\omega - i\nu\nabla\nu\right) \bullet \nabla}_{III} + \underbrace{\left(\nu\nabla\omega - i\nabla\nu\right) \bullet \mathbb{I} \bullet \left(\nu\nabla\omega - i\nabla\nu\right)}_{IV} \tag{78}$$

where the $N-$particle integral kernels ν, ω are functions of the two particle integral kernels $\left\{\nu_1, \ldots, \nu_{\frac{N}{2}}, \omega_1, \ldots, \omega_{\frac{N}{2}}\right\}$ i.e.

$$\nu = \nu\left(\nu_1, \ldots, \nu_{\frac{N}{2}}, \omega_1, \ldots, \omega_{\frac{N}{2}}\right)$$
$$\omega = \omega\left(\nu_1, \ldots, \nu_{\frac{N}{2}}, \omega_1, \ldots, \omega_{\frac{N}{2}}\right) \tag{79}$$

The expansions of the various parts of the effective kinetic energy operator eq. (78) are shown in Appendix G. The expectation value of the one particle potential

$$\mathcal{V}_1(\nu,\omega) = \mathcal{S}(\nu,\omega)^{-1} \langle \varphi_1 \cdots \varphi_N | V_1\ \varphi_1 \cdots \varphi_N \rangle \tag{80}$$

is given in terms of the effective operators

$$V_1 = \sum_{\sigma,\sigma' \in \mathcal{S}_N} \sum_{1 \le j \le N} \int \Big\{ V_1(\mathsf{z}_j)\, T_1\left(\mathsf{z}_{\sigma(1)}, \mathsf{z}_{\sigma(2)}\right)^* \cdots T_{\frac{N}{2}}\left(\mathsf{z}_{\sigma(N-1)}, \mathsf{z}_{\sigma(N)}\right)^*$$
$$T_1\left(\mathsf{z}_{\sigma'(1)}, \mathsf{z}_{\sigma'(2)}\right) \cdots T_{\frac{N}{2}}\left(\mathsf{z}_{\sigma'(N-1)}, \mathsf{z}_{\sigma'(N)}\right) \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N\right| \Big\}\, d\mathsf{z}^N \tag{81}$$

and can be evaluated to give

$$\mathcal{V}_1(\nu,\omega) = \mathcal{S}(\nu,\omega)^{-1} \times$$
$$\sum_{\sigma,\sigma',\sigma'' \in \mathcal{S}_N} \sum_{1 \le j \le N} \int \Big\{ \varphi_1(\mathsf{z}_1)^* \cdots \varphi_N(\mathsf{z}_N)^* (-1)^{\pi(\sigma'')} \varphi_1\left(\mathsf{z}_{\sigma''(1)}\right) \cdots \varphi_N\left(\mathsf{z}_{\sigma''(N)}\right)$$
$$\times V_1(\mathsf{z}_j) \prod_{1 \le k \le \frac{N}{2}} \nu_k\left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \nu_k\left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right)$$
$$e^{i\ \omega_1\left(\mathsf{z}_{\sigma'(1)}, \mathsf{z}_{\sigma'(2)}\right) - \omega_1\left(\mathsf{z}_{\sigma(1)}, \mathsf{z}_{\sigma(2)}\right) + \cdots + \omega_{\frac{N}{2}}\left(\mathsf{z}_{\sigma'(N-1)}, \mathsf{z}_{\sigma'(N)}\right) - \omega_{\frac{N}{2}}\left(\mathsf{z}_{\sigma(N-1)}, \mathsf{z}_{\sigma(N)}\right)} \Big\}\, d\mathsf{z}^N \tag{82}$$

The expectation value $\mathcal{V}_2(\nu)$ of the coulomb potential term is given by

$$\mathcal{V}_2(\nu,\omega) = \mathcal{S}(\nu,\omega)^{-1} \langle \varphi_1 \cdots \varphi_N | V_2\ \varphi_1 \cdots \varphi_N \rangle \tag{83}$$

which can be evaluated in terms of the effective coulomb operator

$$\sum_{\sigma,\sigma'\in\mathcal{S}_N}\sum_{1\leq j<k\leq N}\int\left\{V_2\left(\mathsf{z}_j,\mathsf{z}_k\right)T_1\left(\mathsf{z}_{\sigma(1)},\mathsf{z}_{\sigma(2)}\right)^*\cdots T_{\frac{N}{2}}\left(\mathsf{z}_{\sigma(N-1)},\mathsf{z}_{\sigma(N)}\right)^*\right.$$
$$\left.T_1\left(\mathsf{z}_{\sigma'(1)},\mathsf{z}_{\sigma'(2)}\right)\cdots T_{\frac{N}{2}}\left(\mathsf{z}_{\sigma'(N-1)},\mathsf{z}_{\sigma'(N)}\right)\left|\mathsf{z}^N\right\rangle\left\langle\mathsf{z}^N\right|\right\}d\mathsf{z}^N \tag{84}$$

to give

$$\mathcal{V}_2\left(\nu,\omega\right)=\mathcal{S}\left(\nu,\omega\right)^{-1}\times$$
$$\sum_{\sigma,\sigma',\sigma''\in\mathcal{S}_N}\sum_{1\leq j<k\leq N}\int\left\{\varphi_1\left(\mathsf{z}_1\right)^*\cdots\varphi_N\left(\mathsf{z}_N\right)^*\left(-1\right)^{\pi(\sigma'')}\varphi_1\left(\mathsf{z}_{\sigma''(1)}\right)\cdots\varphi_N\left(\mathsf{z}_{\sigma''(N)}\right)\right.$$
$$\times V_2\left(\mathsf{z}_j,\mathsf{z}_k\right)\prod_{1\leq k\leq\frac{N}{2}}\nu_k\left(\mathsf{z}_{\sigma(2k-1)},\mathsf{z}_{\sigma(2k)}\right)\nu_k\left(\mathsf{z}_{\sigma'(2k-1)},\mathsf{z}_{\sigma'(2k)}\right)$$
$$\left.e^{i\ \omega_1\left(\mathsf{z}_{\sigma'(1)},\mathsf{z}_{\sigma'(2)}\right)-\omega_1\left(\mathsf{z}_{\sigma(1)},\mathsf{z}_{\sigma(2)}\right)+\cdots+\omega_{\frac{N}{2}}\left(\mathsf{z}_{\sigma'(N-1)},\mathsf{z}_{\sigma'(N)}\right)-\omega_{\frac{N}{2}}\left(\mathsf{z}_{\sigma(N-1)},\mathsf{z}_{\sigma(N)}\right)}\right\}d\mathsf{z}^N \tag{85}$$

where

$$V_2\left(\mathsf{z}_j,\mathsf{z}_k\right)=\frac{1}{\left\|\mathbf{r}_j-\mathbf{r}_k\right\|}\delta\left(\xi_j-\xi_k\right) \tag{86}$$

for $\mathsf{z}_j\equiv\left(\mathbf{r}_j,\xi_j\right)$ and $\mathsf{z}_k\equiv\left(\mathbf{r}_k,\xi_k\right)$.

