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SEARCH FOR BOUND STATES IN A ONE-DIMENSIONAL QUANTUM SYSTEM USING THE POWER METHOD: PRACTICAL IMPLEMENTATION

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Abstract. For numerical solution of the time-dependent Schrödinger equation describing the electron evolution in a given potential interacting with the high-intensity ultrashort pulse field, one has to find bound states of this potential with high accuracy. The paper considers the application of power algorithm using Chebyshev operator polynomials to search for bound states of one-dimensional quasi-Coulomb potential. The algorithm convergence improves with increasing polynomial degree m, saturating at $m \geq 8$. For such degree, the ground state is found in ~10^3 Hamiltonian calculation operations, while higher states require ~10^5 operations (several seconds and several minutes respectively).

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One-dimensional quantum systems, where the Hamiltonian $\widehat{H}$ depends on a single coordinate x, have been studied since beginning of quantum era due to the possibility of particle tunneling through a potential barrier [1]. In the 1980–90s, when computational capabilities were limited as compared to the modern ones, the Hamiltonian's dependence on a single spatial coordinate enabled numerical simulation of nonlinear ionization in such systems [2–4]. In the last decade, the relatively low computational complexity of numerical integration of the one-dimensional time-dependent Schrödinger equation has made it possible to self-consistently use quantum calculation results as a nonlinear source in (3D + t) propagation equations [5] and to model quantum electrodynamics effects in strong fields of ultrashort pulses [6].

The interaction of a one-dimensional quantum mechanical system with an electromagnetic field is described by the time-dependent Schrödinger equation for the wave function $\Psi(x,t)$, hereafter the Hartree units are used unless otherwise specified:

$$i\frac{\partial\Psi(x,t)}{\partial t} = \widehat{H}\Psi(x,t) + \widehat{\mathcal{H}}\Psi(x,t), \qquad (1)$$

where

$$\widehat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \widehat{U}(x)$$

is the electron Hamiltonian in the time-independent potential t $\widehat{U}(x)$, $\widehat{\mathcal{H}}(t)$ is the operator describing the interaction of the electron with the electromagnetic wave field, and t is a time. Equation (1) must be provided with the initial condition $\Psi(x,t=-\infty)$. At $t=-\infty$ the system is usually in a bound state, therefore, the initial conditions for equation (1) are the wave functions of bound states $|\Psi_n\rangle$ (most often the ground state with) with $n=0$) the corresponding discrete energy spectrum $E_n < 0$, where $n = 0,1,2,\ldots$ Functions $|\Psi_n\rangle$ are eigenfunctions of the operator $\widehat{H}$ and the search for bound states of the system reduces to solving the time-independent Schrödinger equation:

$$\widehat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle. \qquad (2)$$

For the majority of quantum systems, there is no analytical solution to equation (2), and numerical search for eigenfunctions and eigenvalues is needed. This imposes high requirements on the accuracy of the found solutions for further description of quantum systems' response using the time-dependent

Schrödinger equation, since inaccurate determination of the initial state leads to artifacts in the solution of equation (1).

Various numerical approaches are used for finding eigenfunctions and eigenvalues of the time-independent Schrödinger equation: direct integration [7] of equation (2), matrix approach [8], imaginary time methods [9], spectral [10], power [11] methods, etc. From a computational point of view, the advantage of power methods is that the same Hamiltonian approximation is used in solving equations (2) and (1), which reduces the rate of numerical error accumulation when solving the time-dependent equation. The power method is also free from the boundary conditions problem [12, 13] and can be applied to both one- and multi-dimensional problems. However, for quantum systems with a large number of bound states, the search for eigenfunctions can be extremely time-consuming. Acceleration of power methods convergence can be achieved, in particular, by applying operators that are inverse to the Hamiltonian [14] or Chebyshev polynomials of the Hamiltonian [11], § 16. Let us consider the second case, which is algorithmically simpler and in some sense more universal (inversion of the Hamilton operator is possible if it is approximated by finite differences on a grid, but not in the case when Fourier transform is used to calculate the derivative). Let us briefly outline the idea of the power method.

