Addendum: Considerations about the incompleteness of the Ehrenfest’s theorem in quantum mechanics (2021 Eur. J. Phys. 42 065405)

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Abstract. We describe the analytical solution of the eigenvalue problem introduced in our article mentioned in the title and relative to a punctiform electric charge confined in an one-dimensional box in the presence of an electric field. We also derive and discuss the analytical expressions of the external forces acting on the punctiform charge and associated with the boundaries of the one-dimensional box in the presence of the electric field.

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1. Introduction

The additional reflections described here complement our considerations [1] on the Ehrenfest’s theorem and were inspired by the feedback we received from K. Mouloupolos‡ in a private communication. He and his colleagues also produced interesting contributions [2–4] to the Ehrenfest-theorem theme that, unfortunately and regrettably, escaped the literature survey we carried out when working on our main article [1]; our findings turn out to be in accordance with those exposed in the cited contributions which, by the way, have the valuable feature of not being restricted to spatially one-dimensional cases. Of course, the reading of this short addendum

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presupposes familiarity with our main article and we assume it acquired by the reader. In the sequel, we will use the same notation adopted therein and will make reference to its equations by subscripting the label ‘ma’ (main article); for example, equation (1)\textsubscript{ma} refers to equation (1) in the main article.

Moulopoulos’ comment regards equation (104)\textsubscript{ma} which gives the dimensional expression of the external forces due to the confining walls acting on the punctiform electric charge when the electric field is absent. As duly reported in [1, 5, 6], ter Haar [7] derived the same result in 1964 by following a different approach § and emphasized its coincidence with the classical-mechanics result. With due account of equations (94)\textsubscript{ma} and equation (100)\textsubscript{ma}, the nondimensional version of equation (104)\textsubscript{ma} reads

\[
\frac{\partial^2 \psi_k}{\partial \xi^2} - \alpha \xi \psi_k = \beta_k \tag{1}
\]

Both equation (104)\textsubscript{ma} and equation (1) indicate that, for each eigenstate, the external forces depend linearly on the energy eigenvalue when the electric field is absent. Moulopoulos’ question addresses the circumstance in which the electric field is present; in his own words:

From your later numerical results (the ones that show the several interesting extrema), do I get it correctly that this CLASSICAL relation is no more satisfied for non-zero electric fields?

He refers to the results shown in the graphs of figure 2 of [1] and definitely perceives the appropriate conclusion regarding the “CLASSICAL relation” [equation (104)\textsubscript{ma}]. Indeed, for a given eigenstate \( k \), left and right slopes of the eigenfunction differ when \( \alpha = 10, 100 \) but the energy eigenvalue is unique; therefore, the linear dependence indicated by equation (1), or equation (104)\textsubscript{ma}, must break down somehow. So, what kind of functional dependence is there between external forces and energy eigenvalue in the presence of the electric field? The quantitative answer to this question requires the analytical solution of the eigenvalue problem defined by equations (95)\textsubscript{ma}. This is indeed possible and we will deal with such a task in section 2. In section 3, we will present and discuss the consequences on the external forces that follow from the analytical solution. In section 4, we will present the analytical proof of equation (105)\textsubscript{ma}, which corroborates the numerical verification described in [1].

2. Analytical solution of the eigenvalue problem

For convenience, we rewrite here the equations (95)\textsubscript{ma}

\[
\frac{\partial^2 \psi}{\partial \xi^2} - \alpha \xi \psi = \beta \psi \tag{2a}
\]

§ More bibliographic information is provided in [1].
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\[ \psi(-1) = \psi(+1) = 0 \]  
\[ \frac{1}{2} \int_{-1}^{+1} \psi \psi \, d\xi = 1 \]  
that define the eigenvalue problem. We are interested in the situation with the presence of the electric field and, therefore, we assume \( \alpha \neq 0 \). Then, the independent-variable transformation

\[ \xi = -\frac{\eta}{\alpha^{1/3}} - \frac{\beta}{\alpha} \]  
converts the time-independent Schrödinger equation [equation (2a)] into the Airy differential equation

\[ \frac{\partial^2 \psi}{\partial \eta^2} - \eta \psi = 0 \]  
whose general solution is a linear combination of the Airy functions