The value of the energy functional $E\left(\nu,\omega\right)$ is then the sum

$$E\left(\ominus\left(\nu_1,\ldots,\nu_{\frac{N}{2}},\omega_1,\ldots,\omega_{\frac{N}{2}}\right)\right)=H_0+\mathcal{K}\left(\nu,\omega\right)+\mathcal{V}_1\left(\nu,\omega\right)+\mathcal{V}_2\left(\nu,\omega\right) \tag{87}$$

and the optimal IPS is given by minimizing $E\left(\ominus\left(\nu,\omega\right)\right)$ over $\nu=\left(\nu_1,\cdots,\nu_{\frac{N}{2}}\right)$ and $\omega=\left(\omega_1,\cdots,\omega_{\frac{N}{2}}\right)$. In an analogous fashion to the $\{1,\ldots,1\}$ case the functions $\left\{\nu_1,\cdots,\nu_{\frac{N}{2}},\omega_1,\cdots,\omega_{\frac{N}{2}}\right\}$ can be expanded in terms of a fixed set of s functions $\left\{f_1,\ldots,f_s\right\}$, where now these functions are two particle functions.

VII. SUMMARY

In this article we have shown that

- one can generate all pure states from a cyclic reference state (a pure state that has a wavefunction that is non zero almost everywhere) by transformations that are diagonal in the space-spin coordinate representation,

- these transformations, which form an abelian semigroup C_c, also maintain the local form of the defining space-spin coordinate representation of the Hamiltonian, leading to effective Hamiltonians that have direct physical interpretability in terms of momentum and potential operators and thus have a certain classical flavor,
- one can form an approximation theory by restricting attention to sub semigroups of C_c, that lead to approximations which have a *direct* physical interpretation.

These properties should be contrasted to the effect of the transformation of state in truncated configurational interaction, Multi Configurational Self Consistent Field and couple cluster methods that do not lead to or matrix elements that could identified with such effective Hamiltonians.

To illuminate these points we presented some examples that showed the form of terms that need to be calculated in order to produce an energy functional that can be optimized. Many strategies are obviously possible for the simplification of the expressions we obtained which were, by intention, in a very raw form that need to be simplified in order to produce practical computational formulae.

The approximations that are suggested in this article present a new approach to obtaining approximate solutions to the Schrödinger equation, and offer possibilities for development in many directions.

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APPENDIX A: SUBSPACES OF OPERATORS

The set of trace class operators is defined as

$$\mathcal{B}_1(\mathcal{H}) = \left\{ X | X \in \mathcal{B}(\mathcal{H}); Tr\left\{ \left(X^\dagger X \right)^{\frac{1}{2}} \right\} < \infty \right\} \tag{A1}$$

where $\mathcal{B}(\mathcal{H})$ is the space of bounded operators acting in the Hilbert space $\mathcal{H}$. $\mathcal{B}_1(\mathcal{H})$ is a Banach space equipped with the norm

$$\|X\|_1 = Tr\left\{ \left(X^\dagger X \right)^{\frac{1}{2}} \right\} \tag{A2}$$

The space $\mathcal{B}(\mathcal{H})$ is also a Banach space with a norm defined as

$$\|X\| = \sup_{|\Psi\rangle \in \mathcal{H}} \left\{ \frac{\langle \Psi | X\Psi \rangle}{\langle \Psi | \Psi \rangle} \right\} \tag{A3}$$

The closure of $\mathcal{B}_1(\mathcal{H})$ wrt $\|\|$ produces $\mathcal{B}(\mathcal{H})$. The relationship between these spaces is

$$\mathcal{B}(\mathcal{H}) \supseteq \mathcal{B}_1(\mathcal{H}) \tag{A4}$$

and their norms is

$$\|X\| \leq \|X\|_1 \tag{A5}$$

APPENDIX B: STATES

The states of an N-particle quantum mechanical system correspond to positive, normalized trace class operators and form a convex subset, $\mathcal{S}_N$, of the Banach space, $\mathcal{B}_1\left(\mathcal{H}^N\right)$, of N-particle trace class operators, defined as

$$\mathcal{S}_N = \left\{ D^N | D^N \in \mathcal{B}_1\left(\mathcal{H}^N\right), D^N \geq 0, TrD^N = 1 \right\} \tag{B1}$$

Pure states are idempotent operators i.e.

$$\left(D^N\right)^2 = D^N \tag{B2}$$

and *normalized* pure states can be associated with, in a 1-1 fashion, with a ray $\{\alpha |\Psi\rangle | \alpha \in \mathbb{C}\}$ generated by a vector $|\Psi\rangle$ in the N-particle Hilbert space $\mathcal{H}^N$ by the relationship

$$D^N = \frac{|\Psi\rangle \langle \Psi|}{\langle \Psi | \Psi \rangle} \tag{B3}$$

The set of *unnormalized* states form the set of positive trace class operators, $\mathcal{B}_{1+}(\mathcal{H}^1)$. States that are not idempotent are called mixed or ensemble states and correspond to statistical mixtures of pure states.