Let's choose an arbitrary approximation $|\Psi_n^{(0)}\rangle$ taking into account the parity of the wave function n-th state and its decay in the classically forbidden region. We will repeatedly apply to the trial wave function a certain polynomial operator $P(\widehat{H})$, whose eigenbasis coincides with the basis of $\widehat{H}$. When transitioning from k-th to $(k+1)$-th iteration, we obtain

$$|\Psi_n^{(k+1)}\rangle = P(\widehat{H})|\Psi_n^{(k)}\rangle. \qquad (3)$$

Let's consider the formal expansion $|\Psi_n^{(k)}\rangle$ in the true basis $|\Psi_j\rangle$ of Hamiltonian $\widehat{H}$:

$$|\Psi_n^{(k)}\rangle \propto |\Psi_n\rangle + \sum_{j\neq n} c_j^{(k)} |\Psi_j\rangle,$$

where $c_j^{(k)}$ are the expansion coefficients in basis $|\Psi_j\rangle$ at the k-th iteration. Then for the approximation at the next iteration we get

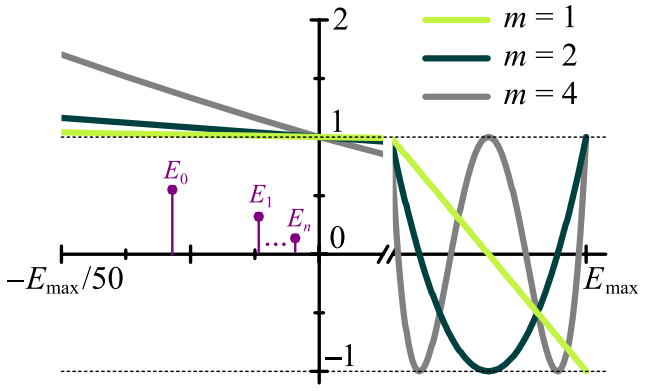

Fig. 1. Dependence of the amplification factor at each iteration of the algorithm on the state energy when using Chebyshev polynomials of different degrees m. Purple lines qualitatively show the levels of discrete spectrum

$$P(\widehat{H})|\Psi_n^{(k)}\rangle \propto |\Psi_n\rangle + \sum_{j\neq n} \underbrace{c_j^{(k)} \frac{P(E_j)}{P(E_n)}}_{c_j^{(k+1)}} |\Psi_j\rangle. \qquad (4)$$

Thus, the decrease in amplitudes for excited states and continuum states (and, accordingly, the convergence rate of the power algorithm $|\Psi_n^{(k)}\rangle \to \Psi_n\rangle$) is determined by the value $\max_{j\neq n}|P(E_j)/P(E_n)|$. The optimal power algorithm should minimize it.

As a result of applying such an algorithm and normalizing the wave function (at each step), we will obtain the eigenfunction $|\Psi_n\rangle$ and eigenvalue $E_n = \langle\Psi_n|\widehat{H}|\Psi_n\rangle$, for which $P(E_n)$ is maximal. After this, the algorithm can be repeated, removing from the wave function the projections onto already found states with lower n:

$$|\Psi_n^{(k+1)}\rangle := |\Psi_n^{(k+1)}\rangle - \sum_{j<n} |\Psi_j\rangle\langle\Psi_j|\Psi_n^{(k+1)}\rangle,$$

i.e., ensuring $c_j = 0$ for $j < n$, and find higher states and energy values.

The convergence rate of the power algorithm is determined by the chosen function $P(\widehat{H})$ and its spectrum, i.e. the values $P(E_n)$ for all energy states in a given potential, including continuum ones. It is desirable to use operator functions that are polynomials of finite degree from the Hamiltonian operator, due to the algorithmic simplicity of their calculation (which is especially important in the multidimensional case). We will use the fact that among all polynomials of a given degree m, whose

absolute values on the segment $[-1, 1]$ do not exceed 1, Chebyshev polynomials of the first kind $T_m(\varepsilon) = \cos[m \arccos(\varepsilon)]$ have maximum values outside this segment. Let $E_{\max} = \pi^2/(2\Delta x^2)$ be the maximum energy state corresponding to the Nyquist frequency on a given computational grid with step Δx. Using the linear transformation

