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# A test of the DV method with an exactly soluble transport problem

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**Abstract.** A special one-dimensional transport equation will be solved by the variational technique of Djukic and Vujanovic Reasonable *ansatz* with one, two and three variational parameters are used. The variational solution is compared with the exact solution and its least mean-square approximation for the same *ansatz*.

## 1. Introduction

The DV method has been introduced by Djukic and Vujanovic (1971) in order to treat dissipative mechanical systems. It has been applied to problems of heat transfer (Vujanovic and Djukic 1972), to hydrodynamical problems (Vujanovic *et al* 1972) and to the Boltzmann equation (Schlup 1975a, b). Its relation to classical variational methods has been discussed by Schlup (1974, 1975c).

Here, we want to treat a one-dimensional diffusion problem without a drift term†. It can be solved exactly and, therefore, the quality of approximate methods can be checked explicitly.

Certainly, the result will depend strongly on the *ansatz* chosen. In order to refine the approach, three variational parameters $A$, $B$, $C$ will be introduced; but in *ansatz* 1, $B$ and $C$ are fixed and only $A$ is optimized; in *ansatz* 2 only $C$ is fixed and $A, B$ are determined by optimization; and only in *ansatz* 3 are all three, ie $A$, $B$ and $C$, considered as variational parameters.

If the *ansatz* is 'exact', ie contains the exact solution for a convenient choice of variational quantities, the optimum solution becomes the exact one. If the *ansatz* is approximate, ie not 'exact' in the above sense, then the result depends on the details of the *ansatz*; if it is a reasonable approximation, it will give good variational results.

In order to compare different approximations, a quality measure will be introduced. A least mean-square approximation for a given *ansatz* to the exact solution will be considered as the ideal approximation. It corresponds to the optimum fitting of the variational quantities. A quality measure for the optimum solution according to the DV method will be the mean-square deviation from the exact result, which always exceeds the ideal deviation for the same *ansatz*. The DV optimum and the ideal deviation are zero for an exact *ansatz* only.

† In one dimension a drift term can always be eliminated by a variable transformation; it is also equivalent to a Fokker–Planck equation in time and momentum.

## 2. The problem

We consider the following one-dimensional diffusion problem† in $x \in (-\infty, \infty)$ for the particle density $n(x, t)$

$$\frac{\partial n}{\partial t} = \frac{\partial^2 n}{\partial x^2} \tag{2.1}$$

with the initial condition

$$n(x, 0) = \begin{cases} 2 & x < 0 \\ 0 & x > 0. \end{cases} \tag{2.2}$$

With the symmetry

$$n(-x, t) = 1 - n(x, t) \tag{2.3}$$

it transforms into a half-space diffusion problem with equation (2.1) in $x \in (0, \infty)$, initial condition

$$n(x, 0) = 0 \tag{2.4}$$

and boundary condition

$$n(0, t) = 1. \tag{2.5}$$

The exact solution (Abramowitz and Stegun 1965) is

$$n(x, t) = 1 - \mathrm{erf}(x/2t^{1/2}) \tag{2.6}$$

where erf is the error function.

## 3. The *ansatz*

We describe the decaying solution by an explicit $x$-dependent *ansatz* of polynomial type, containing at most three variational quantities $q(t)$, $A$, $p$:

$$\textit{ansatz } 1: \quad n^{(1)}(x, t) = \begin{cases} (1 - x/q(t))^2 & x < q(t) \\ 0 & x > q(t) \end{cases} \tag{3.1}$$

$$\textit{ansatz } 2: \quad n^{(2)}(x, t) = \begin{cases} (1 - x/q(t))^A & x < q(t) \\ 0 & x > q(t) \end{cases} \tag{3.2}$$

$$\textit{ansatz } 3: \quad n^{(3)}(x, t) = \begin{cases} [1 - (x/q(t))^p]^A & x < q(t) \\ 0 & x > q(t) \end{cases} \tag{3.3}$$

The results for $x < 0$ are obtained by the symmetry (2.3). The *ansatz* 1 and 2 can be considered as special cases of 3, namely

$$n^{(1)} = n^{(3)} \qquad \text{for } A = 2, p = 1 \tag{3.4}$$

$$n^{(2)} = n^{(3)} \qquad \text{for } p = 1. \tag{3.5}$$

† Diffusion constant $D = 1$; all particles in left half-space with twice the stationary density $n^s = 1$.

