Large-scale diagonalization and effective interactions for quantum dots

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Introduction

Quantum dots are targeted by many research groups, both theoretically and experimentally. Numerical treatments are often done with the so-called *configuration-interaction (CI) method*. It is also called *exact diagonalization*, which is really a misnomer. In this presentation, I analyze this problem and propose a method from nuclear physics that *drastically improves* the convergence properties in a very general setting. See also Ref. [1]

Quantum dots are quasi-two-dimensional electronic systems, usually implemented through etching techniques, thereby confining the electron in one of the spatial directions. The usual stance is that the confining potential in the plane is approximately harmonic, leading to a perturbed two-dimensional n-body harmonic oscillator (h.o.) Hamiltonian, viz,

$$H = \sum_{j=1}^{n} \Big[-\frac{1}{2}\nabla_j^2 + \frac{1}{2}r_j^2 + v(\vec{r}_j) \Big] + \sum_{j<k} \frac{\lambda}{\|\vec{r}_j - \vec{r}_k\|},$$

where v is a perturbation of the h.o., and where λ is the relative strength of electron interactions over confinement. Clearly, expanding the Hamiltonian in h.o. basis functions is a natural approach for solving this problem numerically.

However, a critical analysis of the behaviour of this method is sadly neglected in the literature, leading to inaccurate calculations and conclusions.

★ Important common features in quantum dot models: Many-body problem, singular $1/r$ interaction, non-smooth perturbation v of h.o. potential. See for example Refs. [2, 3]

The CI method

The CI method is a Rayleigh-Ritz projection method:

1. Write $H = H_0 + H_1$, where we have a complete set of eigenfunctions of H_0. In our simple case, H_0 is the (n-body, 2D) h.o.
2. Select a finite-dimensional subspace $\mathcal{H}_N$ spanned by the h.o. states up to shell number N.
3. Let P be the orthogonal projector onto $\mathcal{H}_N$ and construct $H_N = PHP$.
4. Diagonalize H_N using some method, typically Lanczos iterations.

As N grows, the Hilbert space L^2 is spanned, and the eigenvectors and eigenvalues converges to the correct values, see Ref. [4]. But just how quickly does this happen?

★ The *curse of dimensionality* severely restricts the number of shells N used in a many-body calculation, since the dimension of $\mathcal{H}_N$ grows exponentially with n.

Slow convergence for quantum dots

We can illustrate the convergence problems with a simple example. Analytic solutions for $v = 0$, $\lambda = 1$ exists for the two-particle problem, see Ref. [5]. Indeed, by transforming to centre-of-mass coordinates $\vec{R} = (\vec{r}_1 + \vec{r}_2)/\sqrt{2}$ and $\vec{r} = (\vec{r}_1 - \vec{r}_2)/\sqrt{2}$, only the relative motion is non-trivial:

$$H = \underbrace{-\frac{1}{2}\nabla_R^2 + \frac{1}{2}R^2}_{\text{c.o.m. motion}} \underbrace{-\frac{1}{2}\nabla_r^2 + \frac{1}{2}r^2 + \frac{1}{\sqrt{2}r}}_{\text{relative motion}}.$$

Transforming to polar coordinates, the relative problem has the ground state

$$\Psi_0(r) = (r + \sqrt{2})e^{-r^2/2}, \quad E_0 = 2.$$

On the other hand, the h.o. basis functions for this example are:

$$\Phi_n(r) = L_n(r^2)e^{-r^2/2}, \quad (L_n \text{ are Laguerre polys})$$

containing only even powers of r in the polynomial part, while the eigenfunction has odd powers as well. Note the cusp at $r = 0$.

★ This implies very slow convergence of CI. The method needs to approximate r as a polynomial series using only even powers! Similar problems arise when $v(\vec{r})$ is non-smooth.

★ For a many-body calculation, one cannot expect the results to be accurate due to the cusp and the curse of dimensionality!

One-dimensional quantum dots

The model

The 1D dimensional problem is qualitatively similar to the 2D problem, but simpler to analyze numerically and mathematically. First, define the one-dimensional h.o. operator:

$$h(x) = -\frac{1}{2}\frac{\partial}{\partial x^2} + \frac{1}{2}x^2.$$

The eigenfunctions are the well-known Hermite functions, viz,

$$\phi_n(x) = (2^n n! \pi^{1/2})^{-1/2} H_n(x) e^{-x^2/2},$$

with eigenvalues $n + 1/2$.

