Spurious localized highest-frequency modes in Schrödinger-type equations solved by finite-difference methods

T.I. Lakoba*

Department of Mathematics and Statistics, 16 Colchester Ave.,
University of Vermont, Burlington, VT 05401, USA

July 14, 2013

Abstract

High-frequency solutions of one or several Schrödinger-type equations are well known to differ very little from the plane wave solutions $\exp[\pm ikx]$. That is, the potential terms impact the envelope of a high-frequency plane wave by only a small amount. However, when such equations are solved by a finite-difference method, the highest-frequency solutions may, under certain conditions, turn out to be localized. This may puzzle the researcher and suggest that the code may have an error. However, this is not an error but a numerical artifact, and in this note we explain it.

Keywords: Finite-difference methods, Eigenvalue problems, High-frequency modes.

*tlakoba@uvm.edu, 1 (802) 656-2610

The stationary Schrödinger equation is a fundamental model of quantum mechanics. Coupled Schrödinger-type equations also arise in many areas of physics, e.g., in quantum mechanics [1, 2, 3] and in studies of stability of nonlinear waves (solitons) [4]. Often, the problem is posed as an eigenvalue problem whereby localized eigenfunctions and their eigenvalues are sought. The eigenfunction localization occurs due to the presence of potential-like terms (e.g., the second term in Eq. (1) below). A simple approach of solving such an eigenvalue problem is to discretize the equations by a finite-difference scheme and then solve the resulting matrix eigenvalue problem by a commercial software, e.g., Matlab or Fortran. Then, by inspection or otherwise, one selects the localized eigenfunctions and their eigenvalues out of a set of eigensolutions produced by the software.

High-frequency solutions are, typically, *not* sought numerically because their approximate analytical form can be found by perturbation methods, e.g., by the Born or Wentzel–Kramers–Brillouin (WKB) approximations. For example, for a single Schrödinger equation

$$-d^2\psi/dx^2 + V(x)\psi = \lambda\psi, \qquad \lambda > 0, \tag{1}$$

where $\lambda \gg 1$ and $V(x)$ varies on the scale of order one and also $\max|V(x)| = O(1)$, the latter approximation yields:

$$\psi(x) = \left(\frac{\lambda}{\lambda - V(x)}\right)^{1/4} \exp\left[\pm i\left\{\sqrt{\lambda}x - \frac{1}{\sqrt{\lambda}}\int V(x)\,dx\right\}\right]\left(1 + O\left(\frac{1}{\sqrt{\lambda}}\right)\right). \tag{2}$$

Another reason why high-frequency solutions are rarely solved for numerically is that this is computationally expensive. Indeed, according to an empirical rule (see, e.g., Sec. 4.1 in [5] and the end of this paper), one needs about 10 grid points per wavelength to resolve a solution accurately.

While not interested in the numerically obtained high-frequency solutions per se, the researcher may want to inspect them in order to verify that at least in the high-frequency limit, his/her finite-difference code produces reasonable results. The highest-frequency mode resolved on a grid with a step size h has a wavelength $2h$. That is, such a mode has only 2 grid points per wavelength, not 10, as needed per the aforementioned empirical rule. Therefore, one does not expect that such a mode can be resolved with any quantitative accuracy. However, one does expect that it should *qualitatively* look like solution (2): its envelope is to be a finite constant away from the localized potential $V(x)$ and is to have a small "wiggle" around the potential. If the code produces *qualitatively different* profiles of high-frequency modes, the researcher may (and perhaps should) question the correctness of the code and search for a mistake. This can be a time-consuming task when a system of several coupled equations is considered. Thus, it is valuable to know what the highest-frequency modes obtained by a finite-difference method can look like.

Below we show that such modes look not at all as described in the previous paragraph. Rather, their envelopes are the *lowest*-frequency eigenfunctions of the potential $-V(x)$. In short, this occurs because the finite-difference approximation to d^2/dx^2 in (1) evaluated on the highest-frequency carrier $\exp[ikx]$ with $k = \pi/h$ becomes "const $- d^2/dx^2$"; note the change of sign in front of the second derivative. Observing localized envelopes of the numerically obtained highest-frequency

modes may be even more counterintuitive given that they occur for a repulsive potential ($V(x) > 0$). Indeed, such potentials are known from the undergraduate courses of quantum mechanics *not* to support bound states (i.e., localized solutions of (1)); it is attractive potentials ($V(x) < 0$) that support bound states.

