Comment on "Three-dimensional kicked hydrogen atom"

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In a recent paper, Klews and Schweizer [Phys. Rev. A **64**, 053403 (2001)] presented a computational method for the three-dimensional propagation of wave packets in the hydrogen atom driven by a train of short unidirectional electric-field pulses. They argued that their computational scheme is valid for an arbitrary value of the pulse strength. We show, however, that such a scheme leads to both mathematical and physical inconsistences when strong pulses are considered, and, consequently, its validity is limited to the case of weak fields. The generalization to the case of an arbitrary pulse strength is also commented.

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In the recent work [1], an alternative method based on space discretization techniques has been proposed for the treatment of the three-dimensional kicked hydrogen atom. The Hamiltonian of the kicked hydrogen atom can be written in atomic units as [see Eq. (1) in Ref. [1]]

$$H=H_0+\mathbf{r}\cdot\mathbf{F}\sum_{k=0}^{S-1}\delta(t-kT),\qquad H_0=\frac{p^2}{2}-\frac{1}{r},\tag{1}$$

where S is the number of kicks applied, T its period, F is the external field, and H_0 is the Hamiltonian of the field-free hydrogen atom. As between the pulses, the evolution of the wave packet is field-free, Klews and Schweizer [1] implemented a finite-element technique combined with a Cayley expansion of the field-free time propagator $e^{-iH_0\delta t}$ for the wave-packet propagation between two consecutive kicks. For details on this scheme of field-free propagation of wave packets the reader can also consult Ref. [2]. The action of the kicks is incorporated by connecting the wave function immediately before the pulse with the wave function directly after the pulse. The time integration of the kicked system determined by Eq. (1) is then performed by repeating this procedure for each pulse, as represented in Fig. 1 of Ref. [1]. The relation that connects the wave function right before the pulse with the wave function immediately after the pulse is obtained by a direct integration of the formal solution of Hamiltonian (1)

$$\psi(\mathbf{r},t)=e^{-itH_0}\psi(\mathbf{r},0)+\int_0^t e^{-i(t-s)H_0}(-i\mathbf{F}\cdot\mathbf{z})\psi(\mathbf{r},s)\times\delta(s-T)ds.\tag{2}$$

Thus, Klews and Schweizer [1] integrated Eq. (2) and after an *inappropriate* use of the so-called sifting property of the Dirac δ function

$$\int_0^t f(s)\,\delta(s-T)ds=\begin{cases}0 & \text{if } t<T\\ \frac{1}{2}f(T) & \text{if } t=T\\ f(T) & \text{if } t>T,\end{cases}\quad (T>0)\tag{3}$$

they obtained the following relation:

$$\psi(T_+)=\left(1+\frac{i}{2}\mathbf{F}\cdot\mathbf{z}\right)^{-1}\left(1-\frac{i}{2}\mathbf{F}\cdot\mathbf{z}\right)\psi(T_-),\tag{4}$$

with $\psi(T_-)$ and $\psi(T_+)$ representing the wave functions immediately before and right after the pulse applied at $t=T$, respectively. The authors then argued that Eq. (4) [i.e., Eq. (11) in Ref. [1]] "describes exactly the influence of a δ pulse onto the wave function independently from the strength F of this pulse." A more careful analysis, however, reveals that when the pulse strength F is not small, Eq. (4) [i.e., Eq. (11) in Ref. [1]] is inconsistent from both physical and mathematical point of views. Indeed, in the limit of very large pulse strength $F\to\infty$ one has, roughly speaking, that Eq. (4) leads to $|\langle\psi(T_+)|\psi(T_-)\rangle|^2\to 1$, which basically means that for strong enough fields the system behaves as if no pulse was applied. Such a behavior is paradoxical from the physical point of view.

From the mathematical point of view, the procedure for obtaining Eq. (4) by using identity (3) is, in general, inappropriate. The use of this identity requires the continuity of the sub-integral function $f(s)$ at the point $s=T$ (see, e.g., Refs. [3–5]), something that is in clear contradiction with Eq. (4), where a discontinuity of the wave function at $t=T$ is observed. We stress that, actually, the nature of the problem itself requires the wave function to have discontinuities at the moment of application of each pulse. However, for weak enough pulses, the discontinuity of the wave function becomes small [$\psi(T_+)\approx\psi(T_-)$] and the application of Eq. (3) is justified. Nevertheless, it is worth remarking that, contrary to the statements of the authors in Ref. [1], Eq. (4) does not describe exactly the influence of a δ pulse onto the wave function. It is just an approximation that is only justified for weak pulses. We note that the authors of Ref. [6] also made an inappropriate use of the sifting property of the Dirac δ function in their analysis of a kicked nonlinear two-level system. Consequently, the validity of the results in Ref. [6] is also limited to the weak-field regime.