\[ \psi(\eta) = A \cdot \text{Ai}(\eta) + B \cdot \text{Bi}(\eta) \]  
Next step consists in the imposition of the boundary conditions [equation (2b)]. The values of the new independent variable \( \eta \) at the left/right boundaries (\( \xi = \pm 1 \)) are obtained from equation (3) by inversion; they read respectively

\[ \hat{\eta} = -\frac{\beta - \alpha}{\alpha^{2/3}} \]  
\[ \bar{\eta} = -\frac{\beta + \alpha}{\alpha^{2/3}} \]  
Then, the imposition of equation (2b) leads to the algebraic homogeneous system

\[ \begin{cases} 
\psi(-1) \rightarrow \psi(\hat{\eta}) = A \cdot \text{Ai}(\hat{\eta}) + B \cdot \text{Bi}(\hat{\eta}) = 0 & \text{left boundary} \\
\psi(+1) \rightarrow \psi(\bar{\eta}) = A \cdot \text{Ai}(\bar{\eta}) + B \cdot \text{Bi}(\bar{\eta}) = 0 & \text{right boundary} 
\end{cases} \]  
for the coefficients \( A, B \) and its determinant’s vanishing leads to the algebraic equation

\[ \text{Ai}(\hat{\eta}) \cdot \text{Bi}(\bar{\eta}) - \text{Ai}(\bar{\eta}) \cdot \text{Bi}(\hat{\eta}) = 0 \]  
that generates the eigenvalues. Equation (8) requires a numerical solution and we found out that the Newton-Raphson method works very well for that purpose. Table 1 shows the first ten eigenvalues obtained from equation (8) for three values of the electric field \( \alpha = 10, 50, 100 \); for comparison and validation, we have included also the first four eigenvalues \( \alpha = 10, 100 \) only) produced by the finite-difference algorithm described in [1] to solve numerically the complete eigenvalue problem [equations (2)]. With the eigenvalues in hand, the algebraic homogeneous system provides one relation between the coefficients \( A, B \); if we choose to express \( B \) in terms of \( A \)

\[ B = -A \cdot w \]  
| The other way round is obviously equivalent.
Table 1. Eigenvalues calculated from equation (8) and from the numerical algorithm of [1]

| k | \( \alpha = 10 \) | \( \beta \) | \( \alpha = 50 \) | \( \beta \) | \( \alpha = 100 \) | \( \beta \) |
|---|---|---|---|---|---|---|
| 1 | 0.887711281 | 0.887711281 | -18.26699901 | -49.62700286 | -49.62700286 | -49.62700286 |
| 2 | 10.22526410 | 10.22526410 | -11.92779834 | -11.92779834 | -11.92779834 | -11.92779834 |
| 3 | 22.51062910 | 22.51062910 | 18.93712022 | 18.93712022 | 18.93712022 | 18.93712022 |
| 4 | 39.66912539 | 39.66912539 | 46.23552953 | 46.23552953 | 46.23552953 | 46.23552953 |
| 5 | 61.81196016 | 64.82933302 | 71.59210441 | 71.59210441 | 71.59210441 | 71.59210441 |
| 6 | 88.91636665 | 91.09306679 | 97.65486245 | 97.65486245 | 97.65486245 | 97.65486245 |
| 7 | 120.96946456 | 122.58579277 | 127.73430823 | 127.73430823 | 127.73430823 | 127.73430823 |
| 8 | 157.96520055 | 159.20897156 | 163.17600242 | 163.17600242 | 163.17600242 | 163.17600242 |
| 9 | 199.90040917 | 200.88635615 | 204.01483022 | 204.01483022 | 204.01483022 | 204.01483022 |
| 10 | 246.77337411 | 247.57390711 | 250.10294037 | 250.10294037 | 250.10294037 | 250.10294037 |

in which, for brevity, we have set

\[
\psi(\eta) = A \cdot f(\eta)
\]

then the analytical eigenfunction [equation (5)] turns into the form

\[
\psi(\eta) = A \cdot f(\eta)
\]

in which, again for brevity, we have set

\[
f(\eta) = A \cdot f(\eta) - \rho \cdot \text{Bi}(\eta)
\]