$$P_m(\varepsilon) = T_m(1 - 2\varepsilon/E_{\max}),$$

we place the center of the Chebyshev polynomial T_m at $E_{\max}/2$, i.e., transfer the region where the polynomial $|P_m(\varepsilon)| \le 1$, from $[-1, 1]$ to the range of positive energies of continual states $[0, E_{\max}]$; for bound states we have $|P_m(\varepsilon)| \ge 1$, see Fig. 1. For bound state energies $-E_{\max} \ll E_n < 0$

$$P_m(E_n) \approx T_m(1) + T'_m(1)\frac{2|E_n|}{E_{\max}} = 1 + 2m^2\frac{|E_n|}{E_{\max}}, \quad (5)$$

i.e., at each iteration the amplitude of the n-th state will increase approximately by $1 + 2m^2|E_n|/E_{\max}$.

In this work, we use the power algorithm with Chebyshev operator polynomials to find eigenfunctions and eigenvalues of one-dimensional quasi-Coulomb potential (8) with nine bound states. The dependence of the algorithm's speed on the degree of Chebyshev polynomial is investigated. The "optimal" polynomial degree $m \approx 8$ provides search for the ground state $|\Psi_0\rangle$ in $k \approx 125$ iterations (4 s on a workstation with Intel® Xeon® E5–2630 processors), and the bound state with the highest energy $|\Psi_8\rangle$ in $k \approx 8000$ (with calculation time about 4 min). When substituting the found wave functions $|\Psi_n\rangle$ as initial conditions of the time-dependent Schrödinger equation (1) without external field, the artifact value of the electron's mean coordinate deviates from zero by $\le 10^{-10}$ over 50 fs.

In simulations, we use a uniform grid along the coordinate x with step size $\Delta x = 0.125$ and number of nodes $N = 2^{16}$. This provides a sufficiently large region in x, which is important for the time-dependent problem and wave function components related to electrons detached from the atomic core. This relatively coarse resolution complicates the finite-difference approximation of the second derivative in the Hamiltonian, therefore for its determination we used the Fourier transform.

To study the convergence of the Chebyshev power algorithm, let's consider the potential

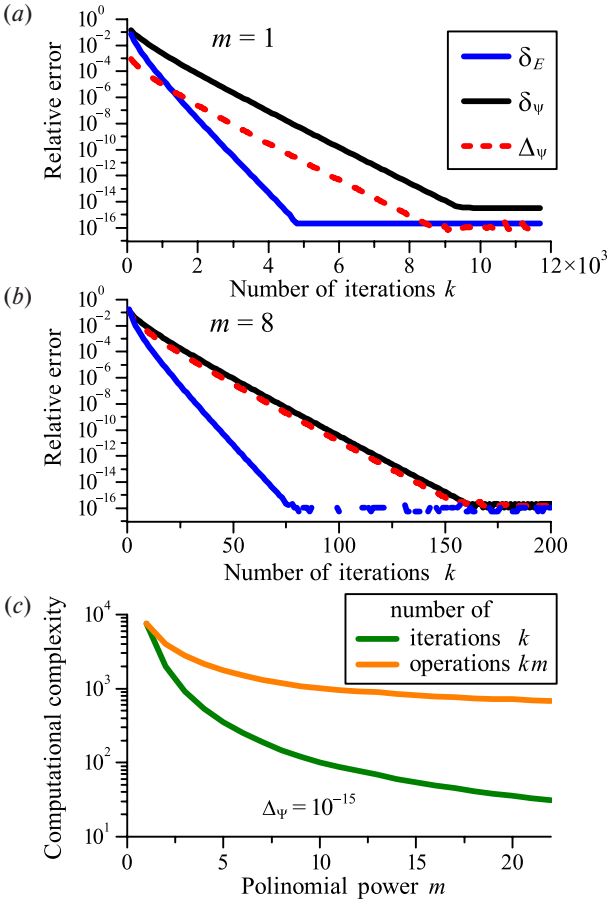

Fig. 2. *a*, *b* – Dependencies on the iteration number k of relative errors in determining the wave function $\delta_\Psi^{(k)}$ and $\Delta_\Psi^{(k)}$, as well as the bound state energy error $\delta_E^{(k)}$ of potential $U(x) = -\mathrm{ch}^{-2}(x)$. Panel *a* corresponds to the power algorithm with Chebyshev polynomial $P_1(\widehat{H})$, *b* – with $P_8(\widehat{H})$. *c* – Number of iterations k and number of operations km, required to determine $|\Psi\rangle$ with relative error $\Delta_\Psi = 10^{-15}$ for polynomials of different degrees m

