A truncated shift–operator technique for the calculation of resonances in Stark systems

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Abstract. A novel method is presented which allows a fast computation of complex energy resonance states in Stark systems, i.e. systems in a homogeneous field. The technique is based on the truncation of a shift–operator in momentum space. Numerical results for space periodic and non-periodic systems illustrate the extreme simplicity of the method.

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Systems in static homogeneous fields appear in many cases in atomic, molecular and solid state physics [1]-[3]. At present, one observes a renewed interest stimulated by dynamical studies of systems, where in addition to the static field the system is affected by a strong time dependent fields [4]-[6].

In the present letter, we confine ourselves to the discussion of a new and extremely simple method for computing complex energy resonance states in such systems. In previous studies complex energy resonances in Stark systems have been almost exclusively calculated by means of complex scaling techniques (see, e.g., [1, 7]). Here we present an alternative method, which seems to be conceptually different and in several aspects also more simpler in numerical applications.

To be specific, we discuss as an illustrating example a system with a single degree of freedom

$$H = H_0 + fx = \frac{p^2}{2} + V(x) + fx \quad \text{with} \quad V(x+L) = V(x)\,, \tag{1}$$

i.e. a periodic potential in a static field ($f > 0$). This setup is well known in solid state physics, but it is also of interest in recent studies of atoms interacting with standing wave fields. In the latter case, the potential is often also modulated in time, e.g. time periodic. We comment on this time dependent case in the concluding remarks below.

It is well known that the field term fx in the time dependent Schrödinger equation

$$\mathrm{i}\hbar\partial_t|\psi(t)\rangle = H|\psi(t)\rangle \tag{2}$$

can be removed by a gauge transformation to the momentum frame

$$|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}fxt/\hbar}|\widetilde{\psi}(t)\rangle = S(t)|\widetilde{\psi}(t)\rangle\,, \tag{3}$$

where

$$i\hbar\partial_t|\widetilde{\psi}(t)\rangle = \widetilde{H}_0(t)|\widetilde{\psi}(t)\rangle \tag{4}$$

with the Hamiltonian

$$\widetilde{H}_0(t) = S^\dagger(t)H_0S(t) = \frac{1}{2}(p - ft)^2 + V(x)\,, \tag{5}$$

which is explicitly time dependent. We note, that $S(t)$ acts as a shift–operator in momentum space ($p = \hbar k$):

$$S(t)|k\rangle = |k - ft/\hbar\rangle\,. \tag{6}$$

The time evolution operators U and $\widetilde{U}$ for a time interval $(0, T)$ are related by

$$U(T, 0) = S(T)\widetilde{U}(T, 0)\,. \tag{7}$$

In addition one can easily see that

$$\widetilde{U}(\nu T, 0) = \mathrm{e}^{+i\nu f x T/\hbar}\left\{S(T)\widetilde{U}(T, 0)\right\}^\nu \tag{8}$$

and, of course,

$$U(\nu T, 0) = U^\nu(T, 0) \tag{9}$$

because the Hamiltonian (1) is time independent.

The Hamiltonian (5) is periodic in space. But as the displacement operator $D(L) = \exp(L\,\partial/\partial x)$ over a period L does not commute with the shift operator $S(T)$, generally $U(T, 0)$ and $D(L)$ do not commute. We have

$$S(T)D(L) = \mathrm{e}^{-ifLT/\hbar}D(L)S(T) \tag{10}$$

and the commutator is

$$[S(T), D(L)] = \left(1 - \mathrm{e}^{ifLT/\hbar}\right)\mathrm{e}^{-ifLT/\hbar}D(L)\,. \tag{11}$$

We observe that both operators commute if the condition

$$\frac{fTL}{\hbar} = 2\pi q\ ,\ \ q = 1,\ 2,\ 3,\ldots \tag{12}$$

is satisfied.