The coefficient \( A \) is determined by the normalization condition [equation (2c)]. The latter’s exploitation requires a bit of care to rephrase the integral in terms of the new independent variable via equation (3) but the normalization operation is rather elementary and leads to

\[
A = \sqrt{\frac{2}{J}}
\]

with

\[
J = J(\alpha) = \int_{\eta}^{\hat{\eta}} f(\eta)^2 d\eta
\]

Obviously, the integral in equation (14) can be evaluated numerically but there is an analytical shortcut which we will return to and describe in more details in section 3. The substitution of equation (13) into equation (11) yields the final form

\[
\psi(\eta) = \sqrt{\frac{2}{J}} f(\eta)
\]

of the analytical eigenfunctions. In figure 1, we provide validation evidence by superposing the numerical eigenfunctions calculated in [1] on the analytical eigenfunctions produced by equation (15) for the first four eigenstates.
3. External forces with the presence of the electric field

The availability of eigenfunctions in analytical form [equation (15)] permits the straightforward determination of their derivative

$$\frac{\partial \psi}{\partial \eta} = \sqrt{\frac{2\alpha^{1/3}}{J}} \cdot f'(\eta)$$  \hspace{1cm} (16)

The prime on the right-hand side of equation (16) indicates derivation with respect to $\eta$. The eigenfunctions’ derivative with respect to the old independent variable $\xi$ is obtained easily by taking advantage of the variable transformation enforced in equation (3)

$$\frac{\partial \psi}{\partial \xi} = -\alpha^{1/3} \frac{\partial \psi}{\partial \eta} = -\sqrt{\frac{2\alpha}{J}} \cdot f'(\eta)$$  \hspace{1cm} (17)
Therefore, the external forces at the left/right boundary turn out to be respectively

\[
\begin{align*}
\left(\frac{\partial \psi}{\partial \xi} \frac{\partial \psi}{\partial \xi}\right)_{\xi=-1} &= \frac{2\alpha}{J} \cdot f'(\eta)^2 \quad \text{left boundary} \\
\left(\frac{\partial \psi}{\partial \xi} \frac{\partial \psi}{\partial \xi}\right)_{\xi=+1} &= \frac{2\alpha}{J} \cdot f'(\eta)^2 \quad \text{right boundary}
\end{align*}
\]

We have plotted them, divided by 2 for convenience, in figure 2 for the first ten eigenstates with increasing electric field.

![Figure 2](image_url)
eigenvalues. The bottom graphs indicate that the number of affected eigenstates increases with the electric-field intensity: there are three for $\alpha = 50$ and four for $\alpha = 100$. For these eigenstates, the left-boundary external force (hollow squares) vanishes and the right-boundary external force (solid circles) is the only one that equilibrates the electric force. For any specified electric-field intensity, there is always a transition from constant to linear dependence but the linearity is different from the one existing without electric field, not only, as expected, in magnitude but also in slope; in order to put in evidence the latter characteristic, we have echoed the trace of the case $\alpha = 0$ from the top-left graph onto the bottom-right graph corresponding to the case $\alpha = 100$. The graphs offer also the evidence that the difference between the external forces keeps constant and coincides with the value of $\alpha$; this is the graphical verification of equation (105)$_{ma}$, perfectly aligned to the numerical one we gave in [1]. The physical interpretation of the situation portrayed in figure 2 is that, as far as the boundary forces are concerned, the effect of the electric field is never negligible and is felt in all the eigenstates, no matter how high-lying they are. This result is in flagrant contraposition with the intuitive expectation that the effect of the electric field should be negligible when $k \to \infty$ because, in that case, $\alpha|\xi| \ll \beta$ and, consequently, the electric-field term in equation (2a) would be looked at as irrelevant with respect to the right-hand side. This occurrence is true for the eigenvalues, as evidenced by Table 2, but not for the boundary forces: they are always affected by the electric field, as proved by the graphs of figure 2, inasmuch as they must balance the same electric force in each eigenstate [equation (105)$_{ma}$].