This *ansatz* will be used for an optimum solution of (2.1), (2.4) and (2.5), according to the DV variational method. The boundary condition (2.5) is identically fulfilled, whereas the initial condition implies

$$q(0) = 0. \tag{3.6}$$

## 4. The DV variational solution

The action integral to be extremized is

$$S = \int_0^\infty \mathrm{d}x \int_0^\infty \mathrm{d}t\, \mathscr{L}(t, x, n, \dot{n}, n') \tag{4.1}$$

where the DV Lagrangian is

$$\mathscr{L} = \psi(t, \lambda)\frac{\dot{n}^2}{2} - \frac{n'^2}{2}. \tag{4.2}$$

$\psi(t, \lambda)$ is a DV auxiliary function with the properties

$$\lim_{\lambda \to 0} \psi(t, \lambda) = 0 \tag{4.3}$$

$$\lim_{\lambda \to 0} \dot{\psi}(t, \lambda) = 1. \tag{4.4}$$

The Euler–Lagrange (EL) equation is

$$\Gamma[n] = \frac{\delta S}{\delta n} = -(\psi(t, \lambda)\dot{n}) + n'' = 0 \tag{4.5}$$

which for $\lambda \to 0$ and (4.3) and (4.4) yields

$$\Gamma_0[n] = \lim_{\lambda \to 0} \Gamma[n] = -\dot{n} + n'' = 0. \tag{4.6}$$

Partially integrated terms in $\delta S$ vanish because of (2.4) and (2.5)†.

According to the rules for application established by Schlup (1975c), a complete *ansatz*‡ in all variables entering the $\psi$ functions has to be made, ie

$$p = p(t), \qquad A = A(t). \tag{4.7}$$

*Ansatz* 1 to 3 are such that the $x$ integration in the action integral can be performed. Using *ansatz* 3 with extension (4.7), $S$ becomes

$$S = \int_0^\infty \mathrm{d}t\, L(t, p, q, A, \dot{p}, \dot{q}, \dot{A}) \tag{4.8}$$

and

$$L = \psi(t, \lambda)(\tfrac{1}{2}I_{11}\dot{p}^2 + \tfrac{1}{2}I_{22}\dot{q}^2 + \tfrac{1}{2}I_{33}\dot{A}^2 + I_{12}\dot{p}\dot{q} + I_{23}\dot{q}\dot{A} + I_{13}\dot{p}\dot{A}) + L_0 \tag{4.9}$$

where $I_{ij}$ and $L_0$ are functions of $p$ and $A$. In the limit $\lambda \to 0$ and for the constants $p$

† There are no contributions from the upper boundaries $x = \infty$ or $t = \infty$, since $\dot{n}$ and $n'$ vanish there.
‡ To avoid the problem of interchange of integration over an infinite range with limit $\lambda \to 0$.

and $A$, the EL equations are

$$\lim_{\lambda\to 0}\frac{\delta S}{\delta p} = 0 \Rightarrow I_{12}\dot{q} = \frac{\partial L_0}{\partial p} \tag{4.10a}$$

$$\lim_{\lambda\to 0}\frac{\delta S}{\delta q} = 0 \Rightarrow I_{22}\dot{q} = \frac{\partial L_0}{\partial q} \tag{4.10b}$$

$$\lim_{\lambda\to 0}\frac{\delta S}{\delta A} = 0 \Rightarrow I_{23}\dot{q} = \frac{\partial L_0}{\partial A}. \tag{4.10c}$$