While we observed the spurious high-frequency eigenfunctions with localized envelopes when numerically solving a certain *system* of coupled Schrödinger-type equations, below we chose to present an explanation for a *single* equation (1), so that the complexity of the problem would not obfuscate the essence of the explanation. We emphasize that spurious localized highest-frequency eigenmodes can be observed in *any* Schrödinger-type eigenvalue problem[1] where the differential operator is approximated by finite differences. Whether such localized numerical eigenmodes *are* observed depends on the sign(s) of the potential term(s), as illustrated below for Eq. (1).

As a finite-difference approximation of (1) in our example, we use the simple central difference scheme:

$$\big(\psi(x_{n+1}) - 2\psi(x_n) + \psi(x_{n-1})\big)/h^2 = \big(V(x_n) - \lambda\big)\,\psi(x_n), \tag{3}$$

where $x_{n\pm1} = x_n \pm h$. Using a more accurate Numerov's scheme [1], where the right-hand side of (3), $\mathrm{RHS}(x_n)$, is replaced with

$$\frac{1}{12}\big(\,\mathrm{RHS}(x_{n-1}) + 10\cdot\mathrm{RHS}(x_n) + \mathrm{RHS}(x_{n+1})\,\big),$$

leads to the same qualitative conclusions.

The matrix eigenvalue problem (3) can be solved by a commercial software; below we show the details using Matlab. The following code computes the four highest-frequency modes and the corresponding eigenvalues of Eq. (1) with $V(x) = 3\,\mathrm{sech}(0.5x)$ and periodic boundary conditions:

```
h=0.1; x=-16:h:16-h; N=length(x);
M=spdiags(repmat([-1 2 -1],N,1),[-1 0 1],N,N)/h^2 + diag(3*sech(0.5*x));
M(1,end)=-1/h^2; M(end,1)=-1/h^2;
[Evecs, Evals]=eigs(M,4,'lm'); absEvecs=abs(Evecs);
k=1; plot(x,sech(0.5*x),'--',x,absEvecs(:,k)/max(absEvecs(:,k)));
```

The envelopes of the first and fourth such modes are shown in Figs. 1(a,b); the carrier is shown in Fig. 1(c). As we have announced above, these envelopes are localized, in contrast to the slightly perturbed plane waves (2) that could have been expected naively. A calculation that explains Fig. 1 is as follows.

As Fig. 1(c) illustrates, one can take $\psi(x_n) = \exp[i\pi n]\,\phi(x_n)$. Here the factor $\exp[i(\pi/h)x_n] = \exp[i\pi n]$ accounts for the highest-frequency carrier, while $\phi(x_n)$ is assumed to vary on the x-scale of order one. Substituting this ansatz into (3), one finds:

$$\frac{4}{h^2}\phi(x) + \frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) + O(h^2) = \lambda\phi. \tag{4}$$

[1]We surmise that this is also true for other types of differential eigenvalue problems, e.g., the Dirac equation with a potential, but investigating this hypothesis is outside the scope of this short communication.