In the following we choose $q = 1$, i.e. a time $T = 2\pi\hbar/fL$, the so-called Bloch period. In this case $[D(L), U(T, 0)] = 0$ and Floquet–Bloch theory can be applied to construct the resonance states, i.e. the eigenstates of the Floquet operator satisfying

$$U(T, 0)|\psi_\alpha\rangle = \lambda_\alpha|\psi_\alpha\rangle = \mathrm{e}^{-i\epsilon_\alpha T/\hbar}|\psi_\alpha\rangle \tag{13}$$

with purely outgoing boundary conditions, i.e. we are interested in solutions, which vanish for $x \to +\infty$ and are purely outgoing for $x \to -\infty$. These are resonance states with complex resonance energies $\epsilon_\alpha = E_\alpha - i\Gamma_\alpha/2$ and decay as

$$\psi_\alpha(nT) = \mathrm{e}^{-in\epsilon_\alpha T/\hbar}|\psi_\alpha\rangle \tag{14}$$

with a lifetime $\tau = \hbar/\Gamma_\alpha$. We point out, that the quasienergy resonances are defined modulo $2\pi\hbar/T = fL$ and we take representative values in the first 'Brillouin zone', where the real part of ϵ_α is in the interval $[-fL/2, +fL/2]$.

It is convenient to carry out the calculations in the momentum representation with an equidistant set of plane wave basis states

$$\langle x|n\rangle = \frac{1}{\sqrt{L}}\,\mathrm{e}^{\mathrm{i}n\,\Delta k\,x} \qquad n = 0,\,\pm 1,\,\pm 2,\ldots \tag{15}$$

with

$$\Delta k = fT/\hbar = 2\pi/L. \tag{16}$$

The shift–matrix is

$$\langle m|S(T)|n\rangle = \langle m|n-1\rangle = \delta_{m,n-1}\,, \tag{17}$$

where the plane wave states are normalized to unity in a period L. Numerically, the time evolution matrix $\widetilde{U}(T,0)$ is calculated by, e.g.,

$$\widetilde{U}(T,0) \approx \prod_{j=1}^{J} \exp\left[-\mathrm{i}\widetilde{H}_0(t_j - \Delta t/2)\,\Delta t/\hbar\right] \tag{18}$$

(with $t_j = j\Delta t = jT/J$) or any other appropriate method.

We now look at the effect of finite basis sets, i. e. of truncating the matrices $S(T)$ and $\widetilde{U}(T,0)$ at $|n| \le N$. First we observe, that the $(2N+1)\times(2N+1)$–matrix $S(T)$ has non-zero entries only on a diagonal, which is shifted by one unit to the upper right. A direct consequence of the truncation is that the eigenvectors $|\psi_\alpha\rangle$ of the truncated system $U(T,0) = S(T)\,\widetilde{U}(T,0)$ automatically satisfy the boundary condition for the resonances states in momentum space, i.e. the components are zero at $k = -\Delta k n_{\mathrm{nmax}}$.

Then the eigenvalues λ_α and eigenvectors of the Floquet matrix $F(T) = U(T,0)$ yield the resonance energies

$$\epsilon_\alpha = E_\alpha - \frac{\mathrm{i}}{2}\Gamma = \mathrm{i}\frac{\hbar}{T}\ln\lambda\,, \tag{19}$$

more precisely, the desired resonance energies are found among the $2N+1$ eigenvalues of the truncated matrix, typically as those energies ϵ_α with the smallest imaginary parts.

Before discussing further details, we will present results of numerical calculations for an illustrating model system

$$H = H_0 + fx = \frac{p^2}{2} + \cos x + fx \tag{20}$$

with parameters $\hbar = 0.5$ and $f = 0.2$, i.e. Bloch period $T = 2.5$. In this case, the matrix elements of the Hamiltonian $\widetilde{H}_0$ are

$$\langle m|H_0|n\rangle = (n\hbar\Delta k - ft)^2\delta_{mn}/2 + V_{mn} \tag{21}$$

with

$$V_{mn} = \frac{1}{2}(\delta_{m,n+1} + \delta_{m,n-1})\,. \tag{22}$$

For the time propagation (18) $J = 256$ steps are used and the matrices are truncated at $N = 30$. It is instructive to look at the iterates $U^\nu(T,0) = U(\nu T,0)$ of the matrix $U(T,0)$. Initially, this matrix is almost diagonal. With increasing ν, due to the static field this diagonal contribution moves to the upper right (in the direction of the outgoing wave) until it disappears for $\nu > N$. In contrast to this the contribution of the resonance states is not shifted by the external field but stays in the center of the matrix. Figure 1 shows an image of the $U^\nu(T,0)$ for $\nu = 20$ (dark regions correspond to large values of the matrix elements), where the shifted diagonal and the contributions of the resonances are clearly visible.