The Hamiltonian for two particles:

$$H = h(x_1) + h(x_2) + v(x_1) + v(x_2) + U(x_1 - x_2),$$

where U is an approximation to the Coulomb repulsion in 1D, viz,

$$U(x) = \frac{\lambda}{|x| + \delta}, \quad \delta > 0.$$

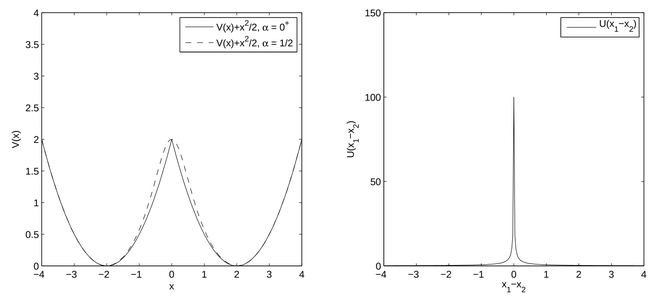
In centre-of-mass coordinates x and X,

$$H = h(X) + h(x) + v\big([X + x]/\sqrt{2}\big) + v\big([X - x]/\sqrt{2}\big) + U(\sqrt{2}x).$$

★ Notice that $h(x_1)+h(x_2)$ is transformed into $h(X)+h(x)$, a symmetry. Holds in general for orthogonal coordinate transformations.

★ Notice that the cases $\lambda = 0$ or $v = 0$ reduce to simple one-dimensional Hamiltonians on the form $h(x)+f(x)$, with $f(x) = v(x)$ or $f(x) = U(\sqrt{2}x)$. In both cases, f vanishes at large $|x|$.

★ Recall that non-smooth functions v are often used.



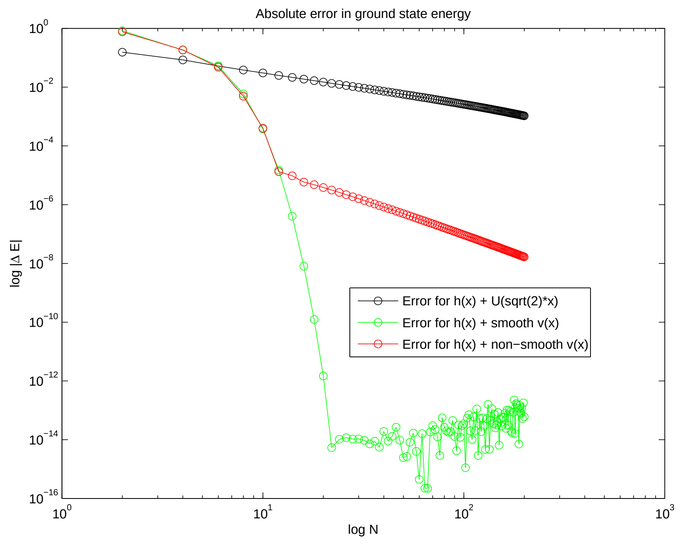
A typical non-smooth and a smooth trap $x^2/2 + v(x)$, and the interaction for $\delta = 0.01$, $\lambda = 1$

Experiments and analysis

Thus, we are concerned with the rather simple eigenproblem

$$\big(h(x) + f(x)\big)\psi(x) = E\psi(x), \tag{1}$$

with $f(x) = v(x)$ or $f(x) = U(\sqrt{2}x)$, respectively. This figure shows the energy error in a CI calculation on these problems:



★ Non-smooth potentials give very slow convergence. An error of about 10^{-3} requires $N \sim 10^3$. Impossible for more particles and/or 2D! Smooth potentials yield exponential convergence.

Decay of h.o. coefficients

We can prove the above results. The Hermite functions $\phi_n(x)$ form a basis for $L^2(\mathbb{R})$, i.e., for any $\psi \in L^2$,

$$\psi(x) = \sum_{n=0}^{\infty} c_n \phi_n(x), \quad \|\psi\|^2 = \sum_{n=0}^{\infty} |c_n|^2 < \infty.$$

The latter implies $|c_n| = o(n^{-1/2})$. Using this, one can show that if (see Ref. [1])

- $\psi(x)$ has k derivatives in L^2
- $x^m\psi(x) \in L^2$ for $m = 0, 1, \ldots, k$

then

$$|c_n| = o(n^{-(n+1)/2}).$$

If $\psi(x)$ is *complex analytic* in a strip of width w around the real axis, then

$$|c_n| = O(n^{-1/4} e^{-w\sqrt{2n+1}}),$$

which decays *much faster* than $o(n^{-(n+1)/2})$.