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The correct relation that connects the wave function right before the pulse $[\psi(T_-)]$ with the wave function immediately after the pulse $[\psi(T_+)]$ can be straightforwardly found by observing that the operator $U(T_+,T_-)$ describing the evolution from $\psi(T_-)$ to $\psi(T_+)[\psi(T_+)=U(T_+,T_-)\psi(T_-)]$ is given by

$$U(T_+,T_-)=\exp\left[-iH_0(T_+-T_-)-i\mathbf{F}\cdot\mathbf{z}\int_{T_-}^{T_+}\delta(t-T)dt\right]. \tag{5}$$

In the limit $(T_+-T_-)\rightarrow 0$, Eq. (5) reduces to

$$U(T_+,T_-)=e^{-i\mathbf{F}\cdot\mathbf{z}}, \tag{6}$$

and, consequently,

$$\psi(T_+)=e^{-i\mathbf{F}\cdot\mathbf{z}}\psi(T_-). \tag{7}$$

The equation above is free of physical inconsistences and is the correct one that exactly describes, instead of Eq. (4), the influence of a δ pulse onto the wave function, independently of the value of its strength F. In fact Eq. (7) is consistent with the expression usually considered for the evolution operator in modeling kicked atoms (see, e.g., Refs. [7,8]). One can also derive the matching condition, Eq. (7), by direct integration of the Schrödinger equation corresponding to the Hamiltonian in Eq. (1). As the wave function is not a continuous function of time at the moment of application of each pulse, it is convenient to introduce the area of the δ function as a new variable. Considering that the Dirac δ function can be represented as

$$\delta(t-T)=\begin{cases}\lim_{\epsilon\rightarrow 0}\dfrac{1}{\epsilon} & \text{for } T_-<t\leqslant T_+\\ 0 & \text{elsewhere,}\end{cases} \tag{8}$$

where $T_-=T-\epsilon/2$ and $T_+=T+\epsilon/2$, the area of the δ function as a function of time in the interval $T_-<t\leqslant T_+$ can be written as follows:

$$a(t)=\int_{T-\epsilon/2}^{t}\delta(t'-T)dt'=\frac{(t-T+\epsilon/2)}{\epsilon}. \tag{9}$$

Thus, right before and after the pulse we have $a(T_-)=0$ and $a(T_+)=1$, respectively. In terms of the new variable $a(t)$ and after performing the limit $\epsilon\rightarrow 0$, the Schrödinger equation reduces to

$$i\frac{\partial\psi}{\partial a}=\mathbf{F}\cdot\mathbf{z}\psi, \tag{10}$$

whose general solution is given by

$$\psi(a)=e^{-ia\mathbf{F}\cdot\mathbf{z}}\psi(a=0). \tag{11}$$

The correct matching condition [Eq. (7)] can then be easily obtained from Eq. (11) by taking into account that $\psi(a=0)=\psi(T_-)$ and $\psi(a=1)=\psi(T_+)$. We stress that this last procedure for integrating kicked systems is rather general and is valid even in the case of kicked nonlinear Schrödinger equations, where the expression for the evolution operator in Eq. (5) does not hold.

Concerning relation (4), the situation now is still more clear. One can notice that the evolution operator given in Eq. (4) is nothing but the result of a Cayley expansion of Eq. (6) that is correct only up to order F^2. Consequently, Eq. (4) [i.e., Eq. (11) in Ref. [1]] is only valid, as was previously commented, for pulses with small strength. This fact also explains why for $F=2\times10^{-3}$ a.u. (i.e., a weak field), the results obtained by Klews and Schweizer in Ref. [1] are in agreement with those reported by Dhar *et al.* [8] who performed a stroboscopical description of the dynamics of the kicked hydrogen atom by using an expression for the evolution operator similar to Eq. (6). The situation can drastically change, however, if intense *kicks* are considered. In the particular case of a Rydberg atom, under the action of half-cycle pulses (HCPs), the actual train of pulses can be simulated within the sudden approximation through a series of kicks where strengths $F=\Delta p$ are given by the momentum transferred to the system by the HCPs [see Eqs. (2) and (3) in Ref. [1]]. Modern laser technologies allow the generation of HCPs with field peaks of hundreds of kV/cm and durations in the picosecond and subpicosecond regimes (see, for instance, Ref. [9]). For such pulses, the transfer of momentum can be considerably large. For a Gaussian-like HCP, the transfer of momentum can be estimated by $F\approx 1.06F_0t_p$ [10], F_0 and t_p being the peak field and the full width at half-maximum of the pulse, respectively. Thus, for a pulse with $F_0=150$ kV/cm and $t_p=1$ ps the corresponding momentum transfer is given by $F\approx 1.28$ a.u. (i.e., several orders of magnitude greater than the values of F used in Ref. [1]). For such HCPs Eq. (4) is no longer valid and, in general, one has to substitute the connecting relation (4) (valid only for very weak fields) by the exact one (7) (valid for arbitrary strengths of the pulses) in order to properly describe the dynamics of wave packets in the hydrogen atom kicked by intense pulses.

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