### 4. Analytical proof of equation (105)$_{ma}$

The presence of $\alpha$ on the right-hand sides of equations (18) caught particularly our attention with regard to equation (105)$_{ma}$ that endorses the equilibrium between the electrical force and the external forces and that we verified numerically, as shown in the
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2nd column from right in Table 1 of [1], and graphically in figure 2. The substitution
of equations (18) into equation (105) gives

\[ \alpha = \frac{1}{2} \left[ \frac{2}{f} \cdot f' (\hat{\eta})^2 - \frac{2}{f} \cdot f' (\hat{\eta})^2 \right] \tag{19} \]

that, after simplification, reduces to

\[ J = f' (\hat{\eta})^2 - f' (\hat{\eta})^2 \tag{20} \]

Equation (20) provides an expression of the integral \( J \) in terms of the first derivatives of the function \( f(\eta) \) evaluated at the boundaries and is the analytical shortcut, mentioned in section 2, that we have systematically used in our calculations. However, according to the way we have obtained it, equation (20) should be read as an expectation required by the force equilibrium established by equation (105) but cannot be considered a rigorous mathematical proof.

The explicit mathematical proof of equation (20), and, by reflection, of equation (105), exists but it requires to follow another path. A few preliminary ingredients are necessary for that purpose. The function \( f(\eta) \) is a linear combination of the Airy functions [equation (12)] and, as such, it is also a solution of the Airy differential equation

\[ f'' - \eta f = 0 \tag{21a} \]

which complies with the boundary conditions

\[ f(\hat{\eta}) = f(\hat{\eta}) = 0 \tag{21b} \]

Further differentiation of equation (21a) gives

\[ f''' - f - \eta f' = 0 \tag{21c} \]

which can be conveniently rearranged as

\[ \frac{f}{\eta} = \frac{f'''}{\eta} - f' \tag{21d} \]

We can proceed now with the calculation of the integral [equation (14)]. We expand the integrand by taking advantage of equations (21)(a,c,d)

\[ J = \int_{\hat{\eta}}^{\hat{\eta}} f^2 \, d\eta = \int_{\hat{\eta}}^{\hat{\eta}} f \cdot f \, d\eta = \int_{\hat{\eta}}^{\hat{\eta}} f \cdot \frac{f''}{\eta} \, d\eta = \int_{\hat{\eta}}^{\hat{\eta}} \frac{f}{\eta} \cdot f'' \, d\eta \]

\[ = \int_{\hat{\eta}}^{\hat{\eta}} \left( \frac{f'''}{\eta} - f' \right) \cdot f'' \, d\eta \tag{22a} \]

\[ = \int_{\hat{\eta}}^{\hat{\eta}} \frac{f'''}{\eta} \cdot f'' \, d\eta - \int_{\hat{\eta}}^{\hat{\eta}} f' \cdot f'' \, d\eta \]

* Check equation (15) evaluated at the boundaries, with due account of equation (10).
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The second integral on the bottom line of equation (22a) is easily calculated

$$\int_\eta^\hat{\eta} f' \cdot f'' \, d\eta = \int_\eta^\hat{\eta} f' \, df' = \frac{1}{2} [f' (\hat{\eta})^2 - f'(\eta)^2] \quad (22b)$$

and returns an encouraging expression in view of reaching equation (20). The first integral on the bottom line of equation (22a) requires further manipulation

$$\int_\eta^\hat{\eta} f'''' \cdot f' \, d\eta = \int_\eta^\hat{\eta} \frac{f'''}{\eta} \cdot f' \, d\eta = \int_\eta^\hat{\eta} f \cdot df'' = \int_\eta^\hat{\eta} d(f \cdot f'') - \int_\eta^\hat{\eta} f' \cdot f' \, d\eta \quad (22c)$$

The underlined integral in equation (22c) vanishes because $f$ and $f''$ themselves vanish at the boundaries as a consequence of the boundary conditions [equation (21b)]. Therefore, equation (22c) reduces to

$$\int_\eta^\hat{\eta} \frac{f'''}{\eta} \cdot f' \, d\eta = - \int_\eta^\hat{\eta} f'' \cdot f' \, d\eta \quad (22d)$$

We can now substitute equation (22d) into the bottom line of equation (22a), take advantage of equation (22b) and obtain the proof we were looking for

$$J = f'(\hat{\eta})^2 - f'(\eta)^2 \quad (22e)$$

Equation (22e) also constitutes the solid analytical proof of equation (105)$_{na}$.

Acknowledgments

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