APPENDIX C: DISCRETE VERSUS CONTINUOUS

The discrete semigroup C_d is given by operators of the form

$$Q = \sum_{1 \leq j \leq \infty} q_j |e_j\rangle \langle e_j| \tag{C1}$$

and the continuous C_c by

$$T = \int T(x) |x\rangle \langle x| \, dx \tag{C2}$$

In the discrete case an invariant one dimensional subspace exists if there is a vector $|v\rangle$ such that

$$Q |v\rangle = \alpha_Q |v\rangle \qquad \forall Q \in C_d \tag{C3}$$

This condition can be expressed as

$$\sum_{1 \le j \le \infty} Q_j |e_j\rangle \langle e_j| \, v\rangle = \alpha_Q \sum_{1 \le j \le \infty} |e_j\rangle \langle e_j| \, v\rangle \qquad \forall Q \in C_d \tag{C4}$$

as the basis $\{e_j\}$ is linearly independent we can treat each component separately to obtain

$$Q_j |e_j\rangle \langle e_j| \, v\rangle = \alpha_Q |e_j\rangle \langle e_j| \, v\rangle \qquad \forall Q_j \quad \forall j \tag{C5}$$

this implies that

$$Q_j = \alpha_Q \qquad \forall v_j \neq 0 \quad \forall Q_j \tag{C6}$$

let

$$v_1 \neq 0 \quad \& \quad v_2 \neq 0 \tag{C7}$$

and all other expansion coefficients of $|v\rangle$ equal to zero then eq. $(C6)$

$$Q_1 = Q_2 = \alpha_Q \quad \forall Q_1, Q_2 \tag{C8}$$

which clearly is not possible. Hence only one coefficient can be nonzero and we obtain

$$|v\rangle = \beta |e_k\rangle \tag{C9}$$

giving

$$\sum_{1 \le j \le \infty} Q_j |e_j\rangle \langle e_j| \, \beta \, e_k\rangle = Q_k \beta |e_k\rangle \quad \forall Q \in C_d \tag{C10}$$

which shows that $\alpha_Q = Q_k$. At the opposite extreme if all the expansion coefficients $\{v_j\}$ are non zero then $|v\rangle$ would be a cyclic vector for C_d i.e. the Hilbert space is generated by the action of C_d on $|v\rangle$.

In the continuous case an invariant one dimensional subspace exists if

$$T |v\rangle = \alpha_T |v\rangle \qquad \forall T \in C_c \tag{C11}$$

which can be expressed as

$$\int T(x)\left|x\right\rangle\left\langle x\right|\left.v\right\rangle dx=\alpha_{T}\int\left|x\right\rangle\left\langle x\right|\left.v\right\rangle dx\qquad\forall T\in C_{c} \tag{C12}$$

$$\Rightarrow t(x)=\alpha_{T}\quad v(x)\neq0\quad\forall t,\quad x\in\Delta \tag{C13}$$

so that for sets of non zero measure Δ

$$T(x)\left\langle x\right|\left.v\right\rangle=\alpha_{T}\left\langle x\right|\left.v\right\rangle\quad\forall T,\quad x\in\Delta \tag{C14}$$

and

$$T(x)=\alpha_{T}\quad\text{when }v(x)\neq0\quad,x\in\Delta\quad\forall T \tag{C15}$$

However now there no single components $\{|x\rangle\}$ as these vectors do not belong to the Hilbert space and there is no such square integrable function $v(x)$ that makes this true for all T (the analogous condition to eq. $(C8)$ in the continuous case cannot be satisfied), so no invariant one dimensional Hilbert subspaces for the semigroup $\{T\}$ exist. If the square integrable function $v(x)$ is non zero almost everywhere then it is a cyclic vector for the semigroup C_c.

APPENDIX D: TRANSFORMATION OF THE KINETIC ENERGY OPERATOR

1. Transition Amplitudes

We consider the commutation relationships between the operators $\mathbf{P}$,$e^{i\breve{\omega}_N}$ and $\breve{\nu}_N$ and observe that

1.

$$\begin{aligned}\mathbf{P}e^{i\breve{\omega}_N}\left|\Psi\right\rangle&=(-i\nabla)\,e^{i\breve{\omega}_N}\left|\Psi\right\rangle=e^{i\breve{\omega}_N}(-i\nabla)\left|\Psi\right\rangle+e^{i\breve{\omega}_N}(\nabla\breve{\omega}_N)\left|\Psi\right\rangle\\&=e^{i\breve{\omega}_N}(-i\nabla+\nabla\breve{\omega}_N)\left|\Psi\right\rangle=e^{i\breve{\omega}_N}\{\mathbf{P}+\nabla\breve{\omega}_N\}\left|\Psi\right\rangle\end{aligned} \tag{D1}$$

2.

$$\begin{aligned}&\mathbf{P}\breve{\nu}_N\left|\Psi\right\rangle=(-i\nabla)\,\breve{\nu}_N\left|\Psi\right\rangle\\&=\breve{\nu}_N(-i\nabla)\left|\Psi\right\rangle+(-i\nabla\breve{\nu}_N)\left|\Psi\right\rangle=\{\breve{\nu}_N\mathbf{P}-i\nabla\breve{\nu}_N\}\left|\Psi\right\rangle\end{aligned} \tag{D2}$$

3.

$$\breve{\nu}_Ne^{i\breve{\omega}_N}\left|\Psi\right\rangle=e^{i\breve{\omega}_N}\breve{\nu}_N\left|\Psi\right\rangle \tag{D3}$$

Which can be summarized in the commutation relationship

$$\begin{aligned}\left[\mathbf{P},e^{i\breve{\omega}_N}\right] &= e^{i\breve{\omega}_N}\nabla\breve{\omega}_N \\ \left[\mathbf{P},\breve{\nu}_N\right] &= i\nabla\breve{\nu}_N \\ \left[\breve{\nu}_N, e^{i\breve{\omega}_N}\right] &= 0\end{aligned} \tag{D4}$$

that produce

$$\begin{aligned}\mathbf{P}\breve{\nu}_N e^{i\breve{\omega}_N}\left|\Psi\right\rangle &= \left\{\breve{\nu}_N\mathbf{P} - i\nabla\breve{\nu}_N\right\}e^{i\breve{\omega}_N}\left|\Psi\right\rangle = \left\{\breve{\nu}_N e^{i\breve{\omega}_N}\left\{\mathbf{P}+\nabla\breve{\omega}_N\right\} - ie^{i\breve{\omega}_N}\nabla\breve{\nu}_N\right\}\left|\Psi\right\rangle \\ &= e^{i\breve{\omega}_N}\left\{\breve{\nu}_N\mathbf{P}+\breve{\nu}_N\nabla\breve{\omega}_N - i\nabla\breve{\nu}_N\right\}\left|\Psi\right\rangle\end{aligned} \tag{D5}$$