★ Hermite coefficients decay faster with smoother functions, and slower with non-smooth functions. In addition one has a decay condition on the function.

★ Eigenfunctions of Eqn. (1) will be $k + 2$ times differentiable, if the potential is k times differentiable. Eigenfunctions will be (complex) analytic at x if and only if the potential is (complex) analytic at x

Effective interactions

Effective interaction theory has been widely used in nuclear physics for decades. We propose to employ the Lee-Suzuki similarity transformed effective interaction [6] on the Coulomb terms in the Hamiltonian to increase the precision for a given number of shells N and for $n \geq 2$ particles.

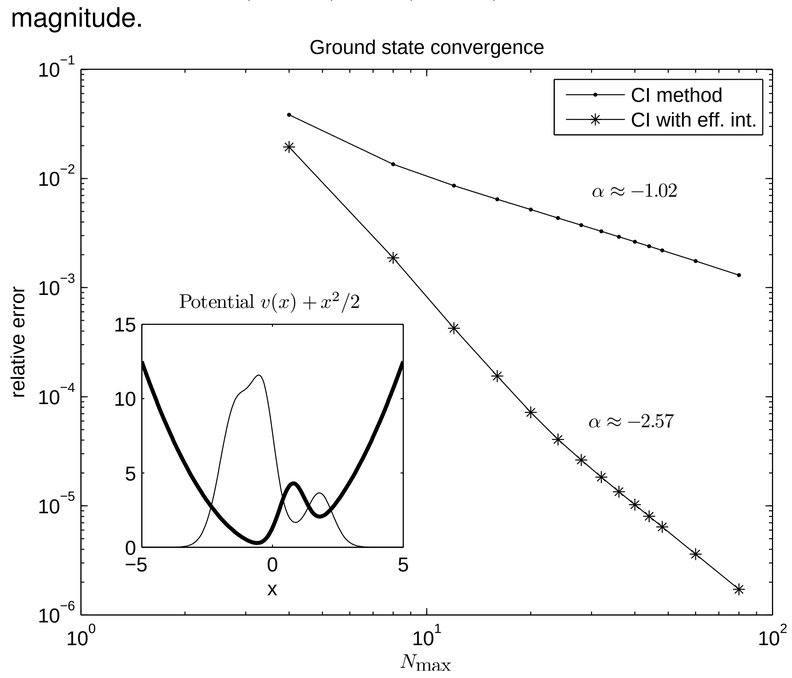
★ One starts with the two-body $v = 0$ case, constructing a *new* operator $\tilde{U}$ with much better approximation properties. Then, v is added as a perturbation to the "renormalized" many-body problem, and $\tilde{U}$ is used for each interaction term.

The effective interaction theory is too complex for a poster presentation. The interested audience is pointed to Refs. [6, 1]. In the quantum dot applications the most important features are:

- Computation of the exact two-electron $v = 0$ eigenvalues and eigenvectors of H. This is possible using a different basis than the h.o. basis.
- Computation of the new renormalized Coulomb matrix based on these.
- Note: The new CI scheme will not be more complex than the original scheme; only the matrix elements differ.

Results in 1D

The figure shows a simple effective interaction experiment in 1D for two electrons. The trap perturbation $v(x)$ is a Gaussian (inset together with ground state electron density). The improvement in the error is from $O(N^{-1.01})$ to $O(N^{-2.57})$, close to two orders of magnitude.



The error in the ground state energy for increasing N using effective interactions.

Conclusion and outlook

Exact diagonalization is far from exact! In Ref. [7] a sophisticated CI implementation for up to 5 particles is given, but unable to yield more than ∼1 % accuracy even when using a large cluster of processors.

I have pointed out that by using effective interaction theory one can drastically improve the bad convergence associated with (but rarely recognized) the CI method.

Numerical experiments for $n \leq 5$ in 2D are in preparation, and will be discussed in a forthcoming sequel to Ref. [1]. With the new method, very good results can be obtained with a single desktop computer. As a by-product, much more accurate time-dependent simulations will be possible, facilitating important decoherence studies in realistic quantum dots.

References

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