In order to find the complex energy resonances, we now compute the eigenvalues λ_α of $U(T,0)$. This yields 61 eigenvalues ϵ_α. For large enough N, we expect the 'true' resonances to be stable with respect to an increase of N. In order to explore this behavior, we have repeated the computation for $N = 40$ and 50. The results are shown simultaneously in Figure 2 in the complex $\lambda = \exp(-\mathrm{i}\epsilon)$ plane. Firstly, because all resonances are decaying states, the λ_α appear inside the unit disk $\lambda_\alpha \leq 1$. Secondly, we observe a number of resonances (the 'true' ones), which are identical in all three cases. The other ones are distributed in the vicinity of a radius $|\lambda| \approx 0.4$ and appear otherwise quite erratic. With increasing N more of these 'false' resonances appear (in addition, more very unstable 'true' may be detected). The two classes can be quite easily distinguished because the 'false' ones are very sensitive against variation of N or other system parameters, as, e.g., the number of time intervals chosen for the numerical computation of $\tilde{U}(T,0)$.

In Table 1 twelve 'true' eigenvalues are listed in comparison with resonance energies obtained by means of exterior complex scaling [8] (the real part is chosen in the first Brillouin zone $[-f\pi, f\pi]$). The agreement is excellent. In addition, we want to emphasise the simplicity of the computational encoding and the reliability of the method even for small basis sets N and only few time steps J. The following MATLAB program

```
f=0.2; hbar=0.5; J=5; N=10;
  M=2*N+1;
  n=1:M; p=hbar*(n-N-1);
  U=eye(M); d=0.5*ones(1,M-1);
  for j=1:J
    h=(p-hbar*(j-0.5)/J ).^2/2;
    U=expm(-i*(diag(h,0)+diag(d,-1)+diag(d,1))/J/f)*U;
  end
S=spdiags(ones(M,1),1,M,M);
D=eig(S*U);
D(length(D))=[];
D= i*log(D);
[a,In]=sort(-imag(D));
E = D(In)*f
```

uses $N = 10$ and $J = 5$ and produces resonances (ordered with respect to increasing imaginary part), where the first six resonances are already in good agreement with the converged ones listed in the table (e.g. one obtains $\epsilon_5 = 0.45059 - \mathrm{i}\,0.26922$ compared to the exact result $\epsilon_5 = 0.45054323 - \mathrm{i}\,0.26932098$).

The discussed method also suggests a simple calculation of the eigenstates associated with the complex energies ϵ_α. Using the Floquet time-dependent eigenstates

$$U(t,0)\,|\psi_\alpha(0)\rangle = \mathrm{e}^{-\mathrm{i}\epsilon_\alpha t/\hbar}\,|\psi_\alpha(t)\rangle, \quad |\psi_\alpha(T)\rangle = |\psi_\alpha(0)\rangle \tag{23}$$

the resonance wave function is calculated by integration over one Bloch period,

$$|\Psi_\alpha(0)\rangle = \int_0^T \mathrm{d}t'\, e^{\mathrm{i}\epsilon_\alpha t'/\hbar}\, U(t',0)|\psi_\alpha(0)\rangle = \int_0^T \mathrm{d}t'\,|\psi_\alpha(t')\rangle\,. \tag{24}$$

In fact, $|\Psi_\alpha(0)\rangle$ solves the time independent Schrödinger equation which follows from

$$|\Psi_\alpha(t)\rangle = \int_0^T \mathrm{d}t'\, e^{\mathrm{i}\epsilon_\alpha t'/\hbar}\, U(t+t',0)|\psi_\alpha(0)\rangle = e^{-\mathrm{i}\epsilon_\alpha t/\hbar}|\Psi_\alpha(0)\rangle\,. \tag{25}$$

As an example, the wave functions $|\langle x|\Psi_\alpha\rangle|^2$ of the four most stable resonances of the system (20) are shown in figure (3).