This allows us to express the transition amplitude

$$\left\langle T\left(\breve{\nu}_{Na},\breve{\omega}_{Na}\right)\Psi\right|\left(\mathbf{P}\bullet\mathbf{P}\right)T\left(\breve{\nu}_{Nb},\breve{\omega}_{Nb}\right)\Psi\right\rangle \tag{D6}$$

as

$$\left\langle e^{i\breve{\omega}_{Na}}\left\{\breve{\nu}_{Na}\mathbf{P}+\breve{\nu}_{Na}\nabla\breve{\omega}_{Na} - i\nabla\breve{\nu}_{Na}\right\}\Psi\right|e^{i\breve{\omega}_{Nb}}\left\{\breve{\nu}_{Nb}\mathbf{P}+\breve{\nu}_{Nb}\nabla\breve{\omega}_{Nb} - i\nabla\breve{\nu}_{Nb}\right\}\Psi\right\rangle \tag{D7}$$

which gives

A

$$\left\langle\breve{\nu}_{Na}e^{i\breve{\omega}_{Na}}\mathbf{P}\Psi\right|\breve{\nu}_{Nb}e^{i\breve{\omega}_{Nb}}\mathbf{P}\Psi\right\rangle = -\left\langle\Psi\right|\left\{\nabla\bullet\left(\breve{\nu}_{Na}\breve{\nu}_{Nb}e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\right)\mathbb{I}\bullet\nabla\right\}\Psi\right\rangle \tag{D8}$$

where

$$\begin{aligned}&\nabla\bullet\left(\breve{\nu}_{Na}\breve{\nu}_{Nb}e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\right)\mathbb{I}\bullet\nabla \\ &= \begin{pmatrix}\nabla_1 & \cdots & \nabla_m\end{pmatrix}\begin{pmatrix}\breve{\nu}_{Na}\breve{\nu}_{Nb}e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \breve{\nu}_{Na}\breve{\nu}_{Nb}e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\end{pmatrix}\begin{pmatrix}\nabla_1 \\ \vdots \\ \nabla_m\end{pmatrix}\end{aligned} \tag{D9}$$

The transition amplitude eq. $(D8)$ is given explicitly by

$$\begin{aligned}&-\int\left\{\breve{\nu}_{Na}\left(\mathsf{z}\right)e^{-i\breve{\omega}_{Na}(\mathsf{z})}\nabla\Psi\left(\mathsf{z}\right)^*\breve{\nu}_{Nb}\left(\mathsf{z}\right)e^{i\breve{\omega}_{Nb}(\mathsf{z})}\nabla\Psi\left(\mathsf{z}\right)\right\}d\mathsf{z} \\ &= -\int\left\{\nabla\Psi\left(\mathsf{z}\right)^\dagger\bullet\nabla\Psi\left(\mathsf{z}\right)e^{i(\breve{\omega}_{Nb}(\mathsf{z})-\breve{\omega}_{Na}(\mathsf{z}))}\breve{\nu}_{Na}\left(\mathsf{z}\right)\breve{\nu}_{Nb}\left(\mathsf{z}\right)\right\}d\mathsf{z}\end{aligned} \tag{D10}$$

B

$$\begin{aligned}&\left\langle\breve{\nu}_{Na}e^{i\breve{\omega}_{Na}}\mathbf{P}\Psi\right|\left\{\breve{\nu}_{Nb}\nabla\breve{\omega}_{Nb} - i\nabla\breve{\nu}_{Nb}\right\}e^{-i\breve{\omega}_{Nb}}\Psi\right\rangle \\ &= -i\left\langle\Psi\right|\left\{\nabla\bullet\breve{\nu}_{Na}e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\mathbb{I}\bullet\left(\breve{\nu}_{Nb}\nabla\breve{\omega}_{Nb} - i\nabla\breve{\nu}_{Nb}\right)\right\}\Psi\right\rangle\end{aligned} \tag{D11}$$

C

$$\begin{aligned}&\left\langle \left(\breve{\nu}_{Na}\nabla\breve{\omega}_{Na} - i\nabla\breve{\nu}_{Na}\right)\Psi | v_b e^{i\breve{\omega}_{Nb}}\mathbf{P}\Psi\right\rangle \\ &= -i\left\langle\Psi\right| \left\{\left(\breve{\nu}_{Na}\nabla\breve{\omega}_{Na} - i\nabla\breve{\nu}_{Na}\right)\bullet v_b e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\mathbb{I}\bullet\nabla\right\}\Psi\right\rangle \end{aligned} \tag{D12}$$

D

$$\begin{aligned}&\left\langle \left(\breve{\nu}_{Na}\nabla\breve{\omega}_{Na} - i\nabla\breve{\nu}_{Na}\right)\Psi\right| \left(\breve{\nu}_{Nb}\nabla\breve{\omega}_{Nb} - i\nabla\breve{\nu}_{Nb}\right)\Psi\rangle \\ &= \left\langle\Psi\right| \left\{\left(\breve{\nu}_{Na}\nabla\breve{\omega}_{Na} - i\nabla\breve{\nu}_{Na}\right)\bullet e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\mathbb{I}\bullet\left(\breve{\nu}_{Nb}\nabla\breve{\omega}_{Nb} - i\nabla\breve{\nu}_{Nb}\right)\right\}\Psi\right\rangle \end{aligned} \tag{D13}$$

collecting together the terms A,B,C and D we obtain

$$\begin{aligned}&\left\langle T\left(\breve{\nu}_{Na},\breve{\omega}_{Na}\right)\Psi\right| \left(\mathbf{P}\bullet\mathbf{P}\right) T\left(\breve{\nu}_{Nb},\breve{\omega}_{Nb}\right)\Psi\rangle = \\ &\qquad\langle\Psi \mid \Big\{-\nabla\bullet\left(\breve{\nu}_{Na}\breve{\nu}_{Nb}e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\right)\mathbb{I}\bullet\nabla \\ &\qquad\quad -\nabla\bullet\breve{\nu}_{Na}e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\mathbb{I}\bullet\left(\breve{\nu}_{Nb}\nabla\breve{\omega}_{Nb} - i\nabla\breve{\nu}_{Nb}\right) \\ &\qquad\quad -\left(\breve{\nu}_{Na}\nabla\breve{\omega}_{Na} - i\nabla\breve{\nu}_{Na}\right)\bullet v_b e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\mathbb{I}\bullet\nabla \\ &+\left(\breve{\nu}_{Na}\nabla\breve{\omega}_{Na} - i\nabla\breve{\nu}_{Na}\right)\bullet e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\mathbb{I}\bullet\left(\breve{\nu}_{Nb}\nabla\breve{\omega}_{Nb} - i\nabla\breve{\nu}_{Nb}\right)\Big\}\Psi\rangle \end{aligned} \tag{D14}$$

