Preliminary results on approximating a wavefunction as an unconstrained \boldsymbol{h}

Ex $\mathbf{k}^{1,*}, \quad \mathbf{k}$, **h** $\mathbf{k}^{2}, \quad \mathbf{n} = \mathbf{k} \mathbf{k}$, $^{-1}$ $\frac{1}{\sqrt{1-\mu}}$ and $\frac{1}{\sqrt{1-\mu}}$ at $\frac{1}{\sqrt{1-\mu}}$ university of Colorado at Boulder, Colorado $\frac{2}{n}$ department of Mathematics, $\frac{M}{n}$, $\frac{1}{n}$ Morton Hall, $\frac{1}{n}$ Morton Hall, $\frac{1}{n}$

 ${\sf A}$ multiparticle wavefunction of the multiparticle solution of the multiparticle ${\sf n}$ solution, satisfies the antisymmetry condition, thus making it natural to approximate it as a sum of \mathbf{n}_1 in \mathbf{n}_2 in addition, \mathbf{n}_3 is addition, \mathbf{n}_4 they impose structural constraints on the Slater determinants, such as or r , n particular excitations or a particular excitation n pattern. By removing these constraints, we have to obtain \mathbf{n}_1 , \mathbf{n}_2 in \mathbf{n}_3 , \mathbf{n}_4 , \mathbf{n}_5 , \mathbf{n}_6 , \mathbf{n}_7 , \mathbf{n}_8 , \mathbf{n}_9 , \mathbf{n}_1 , \mathbf{n}_2 , \mathbf{n}_3 , \mathbf{n}_5 , \mathbf{n}_7 , \mathbf{n}_8

 \overline{m} is an integral formulation of the problem, a fitting problem, and a fitting problem, and a fitting procedure based on the computation, and a fitting problem, and a fitting procedure based on the computation, and tional paradigm of separated representations. For constructions \mathbf{n}_{c} integral system of equations derived from \mathbf{n}_{c} ${\bf n}$ and products, we develop new algorithms with computational computations. T We describe preliminary numerical results and $\mathbf n$.

 \mathbf{n}_c of solving the multiparticle solving the multiparticle \mathbf{n}_c multiparticle \mathbf{n}_c methods in \mathbf{n}_c istry/physics are remarkably successful. Part of the interaction effects gained by \mathbf{n} and \mathbf{n} imposing structural constraints on the wavefunction to match physical intervals such methods scale poorly to high accuracy, \mathbf{n}_i methods scale poorly to high accuracy, \mathbf{n}_i methods scale poorly to high are biased by \mathbf{n}_i to only reveal structures that were part of the in \mathbf{n}_1 , \mathbf{n}_2 , \mathbf{n}_3 , \mathbf{n}_4 , allows better scaling to that allows better scaling to high accuracy and an unbiased exploration of the structure of the wavefunction by approximating it as an unconstrained sum of the wavefunction by approximating it as an unconstrained sum of the wavefunction \mathbf{n} of Slater determinants. In $\mathbf{n}_{\mathrm{max}}$

 \blacksquare the physical intuition that electrons may be excited into higher energy states, the Configuration Interaction Interaction Interaction Interaction Interaction Interaction Interaction Interaction Interaction Interact (Ci) family of methods choose a set of n and then optimize then orbitals, and then optimize the coefficients used to combine them. When it is found insufficient, methods to optimize the orbitals, when \mathbf{r}_i are ference states, etc., are ference states, etc., are ference states, etc., are ference states, etc., are ference states, etc $\mathbf n$ common feature of all these methods is that they impose some structural constraints on the $\mathbf n$ the Slater determinants on the Slater determinants on the Slater determinants on the Slater determinants, $\mathbf n$ the such as orthogonality or an excitation pattern. As the requested accuracy increases, the request ${\bf n}$ and ${\bf n}$ trigger an explosion in the number of determinants used, making the computation intractable for high accuracy. structural constraints present in $\mathbf n$, $\pm \mathbf k$, where we have function to comply with such structure, where $\mathbf n$ it is $\mathbf n$ it is really is the case of the case. For example, if you use a method that \mathbf{n}_i , \mathbf{n}_i , \mathbf{n}_i , \mathbf{n}_i , \mathbf{n}_i , \mathbf{n}_i states, \mathbf{n}_c and that the wavefunction is better as a linear combination is better as \mathbf{n}_c of \mathbf{n}_c and \mathbf{n}_c

- $H_{\rm{max}}(n,n)$ is the sum of kinetic, n is the sum of n and n and n and n
	- \mathcal{H} \mathcal{T} \mathcal{V} \mathcal{W} ,

where \mathtt{k} individually τ $^{-\frac{1}{2}\sum_{i=1}^{N}$ is the i is the particle with index index index i, the nuclear port \mathbf{E} n \mathbf{n} n $\mathbf{R}_{\mathbf{a}}$ n $\mathbf{R}_{\mathbf{a}}$ n \mathbf{V} $\sum_{i=1}^{N} V(\mathbf{r}_i)$, $V(\mathbf{r})$
 $\sum_{a} z_a / ||\mathbf{r} - \mathbf{R}_{\mathbf{a}}||/2$ n \mathbf{n} n \mathbf{n} n \mathbf{n} n \mathbf{n} \mathbf{W} $\frac{1}{2} \sum_{i=1}^{N} V(\mathbf{r}_i)$, $V(\mathbf{r})$ W