Reply to "Comment on 'Kinetic-energy density functional for a special shape-invariant potential of a one-dimensional two-level system'"

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Reply to "Comment on 'Kinetic-energy density functional for a special shape-invariant potential of a one-dimensional two-level system' "

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We thank Jiqiang Chen and M. J. Stott for their helpful remarks [preceding Comment, Phys. Rev. A **44**, 3387 (1991)].

For a harmonic potential, which is the special shape-invariant potential discussed in our paper [1], the relation between the ground state and the first-excited-state wave functions [Eq. (2)] should be

$$\psi_1(x)=-\sqrt{2/\varepsilon}\,\psi_0'(x)\ , \tag{1}$$

and consequently, Eqs. (8)–(10) in our paper become

$$\theta'=\sqrt{\varepsilon/2}+\frac{1}{2}\frac{\rho'}{\rho}\cot\theta\ , \tag{2}$$

$$\theta''=\frac{1}{2}\left[\frac{\rho'}{\rho}\right]'\cot\theta-\frac{1}{2}\frac{\rho'}{\rho}\csc^2\theta\left[\sqrt{\varepsilon/2}+\frac{1}{2}\frac{\rho'}{\rho}\cot\theta\right]\ , \tag{3}$$

and

$$\frac{1}{2}\left[\frac{\rho'}{\rho}\right]'\cot\theta-\frac{1}{2}\frac{\rho'}{\rho}\csc^2\theta\left[\sqrt{\varepsilon/2}+\frac{1}{2}\frac{\rho'}{\rho}\cot\theta\right]+\frac{\rho'}{\rho}\left[\sqrt{\varepsilon/2}+\frac{1}{2}\frac{\rho'}{\rho}\cot\theta\right]+\varepsilon\sin(2\theta)=0\ . \tag{4}$$

Let $\tan\theta=y$ and $\rho'/\rho=\alpha$, then Eq. (11) in our paper reads

$$y^5+\frac{\sqrt{2}}{\alpha\sqrt{\varepsilon}}(\tfrac{1}{2}\alpha'+\tfrac{1}{2}\alpha^2+2\varepsilon)y^4+\tfrac{1}{2}y^3+\frac{\sqrt{2}}{\alpha\sqrt{\varepsilon}}(\tfrac{1}{2}\alpha'+\tfrac{1}{4}\alpha^2)y^2-\tfrac{1}{2}y-\tfrac{1}{4}\sqrt{2/\varepsilon}\,\alpha=0\ , \tag{5}$$

which is derived from the equality

$$\theta''+\frac{\rho'}{\rho}\theta'+\varepsilon\sin(2\theta)=0\ . \tag{6}$$

Obviously, y avoids analytical solution from the Eq. (5).

Note that we forget the point that ε is also a functional of ρ and it has effect on the analycity of y. That y is analytically inaccessible via Eq. (5) does not necessarily mean that one cannot reach the exact θ or θ'.

In fact, as pointed out by Chen and Stott in their Comment [2], there results from Eq. (2)

$$\theta'=\sqrt{2\varepsilon}\cos^2\theta\ . \tag{7}$$

Combining Eq. (2) and Eq. (7) we obtain a cubic equation for θ',

$$\theta'=\frac{\sqrt{2\varepsilon}(\theta'-\sqrt{\varepsilon/2})^2}{[\rho'/(2\rho)]^2+(\theta'-\sqrt{\varepsilon/2})^2} \tag{8}$$

which is analytically solvable.

If one neglects the analycity of the parameter ε, one may get θ' by solving Eq. (8) and then substitute it into the formula of kinetic-energy density derived from the reduced density matrix,

$$t=-\frac{1}{4}\rho''+\frac{1}{8}\left[\frac{\rho'}{\rho}\right]^2+\tfrac{1}{2}\rho(\theta')^2 \tag{9}$$

to obtain the kinetic-energy density in closed form. However, a simple form of kinetic-energy density must not contain a parameter such as ε, which is not a constant for harmonic potentials with different scalings. ε can only be expressed as a function of ρ, and the closed form satisfies our requirement. Let us consider this point now.

Taking θ' and ε as unknown, we solve Eqs. (2) and (7) and find

$$\theta'=\frac{\rho'}{\rho}\frac{\cot\theta\cos^2\theta}{\cos(2\theta)}\ , \tag{10}$$

$$\varepsilon=\frac{1}{2}\left[\frac{\rho'}{\rho}\right]^2\frac{\cot^2\theta}{\cos^2(2\theta)}\ , \tag{11}$$

thus,

$$\theta''=\left[\frac{\rho'}{\rho}\right]'\frac{\cot\theta\cos^2\theta}{\cos(2\theta)}+\left[\frac{\rho'}{\rho}\right]^2\frac{\cot\theta\cos^2\theta}{\cos^3(2\theta)}\times\{2\sin(2\theta)\cos^2\theta\cot\theta-[\cot^2\theta+\sin(2\theta)\cot\theta]\cos(2\theta)\}\ . \tag{12}$$

Substituting Eqs. (10)–(12) into Eq. (6) we have

$$0=\left[\frac{\rho'}{\rho}\right]'\frac{\cot\theta\cos^2\theta}{\cos(2\theta)}+\left[\frac{\rho'}{\rho}\right]^2\frac{\cot\theta\cos^2\theta}{\cos^3(2\theta)}\{2\sin(2\theta)\cos^2\theta\cot\theta-[\cot^2\theta+\sin(2\theta)\cot\theta]\cos(2\theta)\}$$
$$+\left[\frac{\rho'}{\rho}\right]^2\frac{\cot\theta\cos^2\theta}{\cos(2\theta)}+\frac{1}{2}\left[\frac{\rho'}{\rho}\right]^2\frac{\cot^2\theta}{\cos^2(2\theta)}\ , \tag{13}$$

which is an algebraic equation of trigonometric functions of θ and it is not analytically solvable.

Therefore, we have shown that one cannot find a closed form of the kinetic-energy density for the harmonic oscillator.

In the last paragraph of our paper, ρ'/ρ should be θ'/ρ.

[1] Jiushu Shao and John J. Stezowski, Phys. Rev. A **42**, 5767 (1990).

[2] Jiqiang Chen and M. J. Stott, preceding Comment, Phys. Rev. A **44**, 3387 (1991).