We can also consider this as the expectation value wrt the pure state $|\Psi\rangle$ of the effective operator $K\left(\breve{\nu}_{Na},\breve{\omega}_{Na},\breve{\nu}_{Nb},\breve{\omega}_{Nb}\right)$ where

$$\begin{aligned}&K\left(\breve{\nu}_{Na},\breve{\omega}_{Na},\breve{\nu}_{Nb},\breve{\omega}_{Nb}\right) = \\ &-\nabla\bullet\left(\breve{\nu}_{Na}\breve{\nu}_{Nb}e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\right)\mathbb{I}\bullet\nabla - \nabla\bullet\breve{\nu}_{Na}e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\mathbb{I}\bullet\left(\breve{\nu}_{Nb}\nabla\breve{\omega}_{Nb} - i\nabla\breve{\nu}_{Nb}\right) \\ &\qquad -\left(\breve{\nu}_{Na}\nabla\breve{\omega}_{Na} - i\nabla\breve{\nu}_{Na}\right)\bullet v_b e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\mathbb{I}\bullet\nabla \\ &\qquad\quad +\left(\breve{\nu}_{Na}\nabla\breve{\omega}_{Na} - i\nabla\breve{\nu}_{Na}\right)\bullet e^{i(\breve{\omega}_{Nb}-\breve{\omega}_{Na})}\mathbb{I}\bullet\left(\breve{\nu}_{Nb}\nabla\breve{\omega}_{Nb} - i\nabla\breve{\nu}_{Nb}\right) \end{aligned} \tag{D15}$$

2. Expectation Values

If we set $\breve{\nu}_{Na} = \breve{\nu}_{Nb} = \breve{\nu}_N$ and $\breve{\omega}_{Na} = \breve{\omega}_{Nb} = \breve{\omega}_N$ we obtain the expectation value of the Kinetic Energy operator

$$\left\langle T\left(\breve{\nu}_N,\breve{\omega}_N\right)\Psi\right| \left(\mathbf{P}\bullet\mathbf{P}\right) T\left(\breve{\nu}_N,\breve{\omega}_N\right)\Psi\rangle \tag{D16}$$

which can be developed to produce

$$\begin{aligned}\left\langle T\left(\breve{\nu}_N,\breve{\omega}_N\right)\Psi\right|\left(\mathbf{P}\bullet\mathbf{P}\right)T\left(\breve{\nu}_N,\breve{\omega}_N\right)\Psi\rangle = \\ \langle\Psi\mid\{-\nabla\bullet\left(\breve{\nu}_N^2\right)\mathbb{I}\bullet\nabla \\ -\nabla\bullet\left(\breve{\nu}_N^2\nabla\breve{\omega}_N - i\breve{\nu}_N\nabla\breve{\nu}_N\right) \\ -\left(\breve{\nu}_N^2\nabla\breve{\omega}_N - i\breve{\nu}_N\nabla\breve{\nu}_N\right)\bullet\nabla \\ +\left(\breve{\nu}_N\nabla\breve{\omega}_N - i\nabla\breve{\nu}_N\right)\bullet\mathbb{I}\bullet\left(\breve{\nu}_N\nabla\breve{\omega}_N - i\nabla\breve{\nu}_N\right)\}\Psi\rangle\end{aligned} \tag{D17}$$

leading to the definition of an effective Kinetic Energy operator

$$\begin{aligned}K\left(\breve{\nu}_N,\breve{\omega}_N\right) = -\nabla\bullet\left(\breve{\nu}_N^2\right)\mathbb{I}\bullet\nabla - \nabla\bullet\left(\breve{\nu}_N^2\nabla\breve{\omega}_N - i\breve{\nu}_N\nabla\breve{\nu}_N\right) \\ -\left(\breve{\nu}_N^2\nabla\breve{\omega}_N - i\breve{\nu}_N\nabla\breve{\nu}_N\right)\bullet\nabla + \left(\breve{\nu}_N\nabla\breve{\omega}_N - i\nabla\breve{\nu}_N\right)\bullet\mathbb{I}\bullet\left(\breve{\nu}_N\nabla\breve{\omega}_N - i\nabla\breve{\nu}_N\right)\end{aligned} \tag{D18}$$

APPENDIX E: SYMMETRIC KERNELS

The integral kernels of the operators $\breve{T}\left(\nu,\omega\right)$ and in general $\left\{\breve{T}_{n_p}\left(\nu_{n_p},\omega_{n_p}\right)\right\}$ are symmetric functions. Which is shown by considering the wavefunction

$$\left\langle \mathsf{z}^{n_p}\middle|\tilde{\Psi}_{n_p}\right\rangle = \tilde{\Psi}_{n_p}\left(\mathsf{z}^{n_p}\right) = \nu_{n_p}\left(\mathsf{z}^{n_p}\right)e^{i\omega\left(\mathsf{z}^{n_p}\right)}\Psi_{n_p}\left(\mathsf{z}^{n_p}\right) \tag{E1}$$

resulting from the transformation

$$\left|\tilde{\Psi}_{n_p}\right\rangle = \breve{T}_{n_p}\left(\nu_{n_p},\omega_{n_p}\right)\left|\Psi_{n_p}\right\rangle = \int T_{n_p}\left(\mathsf{z}^{n_p}\right)\left|\mathsf{z}^{n_p}\right\rangle\left\langle\mathsf{z}^{n_p}|\Psi\right\rangle d\mathsf{z}^{n_p}. \tag{E2}$$

$\tilde{\Psi}_{n_p}\left(\mathsf{z}^{n_p}\right)$ is antisymmetric wrt coordinate permutation σ i.e.

$$\tilde{\Psi}_{n_p}\left(\mathsf{z}_{\sigma(1)},\cdots,\mathsf{z}_{\sigma(n_p)}\right) = (-1)^{\pi(\sigma)}\,\tilde{\Psi}_{n_p}\left(\mathsf{z}^{n_p}\right) = (-1)^{\pi(\sigma)}\,\tilde{\Psi}_{n_p}\left(\mathsf{z}_1,\cdots,\mathsf{z}_{n_p}\right)\ \text{for}\ \sigma\in S_{n_p} \tag{E3}$$

where S_{n_p} is the $(n_p)^{th}$ order symmetric group and $\pi\left(\sigma\right)$ is the parity of σ. Hence

$$\begin{aligned}\tilde{\Psi}_{n_p}\left(\mathsf{z}_{\sigma(1)},\cdots,\mathsf{z}_{\sigma(n_p)}\right) = (-1)^{\pi(\sigma)}\,\tilde{\Psi}_{n_p}\left(\mathsf{z}_1,\cdots,\mathsf{z}_{n_p}\right) \\ = T_{n_p}\left(\mathsf{z}_{\sigma(1)},\cdots,\mathsf{z}_{\sigma(n_p)}\right)(-1)^{\pi(\sigma)}\,\Psi_{n_p}\left(\mathsf{z}_1,\cdots,\mathsf{z}_{n_p}\right) \\ \Rightarrow T_{n_p}\left(\mathsf{z}_{\sigma(1)},\cdots,\mathsf{z}_{\sigma(n_p)}\right) = T_{n_p}\left(\mathsf{z}_1,\cdots,\mathsf{z}_{n_p}\right)\forall\sigma\in S_{n_p}\end{aligned} \tag{E4}$$

