

# Numerical operator calculus in higher dimensions

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When an algorithm in dimension one is extended to dimension  $d$ , in nearly every case its computational cost is taken to the power  $d$ . This fundamental difficulty is the single greatest impediment to solving many important problems and has been dubbed the *curse of dimensionality*. For numerical analysis in dimension  $d$ , we propose to use a representation for vectors and matrices that generalizes separation of variables while allowing controlled accuracy. Basic linear algebra operations can be performed in this representation using one-dimensional operations, thus bypassing the exponential scaling with respect to the dimension. Although not all operators and algorithms may be compatible with this representation, we believe that many of the most important ones are. We prove that the multiparticle Schrödinger operator, as well as the inverse Laplacian, can be represented very efficiently in this form. We give numerical evidence to support the conjecture that eigenfunctions inherit this property by computing the ground-state eigenfunction for a simplified Schrödinger operator in  $d$  dimensions.

$$\phi(\cdot) \cdot \quad ; \quad \phi(\cdot) \cdot$$

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Abbreviation: SVD, singular value decomposition.



$$\mathcal{H} = \sum_i \left( \frac{p_i^2}{2m} + V(\mathbf{r}_i) \right) + \sum_{i < j} V_{ij}(\mathbf{r}_i, \mathbf{r}_j)$$

**The Multiparticle Schrödinger Operator**

$$\mathcal{H} = \sum_i \left( \frac{p_i^2}{2m} + V(\mathbf{r}_i) \right) + \sum_{i < j} V_{ij}(\mathbf{r}_i, \mathbf{r}_j)$$

$$\mathcal{H} = \left( \frac{p_1^2}{2m} + V_1(\mathbf{r}_1) \right) + \left( \frac{p_2^2}{2m} + V_2(\mathbf{r}_2) \right) + V_{12}(\mathbf{r}_1, \mathbf{r}_2)$$

$$\mathcal{H} = \left( \frac{p_1^2}{2m} + V_1(\mathbf{r}_1) \right) + \left( \frac{p_2^2}{2m} + V_2(\mathbf{r}_2) \right) + V_{12}(\mathbf{r}_1, \mathbf{r}_2)$$

[7]



$\mathbb{B}$

$$B(\cdot, \cdot) = \langle \tilde{\mathbf{V}}, \tilde{\mathbf{V}} \rangle. \quad [22]$$

$\mathbf{b}$

$$V(\cdot) = \langle V(\cdot), \mathbf{V}, \tilde{\mathbf{V}} \rangle. \quad [23]$$

$$\mathbb{B}(\cdot) = \mathbf{b}, \quad [24]$$

$$(\cdot) \quad V(\cdot) \quad (\cdot)$$

$\mathbb{B}, \cdot, M$   $\mathbf{b}$   $\mathbf{b}$   $M$

$F_0$   
 $\mathbf{F}$   
 $\mathbf{F}_{11}$   
 $\varepsilon$

$\mathbb{H} \approx \cdot 10, 2$   
 $\varepsilon 10$   
 $\mathbf{G}$   
 $\rho(\mathbb{A})$   
 $\varepsilon$   
 $2^{-33} \cdot ()$   
 $N 20$   
 $C_1$   
 $(1)$   
 $\cdot 10$   
 $\cdot 12$   
 $10$   
 $\mathbf{F}$   
 $30$   
 $\mathbb{H}$   
 $22$   
 $\varepsilon$   
 $2$

