Lanczos Iteration Applied to the Variational Method in Quantum Mechanics

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CHEG 827

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Quantum Mechanics

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$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

- In general, a difficult PDE to solve.

Variational Approach

- Approximate the wavefunction as the sum of elements in an orthonormal basis set.

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- Orthonormality of basis vectors is desirable.

$$\int_V \phi_i^* \phi_j dV = \delta_{ij}.$$

Matrix Representation of the Hamiltonian Operator

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- Define by how it operates on the basis wavefunctions.

$$\underline{\underline{\hat{H}}} = \begin{bmatrix} \int_V \phi_1^* \hat{\mathrm{KE}} \phi_1 dV & \int_V \phi_1^* \hat{\mathrm{KE}} \phi_2 dV & \cdots \\ \int_V \phi_2^* \hat{\mathrm{KE}} \phi_1 dV & \int_V \phi_2^* \hat{\mathrm{KE}} \phi_2 dV & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} + \begin{bmatrix} \int_V \phi_1^* \hat{\mathrm{PE}} \phi_1 dV & \int_V \phi_1^* \hat{\mathrm{PE}} \phi_2 dV & \cdots \\ \int_V \phi_2^* \hat{\mathrm{PE}} \phi_1 dV & \int_V \phi_2^* \hat{\mathrm{PE}} \phi_2 dV & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

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- Can compute potential part by using an FFT of the potential.

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- $\int_V \phi^*_{ijk} \left(-\frac{\hbar^2}{2m} \nabla^2 \phi_{ijk} \right) dV = \frac{\hbar^2}{2m} |G_{ijk}|^2$
- $\hat{V}(r) = \sum_{ijk} \nu(i, j, k) e^{iG_{ijk} \cdot r}$

$$\frac{1}{\Omega} \int_V \phi_{i+\Delta i, j+\Delta i, k+\Delta i} \hat{V} \phi_{i,j,k} dV = \nu(\Delta i, \Delta j, \Delta k)$$

Lanczos Algorithm

- Krylov method for quickly computing the few top magnitude eigenvalues.

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- A slower method such as QZ decomposition can compute the eigenvalues and eigenvectors of T_k.

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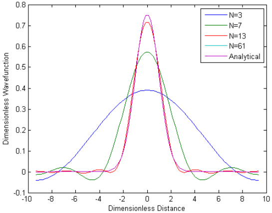
- $\hat{V}(x) = \frac{1}{2}m\omega^2x^2$
- One of the few quantum problems for which an analytical solution exists.

$$\begin{aligned}
\Psi_n(x) &= \frac{1}{\sqrt{2^m n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \\
E_n &= \hbar\omega(n + \frac{1}{2})
\end{aligned}$$

Accuracy



Numerical and analytical solutions

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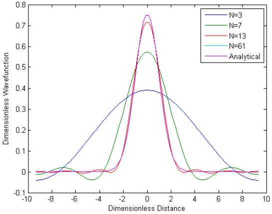

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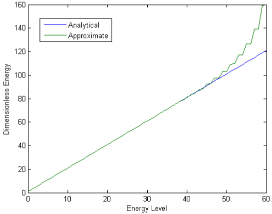

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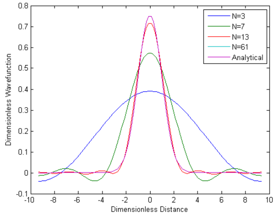

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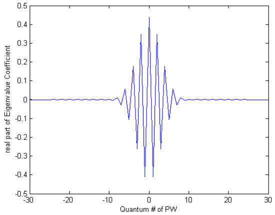
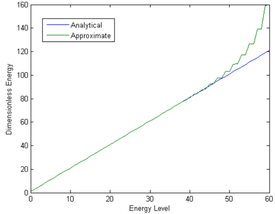


Plane-wave coefficients.



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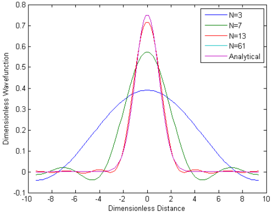

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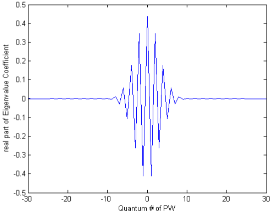

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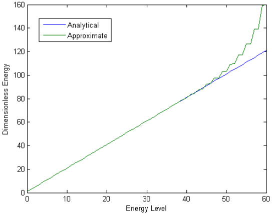

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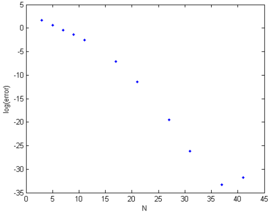
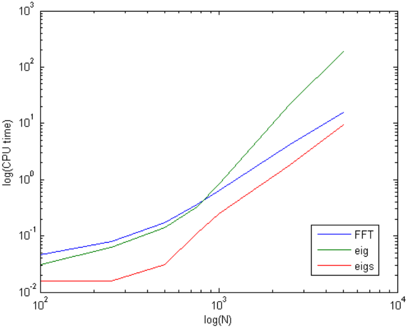


Error behavior.

Speed



Speed of various parts of the calculation.

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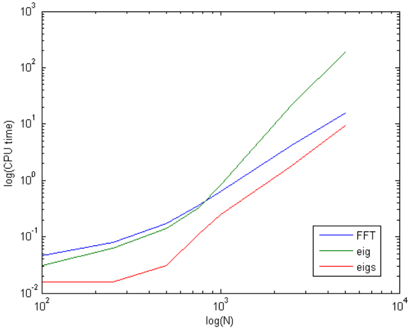

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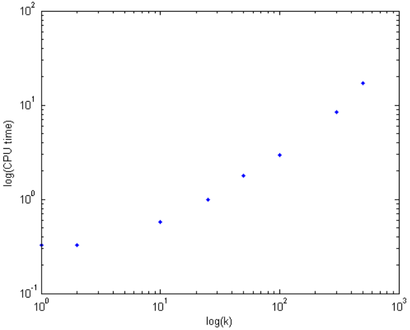

Speed of Lanczos vs. k.

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- The Lanczos Algorithm can quickly compute the smallest eigenvalues, which are the ones well represented by the variational approach.
- Only about 60 basis functions are needed for the case studied, but this will change in higher dimensions.