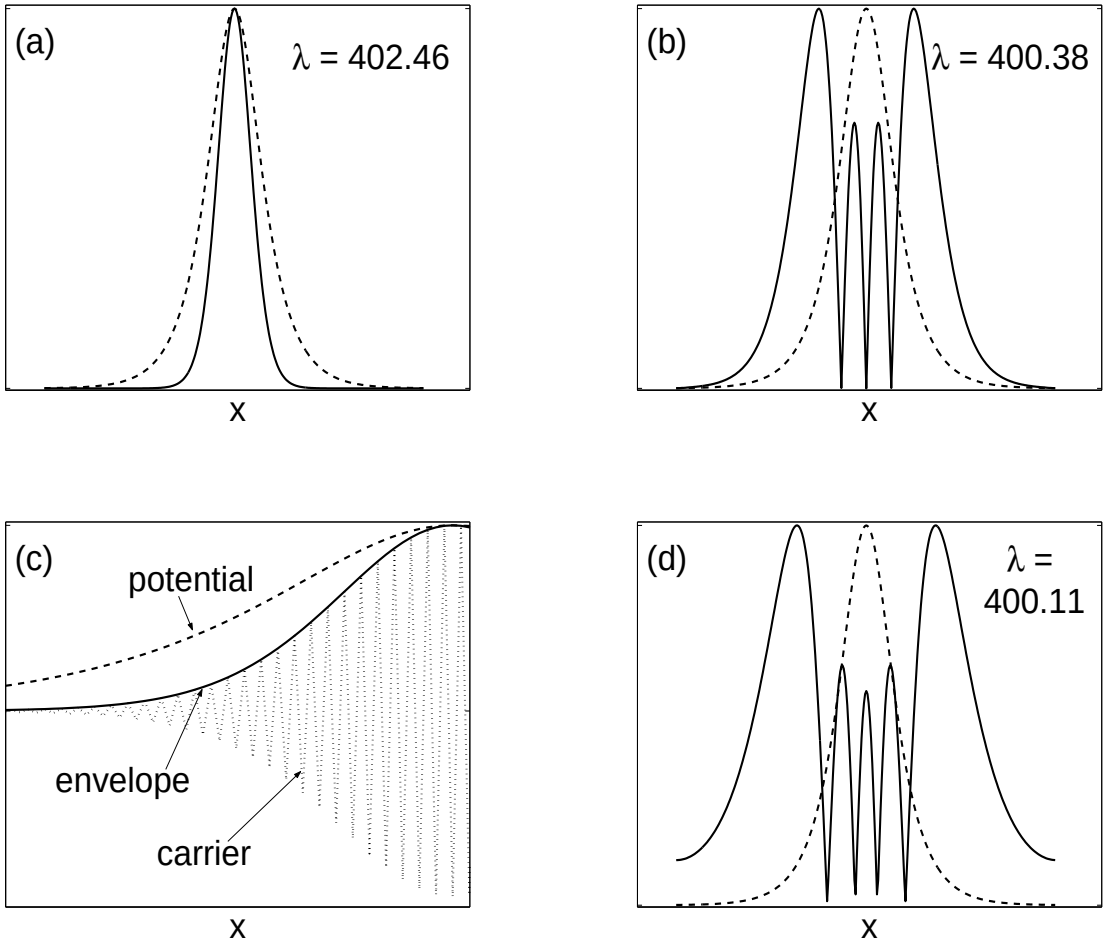

Figure 1: (a,b,d) Solid lines show envelopes of the first, fourth, and fifth highest-frequency modes obtained by the finite-difference approximation of (1) with $V = 3\,\mathrm{sech}(0.5x)$. Dashed line shows the potential $V(x)$. The corresponding eigenvalues are shown in each panel. Note that the fifth mode is essentially non-localized. (c) Part of panel (a), magnified and displaying the highest-frequency carrier.

Here $x \equiv x_n$, and we have used the Taylor expansion $\phi(x_{n\pm1}) = \phi(x) \pm h\phi'(x) + (h^2/2)\phi''(x) + O(h^3)$ for the smooth envelope $\phi(x)$. Neglecting the $O(h^2)$-term in (4), one sees that that equation becomes

$$\phi'' + (V - \Delta\lambda)\phi = 0, \qquad \Delta\lambda = \lambda - (4/h^2). \tag{5}$$

Based on (5), one can make the following conclusions about the appearance of the envelopes of the highest-frequency modes of (1) obtained by a finite-difference approximation. When the potential in the original Eq. (1) is repulsive, $V(x) > 0$ (or, more generally, $\int_{-\infty}^{\infty} V(x)\,dx > 0$), the envelope of the mode with the highest eigenvalue λ is the ground state of (5). It is localized, with the localization scale being comparable to the scale of $V(x)$, as illustrated by Fig. 1(a). For smaller λ's, one obtains consecutive excited states of (5); see Fig. 1(b). The taller and/or wider the

potential, the more high-frequency modes with localized envelopes there exist. The non-localized envelopes, corresponding to $\Delta\lambda < 0$ is (5), still have spatial features on the scale of the potential (see Fig. 1(d)).

On the other hand, for an attractive potential in (1), $V(x) < 0$, there exist no localized solutions of (5). In that case, the envelopes of all high-frequency modes are not localized. Such envelopes of the first and fifth highest-frequency modes for $V(x) = -3\,\mathrm{sech}(0.5x)$ are shown in Fig. 2.