Assuming $p$ and $A$ constant is compatible with equations (4.10), since the ratios

$$\frac{I_{12}}{I_{22}} = \frac{\partial L_0/\partial p}{\partial L_0/\partial q} \tag{4.11a}$$

$$\frac{I_{23}}{I_{22}} = \frac{\partial L_0/\partial A}{\partial L_0/\partial q} \tag{4.11b}$$

are independent of $q$ and are sufficient to determine $p$ and $A$. Finally, (4.10$b$) gives

$$q\dot{q} = \frac{q\partial L/\partial q}{I_{22}} \tag{4.12}$$

where the right-hand side depends only on $p$ and $A$. Therefore, the optimum solution is

$$\frac{q^2}{t} = \frac{2q\partial L_0/\partial q}{I_{22}} \equiv Q(p, A) \tag{4.13}$$

where $p$ and $A$ follow from (4.11) (for explicit formulae see the appendix).

The corresponding results for the *ansatz* (3.1), (3.2) and (3.3) are

1 $p = 1, A = 2 \Rightarrow Q = 10$

$\gamma_{\rm DV}^{(1)} = 0{\cdot}000822$

2 $p = 1 \Rightarrow A = 2{\cdot}118, Q = 11{\cdot}090$

$\gamma_{\rm DV}^{(2)} = 0{\cdot}000524$

3 $\Rightarrow p = 1{\cdot}069, A = 2{\cdot}858, Q = 15{\cdot}542$

$\gamma_{\rm DV}^{(3)} = 0{\cdot}000156$

where $\gamma^{(m)}$ is the least mean-square deviation for $t = 1$ (see § 5).

## 5. The least mean-square approximation

In order to check the variational results of the DV method, we could compare it with the exact solution (2.6). The quality of the approximation naturally depends on the details of the *ansatz*. In order to define the best choice of parameters in a given *ansatz*, we use a least mean-square approximation (LMS) to the exact solution; it can be considered as the ideal approximation with respect to the constraints of a given *ansatz*. This ideal approach should not be confused with the LMS approximation to the equation (Vujanovic and Djukic 1972, Schlup 1975c).

The *ansatz* 1 to 3 contain three variational parameters, if $q(t) = (Qt)^{1/2}$ (see (4.13)) is used, namely $p$, $A$ and $Q$. The quantity to be minimized in the LMS method is

$$R^{(m)} = \int_0^\infty dx\, (n^{(m)}(x,t) - n_{ex}(x,t))^2 \tag{5.1}$$

where $m = 1, 2, 3$ and $n_{ex}(x, t)$ is the exact solution (2.6). This is a reasonable criterion because of: (i) boundary condition (2.4); and (ii) asymptotic behaviour, which makes the integrand 0 in $x = 0$ and integrable for $x \to \infty$†. Since $t$ enters only through $x/t^{1/2}$, the integral $R^{(m)} = t^{1/2}\gamma^{(m)}$, where $\gamma^{(m)}$ depends on the $m$ parameters of the *ansatz* ($m$), regarding $q(t) = (Qt)^{1/2}$.

Minimization of $R^{(m)}$ gave the following numerical results for the *ansatz* 1 to 3:

1 $$p = 1, A = 2$$
$$\Rightarrow Q = 11{\cdot}044,\ \gamma^{(1)}_{\mathrm{MIN}} = 0{\cdot}000324 \tag{5.2}$$

2 $$p = 1$$
$$\Rightarrow A = 2{\cdot}486,\ Q = 15{\cdot}084,\ \gamma^{(2)}_{\mathrm{MIN}} = 0{\cdot}000138 \tag{5.3}$$

3 $$\Rightarrow p = 1{\cdot}129,\ A = 4{\cdot}280,\ Q = 25{\cdot}898$$
$$\gamma^{(3)}_{\mathrm{MIN}} = 0{\cdot}000016. \tag{5.4}$$

## 6. Conclusion

The approximate solution of equation (2.1) according to the DV variational method and the LMS method with respect to the *ansatz* 1 to 3, has been calculated. The deviation from the exact solution $\Delta n = n(x, t) - n_{ex}(x, t)$ is shown in figure 1. The DV result given by the dotted curves—except for *ansatz* 3 and small $x/t^{1/2}$—is smaller everywhere than the exact solution, into which it merges for $x/t^{1/2} > Q^{1/2}$ (full curve). The LMS result