In the rest of the paper we discuss some possible extension of the proposed method. Though designed for space periodic Hamiltonians H_0, the method can also be applied to non-periodic ones with $V(x)\to 0$ for $|x|\to\infty$, provided that their Fourier transform exists. In the plane wave basis (15) with a fixed value of Δk, the system is periodic in the periodicity interval $-L/2 \le x \le L/2$ with $L = 2\pi/\Delta k$. If Δk is chosen small enough, the effects of this artificial periodicity will be neglectable.

As an example, we calculate the resonances for the Gaussian well

$$H = H_0 + fx = \frac{p^2}{2} - A\,\mathrm{e}^{-x^2} + fx \tag{26}$$

with $A = 4.5$, $f = 1.0$ and $\hbar = 1.0$, which has been studied using complex scaling techniques [1]. Here, the matrix elements (22) must be replaced by

$$V_{m,n} = \frac{\sqrt{\pi}}{L}\,\mathrm{e}^{-(n-m)^2\Delta k^2/4}\,. \tag{27}$$

In the computation we used $\Delta k = 1/3$ and $N = 45$. The three most stable resonances are obtained as $\epsilon_0 = -3.2978304 - \mathrm{i}\,4.467066\cdot 10^{-4}$ $\epsilon_1 = -1.460431 - \mathrm{i}\,3.48173\cdot 10^{-1}$ and $\epsilon_2 = +3.01610 - \mathrm{i}\,9.392\cdot 10^{-1}$. The lowest one was reported earlier [1] as $\epsilon_0 = -3.297830 - \mathrm{i}\,4.467\cdot 10^{-4}$, in good agreement with the present result.

In conclusion, we have demonstrated that the truncated shift–matrix technique offers a useful tool for calculating resonances in periodic or non-periodic systems in homogeneous fields. The method can also be applied to systems with more than one degree of freedom. In addition, we would like to point out, that it is also possible to treat explicitly time periodic systems in the same manner, provided that the Bloch period is an integer multiple of the time period. More detailed studies will be reported elsewhere [9].

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Table 1. Resonances for the system (20) ($\hbar = 0.5$, $f = 0.2$) in comparison with results by exterior complex scaling (cs) [8]. The 12 most stable resonances are shown.

α	E_α	$\Gamma_\alpha/2$	$E_\alpha^{\rm cs}$	$\Gamma_\alpha^{\rm cs}/2$
0	-0.15286770	-3.2363851 e-09	-0.15286771	-3.2363488 e-09
1	0.30482723	-2.3630620 e-06	0.30482722	-2.3630619 e-06
2	-0.54109934	-6.0492101 e-04	-0.54109935	-6.0492101 e-04
3	-0.20212214	-2.4735698 e-02	-0.20212215	-2.4735698 e-02
4	0.10823440	-1.3081073 e-01	0.10823439	-1.3081072 e-01
5	0.45054323	-2.6932098 e-01	0.45054319	-2.6932097 e-01
6	-0.43656584	-3.8817725 e-01	-0.43656579	-3.8817729 e-01
7	-0.00657671	-4.7856857 e-01	-0.00657664	-4.7856836 e-01
8	0.48274813	-5.6308779 e-01	0.48274215	-5.6309761 e-01
9	-0.32533902	-6.2769474 e-01	-0.32545833	-6.2766418 e-01
10	2.29998451	-6.2836674 e-01	0.29992308	-6.2835297 e-01
11	-0.16091033	-6.5406891 e-01	-0.16071272	-6.5393565 e-01