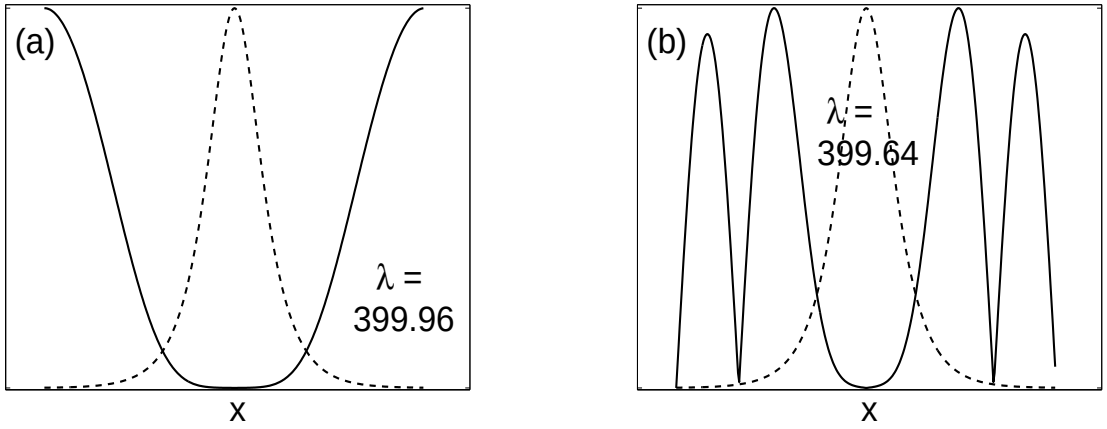

Figure 2: As in Fig. 1, solid and dashed lines show the moduli of the mode envelope and of the potential. First (a) and fourth (b) highest-frequency modes (non-localized) for the potential $V = -3\,\mathrm{sech}(0.5x)$.

As a side note, let us mention that the Matlab code presented above can be easily modified to verify the aforementioned empirical rule that one needs about 10 grid points per wavelength in order to accurately resolve an eigenmode. Replacing `3*sech(0.5*x)` with `3*sech(0.5*x)-lambda0` and the option `'lm'` of `eigs` with `'sm'` allows one to zero in on the modes with $\lambda \approx$`lambda0`. Then, decreasing `lambda0`, one can monitor when the amplitude of the "wiggle" on top of the plane wave in the eigenmode's modulus, will become about $\max V(x)/(4\lambda)$, as predicted by (2). For the parameter $h = 0.1$, selected in our numerical experiments, this occurred for $\lambda \approx 15$, which is approximately $4/(5h)^2$. If we now accept that for high-frequency modes, the eigenvalue is still approximately given by $4/(\lambda/2)^2$ (see (5), where we note that $\Delta\lambda = O(1)$ and $\lambda \gg 1$), we indeed see that $h \approx \lambda/10$ is required for accurate resolution of an eigenmode.

In conclusion, we have shown that the shape of the highest-frequency modes obtained by numerically solving the discretized eigenvalue problem for a differential operator is qualitatively different from that shape predicted by the WKB method. This difference is an artifact of the numerical discretization. Thus, visual inspection of the shape of these high-frequency numerical solutions cannot be used as a means of checking the correctness of one's code.

References

[1] B.R. Johnson, The renormalized Numerov method applied to calculating bound states of the coupled-channel Schroedinger equation, J. Chem. Phys. 69 (1978) 4678–4688.

[2] M. Teubner, Exact solution of coupled Schrdinger equations in a stationary n-state exponential model, Phys. Rev. A 74 (2006) 012704.

[3] A.A. Skorupski, Phase Integral approximation for coupled ODEs of the Schrödinger type, J. Math. Phys. 49 (2008) 053523.

[4] M. Chugunova and D. Pelinovsky, Count of eigenvalues in the generalized eigenvalue problem, J. Math. Phys. 51 (2010) 052901.

[5] K.F. Warnick and W.C. Chew, Numerical simulation methods for rough surface scattering, Waves Rand. Med. 11 (2001) R1–R30.

Figure Captions

Figure 1: Solid lines show envelopes of the first and fourth highest-frequency modes obtained by the finite-difference approximation of (1) with $V = 3\,\mathrm{sech}(0.5x)$. Dashed line show the potential $V(x)$. The corresponding eigenvalues are shown in each panel. (c) Part of panel (a), magnified and displaying the highest-frequency carrier.

Figure 2: As in Fig. 1, solid and dashed lines show the moduli of the mode envelope and of the potential. (a) The fifth (non-localized) highest-frequency mode obtained by the finite-difference approximation of (1) with $V = 3\,\mathrm{sech}(0.5x)$. (b,c) First and fourth highest-frequency modes (non-localized) for the potential $V = -3\,\mathrm{sech}(0.5x)$.