Hence a *sufficient* requirement on the magnitude $\nu_{n_p}\left(\mathsf{z}_{q_p+1},\cdots,\mathsf{z}_{q_p+n_p}\right)$ and phase $\omega_{n_p}\left(\mathsf{z}_{q_p+1},\cdots,\mathsf{z}_{q_p+n_p}\right)$ to produce a symmetric $T_{n_p}\left(\mathsf{z}_{q_p+1},\cdots,\mathsf{z}_{q_p+n_p}\right)$ is that they are also symmetric and all symmetric $T_{n_p}\left(\mathsf{z}_{q_p+1},\cdots,\mathsf{z}_{q_p+n_p}\right)$ can be generated from symmetric $\nu_{n_p}\left(\mathsf{z}_{q_p+1},\cdots,\mathsf{z}_{q_p+n_p}\right)$ and $\omega_{n_p}\left(\mathsf{z}_{q_p+1},\cdots,\mathsf{z}_{q_p+n_p}\right)$, but we note that this is *not a* necessary requirement.

APPENDIX F: TRANSITION AMPLITUDES AND EXPECTATION VALUES WRT IPS

We will need to calculate expectation values and transition amplitudes between IPS composed of non orthogonal 1-particle states, to do this we will follow the presentation [11]. Consider two IPSs $|\Psi\rangle$ and $|\Phi\rangle$ composed of nonorthogonal general spin orbitals $\{\psi_j|1 \leq j \leq N\}$ and $\{\varphi_j|1 \leq j \leq N\}$ and the transition amplitude

$$\langle \Psi | H\Phi \rangle \tag{F1}$$

where the Hamiltonian is a sum of one and two particle operators

$$H = \sum_{1 \leq j \leq N} h(j) + \frac{1}{2} \sum_{1 \leq j \neq k \leq N} g(j,k) \tag{F2}$$

The transition amplitude of the 1-particle part is given by

$$\left\langle \Psi \left| \sum_{1 \leq j \leq N} h(j) \, \Phi \right. \right\rangle = Tr\left\{ \mathbf{h} \operatorname{adj}(\mathbf{S}) \right\} \tag{F3}$$

where the matrix $\mathbf{h}$ has matrix elements $\{h_{jk}|1 \leq j,k \leq N\}$ given by

$$h_{jk} = \langle \psi_j | h(1) \varphi_k \rangle = \int \psi_j(\mathsf{z})^* h(\mathsf{z},\mathsf{z}') \varphi_k(\mathsf{z}') \, d\mathsf{z} d\mathsf{z}' \tag{F4}$$

and the classical $N \times N$ adjugate matrix $\operatorname{adj}(\mathbf{S})$ of the overlap matrix $\mathbf{S} \equiv \{\langle \psi_j | \varphi_k \rangle | 1 \leq j,k \leq N\}$ is defined by

$$(\operatorname{adj}(\mathbf{S}))_{jk} = (-1)^{j+k} \det(\mathbf{S}[k|j]) \tag{F5}$$

where $\mathbf{S}[k|j]$ is the $(N-1) \times (N-1)$ matrix obtained from $\mathbf{S}$ by deleting the row k and the column j.

The transition amplitude of the 2-particle part is given by

$$\left\langle \Psi \left| \frac{1}{2} \sum_{1 \leq j \neq k \leq N} g(j,k) \, \Phi \right. \right\rangle = \frac{1}{2} Tr\left\{ \mathbf{G} \operatorname{adj}^{(2)}(\mathbf{S}) \right\} \tag{F6}$$

where the matrix $\mathbf{G}$ has matrix elements $\{g_{jklm}|1 \leq j < k \leq N; 1 \leq l < m \leq N\}$ given by

$$\begin{aligned} g_{jklm} &= \langle \psi_j \psi_k | g(1,2) \varphi_l \varphi_m \rangle \\ &= \int \left\{ \psi_j(\mathsf{z}_1)^* \psi_k(\mathsf{z}_2)^* g\left(\mathsf{z}_1, \mathsf{z}_2, \mathsf{z}_1', \mathsf{z}_2'\right) \varphi_l(\mathsf{z}_1') \varphi_m(\mathsf{z}_2') \right. \\ &\qquad \left. - \psi_j(\mathsf{z}_1)^* \psi_k(\mathsf{z}_2)^* g\left(\mathsf{z}_1, \mathsf{z}_2, \mathsf{z}_1', \mathsf{z}_2'\right) \varphi_m(\mathsf{z}_1') \varphi_l(\mathsf{z}_2') \right\} d\mathsf{z}^2 d\mathsf{z}'^2 \end{aligned} \tag{F7}$$

and the second order $\binom{N}{2} \times \binom{N}{2}$ adjugate matrix $\mathrm{adj}^{(2)}(\mathbf{S})$ is defined by

$$\left(\mathrm{adj}^{(2)}(\mathbf{S})\right)_{jklm} = (-1)^{j+k} \det(\mathbf{S}[lm|jk]) \tag{F8}$$

where $\mathbf{S}[lm|jk]$ is the $(N-2) \times (N-2)$ matrix obtained from $\mathbf{S}$ by deleting the rows l, m and the columns j, k.