$$U(x) = -\mathrm{ch}^{-2}(x),$$

with the analytical solution for single bound state

$$\Psi_a(x) = \frac{1}{\sqrt{2}}\mathrm{ch}^{-1}(x)$$

and energy

$$E_a = -\frac{1}{2} = -13.6\,\mathrm{eV}.$$

To determine the accuracy of the eigenfunctions $\Psi^{(k)}(x)$ in such potential we will use relative errors

$$\delta_\Psi^{(k)} = \max_i \left|\frac{\Psi_a(x_i) - \Psi^{(k)}(x_i)}{\Psi_a(x_i)}\right| \quad (6)$$

and

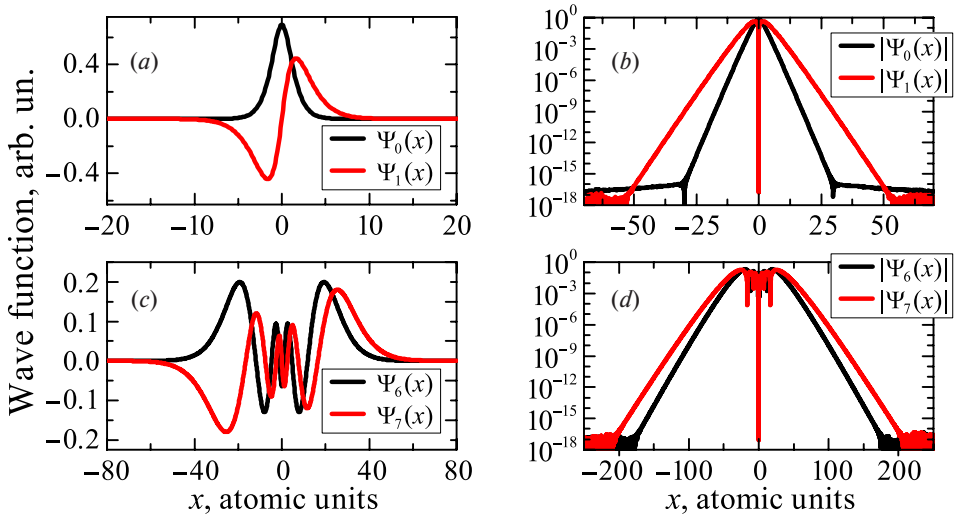

Fig. 3. *a*, *b* – Wave functions $\Psi_0(x)$, $\Psi_1(x)$, *c*, *d* – $\Psi_6(x)$, $\Psi_7(x)$. Figures are plotted on a linear scale, *b*, *d* – on a semi-logarithmic scale. The simulation was conducted for potential (8) using Chebyshev polynomial $P_8(\widehat{H})$

$$\Delta_\Psi^{(k)} = \max_i \left| \frac{\Psi^{(k)}(x_i) - \Psi^{(k-1)}(x_i)}{\Psi^{(k-1)}(x_i)} \right|. \qquad (7)$$

The first of these expressions is applicable only for potentials with analytical eigenfunction, while the second is for an arbitrary one-dimensional potential. The relative error in the state energy is defined as

$$\delta_E^{(k)} = |(E_a - E^{(k)})/E_a|.$$

In Figs. 2*a*, *b* for polynomials of degrees $m = 1$ and $m = 8$, the dependencies of relative errors $\delta_\Psi^{(k)}$, $\Delta_\Psi^{(k)}$ and $\delta_E^{(k)}$ in the studied potential on the iteration number k are shown. The error of energy $\delta_E^{(k)}$ with increasing k decreases faster than $\delta_\Psi^{(k)}$ and $\Delta_\Psi^{(k)}$, therefore, in the following, we will evaluate the algorithm execution speed via the errors in determining the wave function. Errors $\delta_\Psi^{(k)}$ and $\Delta_\Psi^{(k)}$ decrease with the same slope and almost simultaneously reach the "noise level" $\sim 10^{-15}$ associated with errors of double precision numbers (Figs. 2*a*, *b*). Thus, the termination condition for the iterative algorithm can be chosen based on $\Delta_\Psi^{(k)} \approx 10^{-15}$.

