On the Q-BOR-FDTD method

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Abstract
We discuss a recently proposed approach termed Q-BOR-FDTD method and develop its main equations in a clearer and more rigorous way. We show that it is unsuitable for the calculation of the eigenfunctions in the case of degenerate states and propose an improvement to overcome such limitation.

1 Introduction
In a recent paper Firoozi et al [1] proposed a numerical approach, named quantum body of revolution finite-difference time-domain (Q-BOR-FDTD) method, for the calculation of eigenvalues and eigenfunctions of the Schrödinger equation. They applied it to a variety of simple models (some of them rather trivial) like the particle in a spherical box, the three-dimensional harmonic oscillator, the particle in a cylindrical box, a cone-like quantum dot and the spherical quantum dot with hydrogenic impurity. They obtained some of the lowest eigenvalues and eigenfunctions for each of them.

The purpose of this paper is a somewhat more rigorous discussion of the approach. In section 2 we outline the main ideas about the method; in section 3 we disclose a deficiency of the method by means of one of the examples and put

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forward an improvement; finally, in section 4 we summarize the main results and draw conclusions.

2 The Method

The purpose of this section is a more rigorous discussion of the Q-BOR-FDTD method with the purpose of disclosing some of the limitations overlooked by Firoozi et al [1].

In order to obtain the eigenvalues \( E_n \) and eigenfunctions \( \phi_n \) of a given Hamiltonian operator \( H \)

\[
H \phi_n = E_n \phi_n, \ n = 0, 1, \ldots,
\]  

(1)

Firoozi et al proposed an approach based on the equation

\[
\frac{\partial \psi(r, \tau)}{\partial \tau} = -H \psi(r, \tau).
\]  

(2)

If

\[
\psi(r, 0) = \chi = \sum_{j=0}^{\infty} c_j \phi_j, \quad \langle \phi_i | \phi_j \rangle = \delta_{ij},
\]  

(3)

then, the solution to equation (2) is

\[
\psi(r, \tau) = e^{-\tau H} \chi = \sum_{j=0}^{\infty} c_j \phi_j e^{-\tau E_j},
\]  

(4)

The main idea behind the approach is that

\[
\lim_{\tau \to \infty} \langle H \rangle = E_0, \quad \langle H \rangle = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}.
\]  

(5)

Therefore, it is only necessary to solve equation (2) for sufficiently large values of \( \tau \). To this end Firoozi et al [1] resorted to a straightforward discretization algorithm that produces \( \psi(r_i, \tau_j) \) at the points of a suitably chosen mesh. Since

\[
\frac{\partial \langle H \rangle}{\partial \tau} = 2 \left( \langle H \rangle^2 - \langle H^2 \rangle \right) < 0,
\]  

(6)

we conclude that the numerical eigenvalue should approach the exact one from above as \( \tau \) increases. This expression, which was not mentioned by Firoozi et al, is a useful test for the accuracy of the calculation.
In order to obtain the ground-state eigenfunction Firoozi et al. [1] resorted to the obvious expression

\[ \tilde{\varphi}_0 = \lim_{\tau \to \infty} \frac{\psi}{\sqrt{\langle \psi | \psi \rangle}} = \frac{c_0}{|c_0|} \varphi_0, \]  

that they wrote in a rather imprecise way. We can extend this procedure to excited states quite easily if we take into account that

\[ \psi_1 = (1 - |\tilde{\varphi}_0 \rangle \langle \tilde{\varphi}_0|) \psi = \sum_{j=1}^{\infty} c_j \varphi_j e^{-\tau E_j}, \]

that Firoozi et al also expressed unclearly. Therefore, we can repeat the procedure outlined above and obtain \( E_1 \) and \( \tilde{\varphi}_1 \) and then proceed to other excited states. Obviously, we have tacitly assumed that there are no degenerate states; that is to say: \( E_j < E_{j+1} \), \( j = 0, 1, \ldots \). Firoozi et al [1] did not pay attention to this point and applied the approach to problems with degenerate states.

Suppose that

\[ H \varphi_{n,i} = E_n \varphi_{n,i}, \quad n = 0, 1, \ldots, i = 1, 2, \ldots, g_n, \quad \langle \varphi_{n,i} | \varphi_{n',i'} \rangle = \delta_{nn'} \delta_{ii'}. \]  

In this case we have

\[ \chi = \sum_{n=0}^{\infty} \sum_{i=0}^{g_n} c_{n,i} \varphi_{n,i}, \]

and

\[ \psi(r, \tau) = \sum_{n=0}^{\infty} e^{-\tau E_n} \sum_{i=0}^{g_n} c_{n,i} \varphi_{n,i}. \]  