In general the transition amplitude of the p-particle part is given by

$$\left\langle \Psi \left| \frac{1}{p!} \sum_{1 \leq j_1 \neq \cdots \neq j_p \leq N} O_p(j_1, \cdots, j_p)\, \Phi \right\rangle = \frac{1}{p!} Tr\left\{ \mathbf{O}_p\, \mathrm{adj}^{(p)}(\mathbf{S}) \right\} \right. \tag{F9}$$

where the matrix $\mathbf{O}_p$ has matrix elements

$$\left\{ [\mathbf{O}_p]_{j_1,\cdots,j_p;k_1,\cdots,k_p} \,|\, 1 \leq j_1 < \cdots < j_p \leq N; 1 \leq k_1 < \cdots < k_p \leq N \right\} \tag{F10}$$

given by

$$\begin{aligned} &[\mathbf{O}_p]_{j_1,\cdots,j_p;k_1,\cdots,k_p} = \left\langle \psi_{j_1} \cdots \psi_{j_p} | g(j,k)\, \varphi_{k_1} \cdots \varphi_{k_p} \right\rangle \\ &= \int \left\{ \psi_{j_1}(\mathsf{z}_1)^* \cdots \psi_{j_p}(\mathsf{z}_p)^* O_p\left(\mathsf{z}_{1\ldots}\mathsf{z}_p, \mathsf{z}'_{1\ldots}\mathsf{z}'_p\right) \sum_{\sigma \in S_p} (-1)^{\pi(\sigma)} \varphi_{k_{\sigma(1)}}(\mathsf{z}'_1) \cdots \varphi_{k_{\sigma(p)}}\left(\mathsf{z}'_p\right) \right\} d\mathsf{z}^p d\mathsf{z}'^p \end{aligned} \tag{F11}$$

and the p^{th} order $\binom{N}{p} \times \binom{N}{p}$ adjugate matrix $\mathrm{adj}^{(p)}(\mathbf{S})$ is defined by

$$\left(\mathrm{adj}^{(p)}(\mathbf{S})\right)_{j_1,\cdots,j_p;k_1,\cdots,k_p} = (-1)^{\sum\limits_{1 \leq l \leq p}^{\{j_l+k_l\}}} \det(\mathbf{S}[j_1, \cdots, j_p | k_1, \cdots, k_p]) \tag{F12}$$

where $\mathbf{S}[j_1, \cdots, j_p | k_1, \cdots, k_p]$ is the $(N-p) \times (N-p)$ matrix obtained from $\mathbf{S}$ by deleting the rows $j_1, \cdots, j_p$ and the columns $k_1, \cdots, k_p$.

APPENDIX G: KINETIC ENERGY EXPANSION IN THE $\{2, \ldots, 2\}$ APPROXIMATION

The effective kinetic energy operator $K(\nu, \omega)$ is given by

$$\begin{aligned} K(\nu,\omega) = &\underbrace{-\nabla \bullet \left(\nu^2\right) \mathbb{I} \bullet \nabla}_{I} - \underbrace{\nabla \bullet \left(\nu^2 \nabla\omega - i\nu\nabla\nu\right)}_{II} \\ &- \underbrace{\left(\nu^2\nabla\omega - i\nu\nabla\nu\right) \bullet \nabla}_{III} + \underbrace{\left(\nu\nabla\omega - i\nabla\nu\right) \bullet \mathbb{I} \bullet \left(\nu\nabla\omega - i\nabla\nu\right)}_{IV} \end{aligned} \tag{G1}$$

I

$$
\begin{aligned}
&-\nabla \bullet \left(\nu^2\right) \mathbb{I} \bullet \nabla = \\
&-\sum_{\sigma,\sigma' \in \mathcal{S}_N} \sum_{1 \leq j \leq N} \nabla_j \bullet \int \left\{ \prod_{1 \leq k \leq \frac{N}{2}} \nu_k \left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \nu_k \left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) \right. \\
&\left. \exp\left\{ i \sum_{1 \leq k \leq \frac{N}{2}} \left\{ \omega_k \left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) - \omega_k \left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \right\} \right\} \right\} \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N \right| d\mathsf{z}^N \mathbb{I} \bullet \nabla_j
\end{aligned}
\tag{G2}
$$

II

$$
\begin{aligned}
&-\nabla \bullet \left(\nu^2 \nabla\omega - i\nu\nabla\nu\right) = \\
&-\sum_{\sigma,\sigma' \in \mathcal{S}_N} \sum_{1 \leq j \leq N} \nabla_j \bullet \int \left\{ \nabla_j \left\{ \sum_{1 \leq k \leq \frac{N}{2}} \left\{ \omega_k \left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) \right\} \right\} \times \right. \\
&\qquad \left. \prod_{1 \leq k \leq \frac{N}{2}} \nu_k \left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \nu_k \left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) \right. \\
&\left. -i\nabla_j \left\{ \prod_{1 \leq k \leq \frac{N}{2}} \nu_k \left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) \right\} \prod_{1 \leq k \leq \frac{N}{2}} \nu_k \left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \right\} \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N \right| d\mathsf{z}^N
\end{aligned}
\tag{G3}
$$

III

$$
\begin{aligned}
&-\left(\nu^2 \nabla\omega - i\nu\nabla\nu\right) \bullet \nabla = \\
&-\sum_{\sigma,\sigma' \in \mathcal{S}_N} \sum_{1 \leq j \leq N} \int \left\{ \prod_{1 \leq k \leq \frac{N}{2}} \nu_k \left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \nu_j \left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) \times \right. \\
&\qquad \left. \nabla_j \left\{ \sum_{1 \leq k \leq \frac{N}{2}} \left\{ \omega_k \left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) \right\} \right\} \right. \\
&\left. -i \prod_{1 \leq k \leq \frac{N}{2}} \nu_k \left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \nabla_j \left\{ \prod_{1 \leq k \leq \frac{N}{2}} \nu_k \left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) \right\} \right\} \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}'^N \right| d\mathsf{z}^N \bullet \nabla_j
\end{aligned}
\tag{G4}
$$

IV

$$
\begin{aligned}
&(\nu\nabla\omega - i\nabla\nu) \bullet \mathbb{I} \bullet (\nu\nabla\omega - i\nabla\nu) = \\
&\sum_{\sigma,\sigma'\in\mathcal{S}_N} \sum_{1\leq j\leq N} \int \prod_{1\leq k\leq \frac{N}{2}} \nu_k\left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \times \\
&\left\{ \nabla_j \left\{ \sum_{1\leq k\leq \frac{N}{2}} \left\{ \omega_k\left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right)\right\}\right\} - i\nabla_j \left\{ \prod_{1\leq k\leq \frac{N}{2}} \nu_k\left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right)\right\}\right\} \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N\right| d\mathsf{z}^N \\
&\bullet \mathbb{I} \bullet \sum_{\sigma,\sigma'\in\mathcal{S}_N} \sum_{1\leq j\leq N} \int \left\{ \prod_{1\leq k\leq \frac{N}{2}} \nu_k\left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) \times \right. \qquad \text{(G5)} \\
&\left. \nabla_j \left\{ \sum_{1\leq k\leq \frac{N}{2}} \left\{ \omega_k\left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right)\right\}\right\} - i\nabla_j \left\{ \prod_{1\leq k\leq \frac{N}{2}} \nu_k\left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right)\right\}\right\} \left|\mathsf{z}^N\right\rangle \left\langle \mathsf{z}^N\right| d\mathsf{z}^N \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(G6)}
\end{aligned}
$$