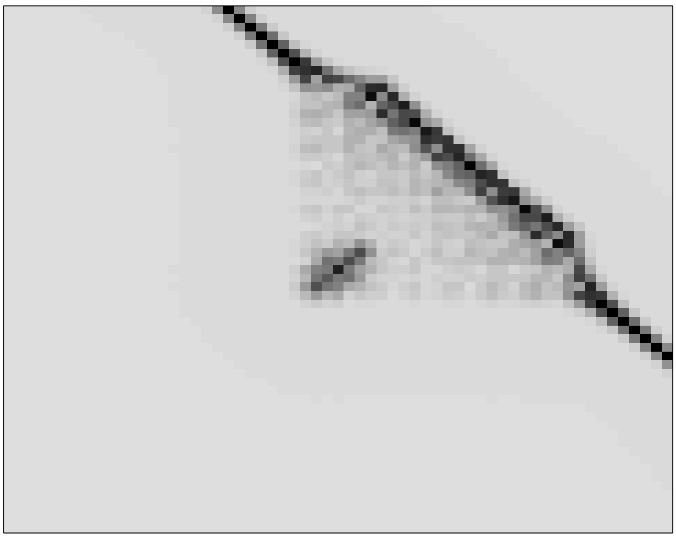

Figure 1. Image of the matrix $U^\nu(T,0) = U(\nu T, 0)$ ($\nu = 20$, $N = 30$) for the periodic potential (20). Dark regions mark large values of the matrix elements. The resonances manifest inside the dark region in the center.

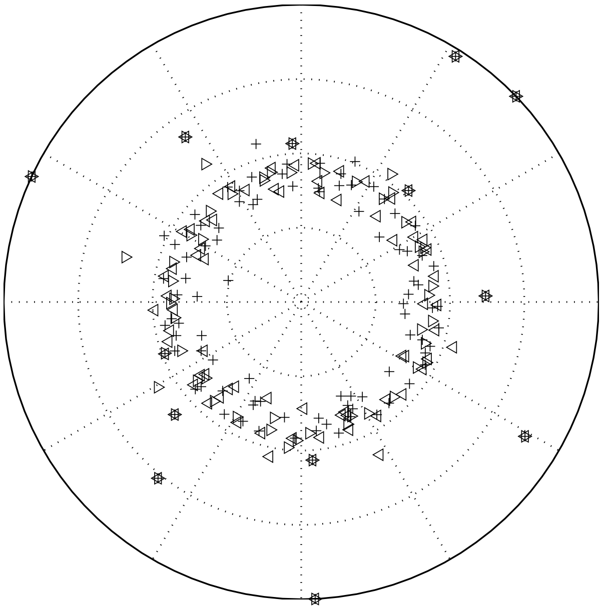

Figure 2. Complex energy resonances ϵ_α for the periodic potential (20) for $f = 0.2$, $\hbar = 0.5$ in the complex $\lambda = \exp(-\mathrm{i}\epsilon T/\hbar)$ plane (for a clearer presentation the radial coordinate is scaled as $|\lambda|^f$). Results obtained from different values of the N are shown simultaneously ($N = 30$ ($\triangleleft$), $N = 40$ ($\triangleright$), $N = 50\,(+)$). The 'true' resonances are identified by coincidence.

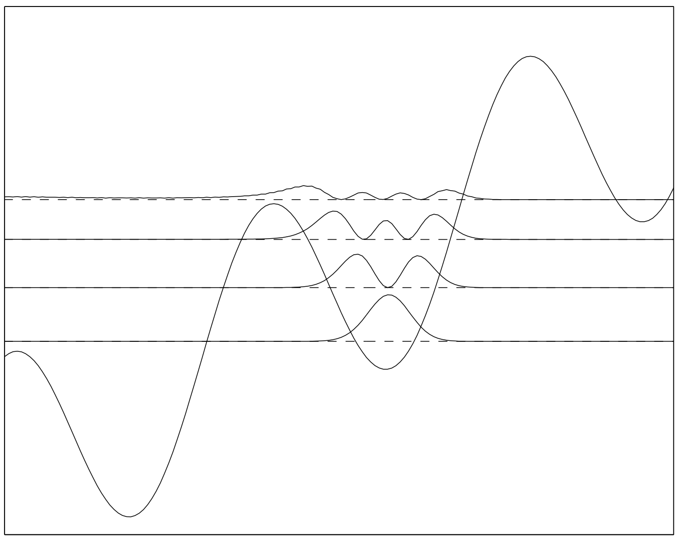

Figure 3. Resonance wave functions $\psi_\alpha(x)$ for the four most stable states $\alpha = 0, 1, 2, 3$ for the cosine potential in a homogeneous field (20). Parameters are the same as in Fig. (2) and Tab. (1). Shown are $|\psi_\alpha(x)|^2$, the energy levels (dashed lines) and the potential. The state $\alpha = 3$ is already located above the barrier.