Comments

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Further comment on "Optimization of approximate solutions to the time-dependent Schrödinger equation"

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We show that the Reply of Weglein [Phys. Rev. A 31, 4025 (1985)] to our previous Comment [Phys. Rev. A 31, 4023 (1985)] is not valid.

Recently we presented a Comment[1] (hereafter denoted as MP) where we showed some deficiencies in the optimization method developed by another author[2] in order to build approximate solutions to the time-dependent Schrödinger equation. In his reply[3] (hereafter denoted as W) the author claims that our conclusions are based on the wrong argument $\dot{N}(t_f)=0 \Longrightarrow N(t_f)=0$. That argument was never used by us.

The principal aim of MP was to alert researchers working in collisional problems about the inadequacy of the linear parametrization developed in Ref. 2, in order to minimize a non-negative functional (which is zero if the norm of the trial wave function vanishes) without normalization constraint. The problem with the method developed in Ref. 2 is that it leads to noncausal evolution, due to the final conditions $P_{\alpha_j^*}(t_f)=0$ [see Eqs. (4) and (6) of MP]. There is a set of initial $P_{\alpha_j^*}(t_i)$ which leads to the imposed mixed boundary conditions. But this set of initial values depends on the *full process,* so that the variation of the wave function is, in part, due to the future action of the perturbation V. The main consequence of this fact is the strong dependence of the approximate solution on the *initial* integration time t_i. In what follows, we shall show that the solution obtained taking t_i far away from the interaction region becomes the zero function *before the perturbation starts to work.* During the initial unperturbed evolution (between t_i and the beginning of the interaction region, in the surroundings of, say, $t=0$) the error $\langle \epsilon \mid \epsilon \rangle$ has the lower bound $| P_{\alpha_1^*}(t) |^2$ [see Eq. (7) of MP]. Since in this region $\dot{P}_{\alpha_j^*}(t)=0$ [see Eq. (4b) of MP], the lower bound is J^2 [see Eq. (9) of MP]. So, we have $\langle \epsilon \mid \epsilon \rangle \geq J^2$. If this inequality is integrated throughout its region of validity (the initial unperturbed region of extension, say, Δt) we have

$$J \geq \int_{\Delta t} dt \langle \epsilon \mid \epsilon \rangle \geq J^2 \Delta t \ , \tag{1}$$

where we have taken into account the fact that $\langle \epsilon \mid \epsilon \rangle \geq 0$ in order to obtain the first inequality. Then the inequality $J\Delta t \leq 1$ which arises from (1) shows that the deviation J can be made small enough taking t_i far away from the interaction region. In the limit $t_i = -\infty$ we have $J=0$. This result proves that, in the above limit, $\langle \epsilon \mid \epsilon \rangle = 0$ for *all times.* But there are only two functions which do not generate error in the interaction region: the exact solution and the zero function. This shows that, in every approximate calculation, the trial wave function disappears before the perturbation is turned on. As can be easily understood from the last discussion, there is no problem in the final unperturbed region (where Weglein focussed his attention). In this region there is no norm reduction in any case (whichever t_i is taken) since the trial wave function can be chosen to be an exact solution [see discussion below Eq. (10) of MP]. In the case where t_i is finite, the reduction of the norm, of course, cannot be completed and $\alpha_j \neq 0$ will be obtained. But its physical meaning cannot be seriously supported.

[1] J. M. Maidagan and R. D. Piacentini, Phys. Rev. A 31, 4023 (1985).
[2] A. B. Weglein, Phys. Rev. A 17, 1810 (1978).
[3] A. B. Weglein, Phys. Rev. A 31, 4025 (1985).