leading to the expectation values

I

$$
\begin{aligned}
&\mathcal{K}(\nu,\omega) = \left\langle \varphi_1 \cdots \varphi_N \right| K(\nu,\omega) \left| \varphi_1 \cdots \varphi_N \right\rangle = \\
&\sum_{\sigma,\sigma',\sigma''\in\mathcal{S}_N} \int \left\{ \left\{ \varphi_1\left(\mathsf{z}_1\right)^* \cdots \nabla_j \varphi_j\left(\mathsf{z}_j\right)^* \cdots \varphi_N\left(\mathsf{z}_N\right)^* \right\} \bullet \nabla_j \left\{ (-1)^{\pi(\sigma'')} \varphi_1\left(\mathsf{z}_{\sigma''(1)}\right) \cdots \varphi_N\left(\mathsf{z}_{\sigma''(N)}\right)\right\} \right. \\
&\left. \prod_{1\leq k\leq \frac{N}{2}} \nu_k\left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \nu_k\left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) e^{\,i \sum\limits_{1\leq k\leq \frac{N}{2}} \left\{ \omega_k\left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) - \omega_k\left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right)\right\}} \right\} d\mathsf{z}^N \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(G7)}
\end{aligned}
$$

II

$$
\begin{aligned}
&- \sum_{\sigma,\sigma',\sigma''\in\mathcal{S}_N} \sum_{1\leq j\leq N} \int \left\{ \left\{ (-1)^{\pi(\sigma'')} \varphi_1\left(\mathsf{z}_{\sigma''(1)}\right) \cdots \varphi_N\left(\mathsf{z}_{\sigma''(N)}\right)\right\} \right. \\
&\varphi_1\left(\mathsf{z}_1\right)^* \cdots \nabla_j \varphi_j\left(\mathsf{z}_j\right)^* \cdots \varphi_N\left(\mathsf{z}_N\right)^* \bullet \left\{ \nabla_j \left\{ \sum_{1\leq k\leq \frac{N}{2}} \left\{ \omega_k\left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right)\right\}\right\} \right. \\
&\qquad\qquad \prod_{1\leq k\leq \frac{N}{2}} \nu_k\left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \nu_k\left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right) \\
&\left.\left. \qquad - i\nabla_j \left\{ \prod_{1\leq k\leq \frac{N}{2}} \nu_k\left(\mathsf{z}_{\sigma'(2k-1)}, \mathsf{z}_{\sigma'(2k)}\right)\right\} \prod_{1\leq k\leq \frac{N}{2}} \nu_k\left(\mathsf{z}_{\sigma(2k-1)}, \mathsf{z}_{\sigma(2k)}\right) \right\} d\mathsf{z}^N \qquad \text{(G8)}
\end{aligned}
$$

III

$$-\sum_{\sigma,\sigma',\sigma''\in\mathcal{S}_N}\sum_{1\leq j\leq N}\int\varphi_1\left(\mathsf{z}_1\right)^*\cdots\varphi_N\left(\mathsf{z}_N\right)^*\left\{\prod_{1\leq k\leq\frac{N}{2}}\nu_k\left(\mathsf{z}_{\sigma(2k-1)},\mathsf{z}_{\sigma(2k)}\right)\nu_k\left(\mathsf{z}_{\sigma'(2k-1)},\mathsf{z}_{\sigma'(2k)}\right)\right.$$
$$\times\sum_{1\leq k\leq\frac{N}{2}}\nabla_j\left\{\omega_k\left(\mathsf{z}_{\sigma'(2k-1)},\mathsf{z}_{\sigma'(2k)}\right)\right\}-i\prod_{1\leq k\leq\frac{N}{2}}\nu_k\left(\mathsf{z}_{\sigma(2k-1)},\mathsf{z}_{\sigma(2k)}\right)\times$$
$$\left.\nabla_j\left\{\prod_{1\leq k\leq\frac{N}{2}}\nu_k\left(\mathsf{z}_{\sigma'(2k-1)},\mathsf{z}_{\sigma'(2k)}\right)\right\}\bullet\nabla_j\left\{\left(-1\right)^{\pi(\sigma'')}\varphi_1\left(\mathsf{z}_{\sigma''(1)}\right)\cdots\varphi_N\left(\mathsf{z}_{\sigma''(N)}\right)\right\}\right\}d\mathsf{z}^N \tag{G9}$$

IV

$$+\sum_{\sigma,\sigma',\sigma''\in\mathcal{S}_N}\sum_{1\leq j\leq N}\int\varphi_1\left(\mathsf{z}_1\right)^*\cdots\varphi_N\left(\mathsf{z}_N\right)^*\left(-1\right)^{\pi(\sigma'')}\varphi_1\left(\mathsf{z}_{\sigma''(1)}\right)\cdots\varphi_N\left(\mathsf{z}_{\sigma''(N)}\right)\times$$
$$\left\{\prod_{1\leq k\leq\frac{N}{2}}\nu_k\left(\mathsf{z}_{\sigma(2k-1)},\mathsf{z}_{\sigma(2k)}\right)\nabla_j\left\{\sum_{1\leq k\leq\frac{N}{2}}\left\{\omega_k\left(\mathsf{z}_{\sigma(2k-1)},\mathsf{z}_{\sigma(2k)}\right)\right\}\right\}\right.$$
$$-i\nabla_j\left\{\prod_{1\leq k\leq\frac{N}{2}}\nu_k\left(\mathsf{z}_{\sigma(2k-1)},\mathsf{z}_{\sigma(2k)}\right)\right\}\bullet\left\{\nabla_j\left\{\sum_{1\leq k\leq\frac{N}{2}}\left\{\omega_k\left(\mathsf{z}_{\sigma'(2k-1)},\mathsf{z}_{\sigma'(2k)}\right)\right\}\right\}\times\right.$$
$$\left.\left.\prod_{1\leq k\leq\frac{N}{2}}\nu_k\left(\mathsf{z}_{\sigma'(2k-1)},\mathsf{z}_{\sigma'(2k)}\right)-i\nabla_j\left\{\prod_{1\leq k\leq\frac{N}{2}}\nu_k\left(\mathsf{z}_{\sigma'(2k-1)},\mathsf{z}_{\sigma'(2k)}\right)\right\}\right\}d\mathsf{z}^N \tag{G10}$$

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