It is convenient to define

\[ u_n = \frac{\sum_{i=0}^{g_n} c_{n,i} \varphi_{n,i}}{\sqrt{\sum_{i=0}^{g_n} |c_{n,i}|^2}}, \quad \langle u_i | u_j \rangle = \delta_{ij}, \]

and rewrite equation (11) as

\[ \psi(r, \tau) = \sum_{n=0}^{\infty} a_n u_n e^{-\tau E_n}, \quad a_n = \sqrt{\sum_{i=0}^{g_n} |c_{n,i}|^2}. \]  

We appreciate that the approach outlined above provides the eigenvalues but not the eigenfunctions. Instead of \( \tilde{\varphi}_{n,i} \) we obtain just some linear combinations \( \tilde{u}_n \).
3 Examples

Firoozi et al [1] applied the approach to one-particle Hamiltonian operators of the form

$$H = -\frac{1}{2} \nabla^2 + V(x, y, z),$$  \hspace{1cm} (14)

where, for simplicity, we have resorted to a suitable dimensionless form [2]. They proposed an improvement in the case of rotationally-invariant potentials $V(x, y, z) = V(\rho, z)$, $\rho = \sqrt{x^2 + y^2}$, and chose $\psi(r, \tau) = U(\rho, z, \tau)e^{im\phi}$, $m = 0, \pm 1, \ldots$. Therefore,

$$\frac{\partial U(\rho, z, \tau)}{\partial \tau} = \left[ -\frac{1}{2\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{m^2}{2\rho^2} - \frac{1}{2} \frac{\partial^2}{\partial z^2} + V(\rho, z) \right] U(\rho, z, \tau).$$  \hspace{1cm} (15)

It is quite obvious that in this way one gets rid of the degeneracy of the problems with this kind of symmetry. However, they applied this approach to spherically symmetric models $V(x, y, z) = V(r)$, $r = \sqrt{x^2 + y^2 + z^2}$, and, consequently, they failed to remove the degeneracy completely. For example, in the case of the harmonic oscillator $V(r) = \frac{1}{2} r^2$ the energy levels are

$$E_n = n + \frac{3}{2}, \quad n = n_x + n_y + n_z, \quad n_x, n_y, n_z = 0, 1, \ldots, \quad g_n = \frac{(n + 1)(n + 2)}{2}. \hspace{1cm} (16)$$

For the ground state $g_0 = 1$ and they obtained the correct wavefunction that depends only on $r$. However, for the first two excited energy levels they showed only one eigenfunction for each of them when there are $g_1 = 3$ and $g_2 = 6$.

For example, for $n = 1$ we have the following eigenfunctions

$$\varphi_{1, \pm 1} = \frac{re^{-r^2/2} \sin(\theta)}{\pi^{\frac{1}{4}}} e^{\pm i\phi},$$

$$\varphi_{1, 0} = \frac{\sqrt{2}re^{-r^2/2} \cos(\theta)}{\pi^{\frac{1}{4}}}. \hspace{1cm} (17)$$

Note that, even when removing the dependence on $\phi$, they still depend on the other angle $\theta$. Surprisingly, Firoozi et al [1] plotted wavefunction vs $R(nm)$ in their figure 2. If we assume that $R$ stands for the radial variable $r$ there is something else amiss because the plot range is $0 \leq R \leq 0.4$ when one of the calculations was carried out with a mesh size of $0.4 \text{ nm}$. Besides, those authors
suggest that their calculation provides $U(\rho_i, z_j, \tau_k)$ which casts doubts on those plots of wavefunction vs $R$ because the eigenfunctions (17) exhibit an angular dependence.

In order to improve the approach in the case of spherically-symmetric potentials we may choose $\psi(x, y, z, \tau) = R_l(r, \tau)Y_m(\theta, \phi)$, where $Y_m(\theta, \phi)$ are the spherical harmonics and $l = 0, 1, \ldots, m = 0, \pm 1, \ldots, \pm l$ the rotational quantum numbers. The radial factor $R_l(r, \tau)$ is a solution to the equation

$$\frac{\partial R_l(r, \tau)}{\partial \tau} = \left[ -\frac{1}{2r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{l(l+1)}{2r^2} + V(r) \right] R_l(r, \tau),$$

(18)

and we can apply the approach safely because there are no degenerate states left.

4 Conclusions

Throughout this paper we have reviewed a recently proposed approach termed Q-BOR-FDTD method [1] and developed the main equations in a clearer and more rigorous way. It has been shown that, although it provides the eigenvalues, it fails to yield the eigenfunctions in the case of degenerate states. This shortcoming affects the application of the method to the spherically-symmetric potentials exhibited by some of the examples chosen by the authors. For this reason, one may reasonably cast doubts on the validity of some of their results. We have shown how to overcome this difficulty by means of a simple and straightforward strategy that generalizes and improves the one proposed by the authors.

References

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