With increasing polynomial degree m, the number of iterations required to achieve the same accuracy $\Delta_\Psi = 10^{-15}$ monotonically decreases by 2 orders of magnitude when m changes from 1 to 24 (see Fig. 2*c*). However, one iteration using polynomial $P_m(\widehat{H})$ requires m times more operations than for polynomial $P_1(\widehat{H})$. Therefore, the choice of polynomial order was determined by the saturation of the number of

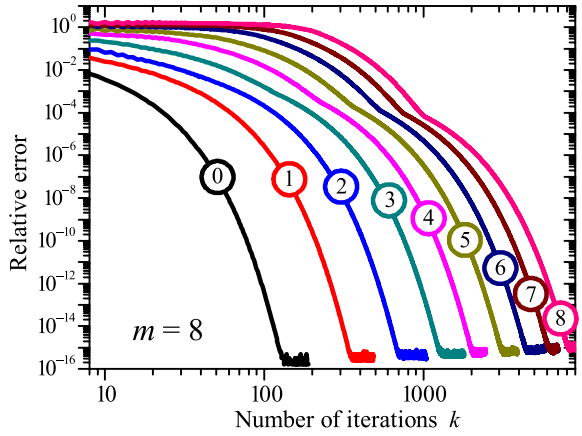

Fig. 4. The dependence of the relative error of wave functions Δ_Ψ on the number of iterations k for potential (8). Numbers indicate state numbers (0 corresponds to the ground state)

operations km, allowing to find $|\Psi\rangle$ with relative error $\Delta_\Psi = 10^{-15}$, which in our case is $\sim 10^3$ and is achieved at $m \approx 8$. Thus, the degree of Chebyshev polynomial $m = 8$ is optimal for the practical implementation of the power algorithm for solving the time-independent Schrödinger equation (2).

Now let's apply the power algorithm with the "optimal" value $m = 8$ to the potential $U(x)$, with no analytical solution to equation (2):

$$U(x) = -\frac{A}{\sqrt{x^2 + B^2}} \exp\left[-\left(\frac{x}{C} \right)^{16} \right]. \qquad (8)$$

The first factor here corresponds to the quasi-Coulomb potential with an infinite number of levels