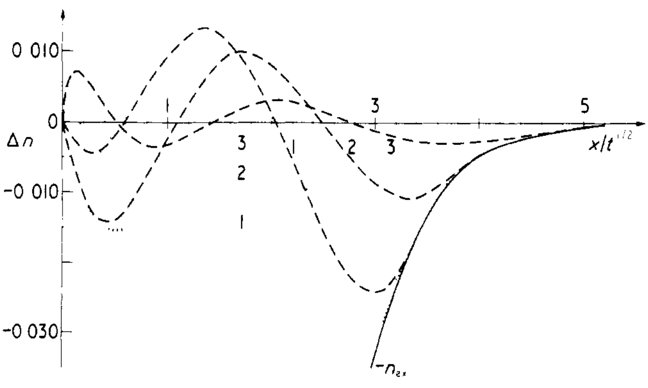


**Figure 1.** The deviation $\Delta n = n(x, t) - n_{ex}(x, t)$ against $x/t^{1/2}$ for the different *ansatz* 1, 2, 3 by the variational method of Djukic and Vujanovic (dotted curves) and the least mean-square method (broken curves).

† Otherwise, instead of the ordinate distance a normal distance should be used and also some weight factor $\rho(x)$ would be necessary.

given by the broken curves cuts the exact solution several times (zeros). If one compares curves corresponding to the same *ansatz* $(m)$, the maximal deviation is practically of the same order (ratio DV/LMS $\simeq 2$). Therefore, the DV method yields results which are, for reasonable *ansatz*, nearly as reliable as the ideal approximation.

The relative error for $x/t^{1/2} < 1$ is of the order of a few per cent; it increases to 100% (for $x/t^{1/2} \geqslant Q$) for increasing $x/t^{1/2}$, because of the special asymptotic form of the *ansatz* 1 to 3. In this range, the relative error is not a good measure as to the quality of the approximation. The LMS deviation (for $t = 1$) $\gamma^{(m)}$ is much smaller for the ideal approximation (ratio $\gamma^{(m)}_{\mathrm{DV}}/\gamma^{(m)}_{\mathrm{MIN}} \simeq 3$ to 10) than the linear deviation, especially for a more-parameter *ansatz*. This is a consequence of the essentially unilateral deviation of the DV result, which gives a much larger contribution to $\gamma^{(m)}$.

Finally, it should be noted that the diffusion problem has the same variational solution, if the limit $(\lambda \to 0)$ Lagrangian

$$\mathscr{L} = \mathrm{e}^{t/\lambda}(\tfrac{1}{2}\lambda\dot{n}^2 - \tfrac{1}{2}n'^2) \qquad (6.1)$$

is used as the starting point (see variational equivalence: Schlup 1975c).

## Appendix

$$\frac{\delta S}{\delta q} = 0 \Rightarrow (4{\cdot}13)$$

$$Q(p, A) = \frac{\Gamma(2-1/p)\Gamma(2A+1+1/p)}{\Gamma(2+1/p)\Gamma(2A+1-1/p)} \qquad (\mathrm{A}1.1)$$

$$p = 1: \qquad Q(1, A) = A(2A+1).$$

$$\frac{\delta S}{\delta q} = \frac{\delta S}{\delta A} = 0 \Rightarrow (4.11b)$$

$$\begin{aligned} &2A(p+1)(\psi(2A+1-1/p)-\psi(2A-1)-1/A) \\ &\qquad +(2A-1)(\psi(2A+1+1/p)-\psi(2A)) = 0 \end{aligned} \qquad (\mathrm{A}1.2)$$

$$p = 1, \qquad (\mathrm{A}1.2) \Rightarrow 4A^2 - 8A + 1 = 0.$$

$$\frac{\delta S}{\delta q} = \frac{\delta S}{\delta p} = 0 \Rightarrow (4.11a)$$

$$\psi(2A+1+1/p)-\psi(2A+1-1/p)-\psi(2+1/p)+\psi(2-1/p)+p = 0. \qquad (\mathrm{A}1.3)$$

For transcendental functions see Abramowitz and Stegun (1965).

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