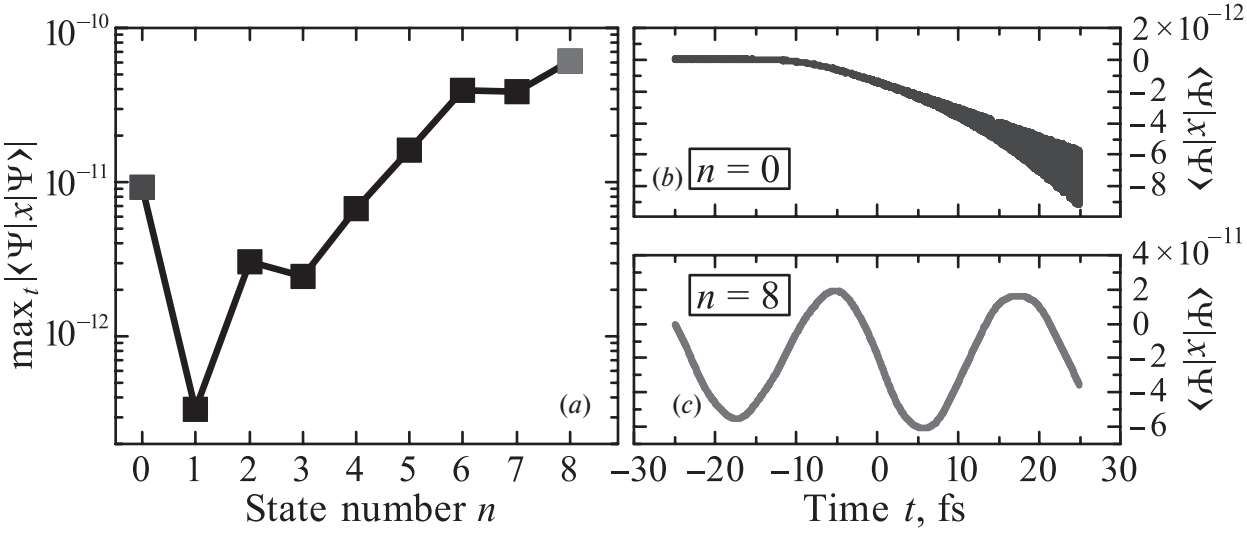

Fig. 5. *a* – Dependence of the maximum artifact deviation from zero of the electron mean coordinate over 50 fs on the number of the bound state of potential (8), obtained by numerical integration of the time-dependent Schrödinger equation (1) in the absence of external field ($\hat{\mathcal{H}} = 0$) with initial condition $\Psi(x,t = -\infty) = \Psi_n(x)$. *b, c* – Examples of artifact dependencies of the electron mean coordinate on time for $n = 0$ and $n = 8$ respectively

[2], while the second one makes their number finite. To obtain a sufficiently large number of bound states, we fixed the constant $C = 512$. Then we selected the parameters $A = 1.13$ and $B = 0.827$ in such a way that the ground state energy corresponds to the ionization potential of the helium atom. In the resulting potential, we found nine bound states. The wave functions of the ground $\Psi_0(x)$ and some excited $\Psi_1(x)$, $\Psi_6(x)$, and $\Psi_7(x)$ states are shown in Fig. 3 in linear (*a*, *c*) and semi-logarithmic (*b*, *d*) scales respectively. The energies of these states are $E_0 = -24.61$ eV, $E_1 = -9.84$ eV, $E_6 = -1.20$ eV, and $E_7 = -0.92$ eV. In agreement with known analytical solutions [15], outside the well, the wave functions $\Psi_n(x)$ decrease as $\exp\left(-|x|\sqrt{-2E_n}\right)$ down to the "noise" associated with double precision errors (Figs. 3*b*, *d*).

Let's examine the convergence of the power algorithm for bound states with different quantum numbers *n*. Figure 4 shows the dependence of relative error Δ_Ψ on iteration number *k*. At $n = 0$ the value $\Delta_\Psi = 10^{-15}$ is achieved in $k \approx 125$ iterations, which corresponds to program execution time of 4 s, at $n = 1$ – in $k \approx 125$ iterations and 11 s, and at $n = 8$ the value *k* increases to ~8000 and computation time increases to ~4 min (on a workstation with Intel® Xeon® E5–2630 processors).

We used the obtained wave functions $\Psi_n(x)$ as initial conditions for the time-dependent Schrödinger equation (1) with $\widehat{H} = 0$, which was numerically integrated according to the method described in [16]. The average value $\langle\Psi \mid \hat{x} \mid \Psi\rangle$ of the electron coordinate operator $\hat{x}$ obtained during simulation changes by $\leq 10^{-10}$ over 50 fs for all found wave functions $\Psi_n(x)$ (see Fig. 5). Such magnitude of the average electron coordinate is 6–7 orders smaller than the value $\langle\Psi \mid \hat{x} \mid \Psi\rangle$, achieved in a one-dimensional quantum system under the action of a pulse with intensity $\sim 1 - 100$ TW/cm^2 [16]. This indicates that the power algorithm for finding eigenstates of a one-dimensional system determines $|\Psi_n\rangle$, with an accuracy sufficient for quantum mechanical simulations of the evolution of a one-dimensional system under the action of an intense ultrashort pulse.

In conclusion, we applied the power algorithm using Chebyshev operator polynomials to determine wave functions $\Psi_n(x)$ and energy levels E_n of bound states of one-dimensional potentials with accuracy sufficient for their use as initial conditions $\Psi(x,t = -\infty) = \Psi_n(x)$ of the time-dependent Schrödinger equation. We have shown that the increase in polynomial degree *m* results in the faster convergence of the power method: the number of iterations required to achieve the specified accuracy decreases rapidly. However, the number of operations *km* of calculating the Hamiltonian decreases much more slowly, and saturates at $m \geq 8$. Thus, using Chebyshev polynomials of degree higher than eight in the power method for finding bound states appears redundant.

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