Calculation of Transport Coefficient Profiles in Modulation Experiments as an Inverse Problem

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The calculation of transport profiles from experimental measurements belongs in the category of inverse problems which are known to come with issues of ill-conditioning or singularity. A reformulation of the calculation, the matricial approach, is proposed for periodically modulated experiments, within the context of the standard advection-diffusion model where these issues are related to the vanishing of the determinant of a 2×2 matrix. This sheds light on the accuracy of calculations with transport codes, and provides a path for a more precise assessment of the profiles and of the related uncertainty.

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Inverse problems, i.e., going from data to model parameters, are ubiquitous in science and engineering. They are known to come with issues of ill-conditioning or singularity, which make difficult relating the accuracy of the computed model parameters to the errors in the input data. Inferring transport properties of magnetically confined plasmas from perturbative experiments [1] belongs in this category. This issue is crucial to both the theoretical understanding of transport processes and the practical control of fusion plasmas. Classical reconstructions of transport coefficients rely on standard transport codes, which ignore the possible ill-posedness of the problem by employing *ad hoc* regularizations. To the best of our knowledge, so far the only authors that took it into account were Andreev and Kasyanova [2], who provided a detailed analysis of the uncertainties present in the case of a localized impulsive source. However, as shown later, experimentalists happened unwittingly to avoid ill-conditioning and singularity by trying naturally to separate the domain where transport is measured from that where sources are present. Unfortunately, this separation is almost impossible for measuring the transport of angular momentum, and only partially possible for heat transport. It is therefore most important to warn the users of transport codes, and to benefit from an alternative safer approach. For the first time this Letter proposes such an alternative. The corresponding technique is elementary, quite general, and requires much less numerical calculations than with transport codes. It may be applied to any experiment aiming at the calculation of transport coefficients, also in media other than plasmas. Its only limitations are: (i) it works in effectively one-dimensional geometries; (ii) applies to perturbative regimes, i.e., where relevant equations may be linearized around unperturbed equilibria; (iii) the forcing term causing the perturbation must be periodic in time.

The standard procedure for inferring transport coefficients is through solving the advection-diffusion for the generic quantity $\zeta(r, t)$ (which may stand for the perturbation to particle density, temperature, momentum,...):

$$\partial_t \zeta = -\nabla \cdot \Gamma(\zeta) + S, \qquad \Gamma = -\chi \nabla \zeta + V\zeta. \tag{1}$$

In (1) χ, V are functions taken out of a set of trial profiles guessed *a priori*, usually simple analytical expressions containing a certain number of free coefficients which are given explicit values by minimizing under some norm the gap between the experimental ζ profiles and the reconstructed ones. The regularization built in this approach is straightforward: it consists in choosing well-behaved trial functions for χ, V.

In this work we address the problem of solving Eq. (1) as an inverse problem in the case of periodically modulated perturbations. We present a simple algebraic method to recover *exact* solutions; that is, χ, V, may be exactly and directly (not by means of iterative procedures) obtained from the smoothed data without the recourse to any adjustable trial function and minimization procedure. We identify under which conditions the problem is well- or ill-posed, i.e., the solution (χ, V) does sensitively depend from the input data. We discuss how error bars in the raw measurements are propagated to final estimates of (χ, V). This is a delicate issue when Eq. (1) is addressed as a least-squares problem using smooth trial functions for (χ, V): on the one hand, they prevent any oscillation to blow up, thereby constraining the apparent error bars to values smaller than ought be. On the other hand the opposite limit is also possible: if trial functions are chosen that cannot match the true (χ, V) profiles, the minimization procedure necessarily converges towards just a local minimum that is far away from the true global minimum. In this case, the error on the final (χ, V) values is larger than expected from the raw data alone. Finally, we point out how data from different experiments can be combined to reduce the effective margin of error and thus yield a more accurate final estimate of (χ, V).

We consider a case with cylindrical symmetry and a purely sinusoidal forcing term. Calculations are easier using complex notation, thus the temporal behavior is factored out in the term $\exp(-i\omega t)$ and Eq. (1) writes

$$-i\omega\zeta = r^{-1}\partial_r[r(\chi\partial_r\zeta - V\zeta)] + S. \quad (2)$$

After rearranging, integrating over the radial coordinates and using the boundary condition $\Gamma(r=0)=0$ we get

$$\chi\partial_r\zeta - V\zeta = -r^{-1}\int_0^r dz\, z(i\omega\zeta + S). \quad (3)$$

The previous equation is reduced to an algebraic system of two real equations by expressing the signal in terms of amplitude and phase, $\zeta = Ae^{i\phi}$, and $S = S_r + iS_i$:

$$\mathbf{M}\cdot\mathbf{Y} = \mathbf{\Gamma} \qquad \mathbf{Y} = \begin{pmatrix}\chi\\ V\end{pmatrix},$$
$$\mathbf{M} = \begin{bmatrix} -A'\cos\phi + A\phi'\sin\phi & A\cos\phi \\ -A'\sin\phi - A\phi'\cos\phi & A\sin\phi \end{bmatrix}, \quad (4)$$
$$\mathbf{\Gamma} = \begin{bmatrix} \frac{1}{r}\int_0^r dz\, z(S_r(z) - \omega A(z)\sin\phi(z)) \\ \frac{1}{r}\int_0^r dz\, z(S_i(z) + \omega A(z)\cos\phi(z)) \end{bmatrix}$$

where the primes stand for differentiation with respect to r. Provided $\mathbf{\Gamma}(r)$ is known, $\mathbf{Y}(r)$ can be computed by inverting the matrix $\mathbf{M}(r)$. For this reason, in the following we refer to this method as the matricial approach. It should be mentioned that considering just time-periodic quantities in (1) leads to a considerable simplification: this reduces Eq. (1) from a partial differential equation to an ordinary differential equation (2). Several efforts were devoted to solving Eq. (2) using simpler techniques than its numerical integration, possibly even analytical methods [3].

We now solve Eq. (4) for $\mathbf{Y}(r)$ in terms of the eigenvalues $\lambda(r)$ and eigenvectors $\mathbf{E}(r)$ of the matrix $\mathbf{M}(r)$

$$\mathbf{Y} = y_0\mathbf{E}_0 + y_1\mathbf{E}_1, \qquad y_j = \lambda_j^{-1}\mathbf{\Gamma}\cdot\mathbf{E}_j \quad (j=0,1). \quad (5)$$

A solution exists wherever the matrix $\mathbf{M}$ is invertible, i.e., where none of the λ_j's vanishes, which would imply

$$\det(M) = A^2\phi' = 0. \quad (6)$$

Excluding exceptional cases where $A=0$, the singular points are those where $\phi'=0$. The origin is one such point, but there $\mathbf{\Gamma}=0$, too; thus ultimately $r=0$ is a regular point. Inspection of literature (see, e.g., [4–9]) shows instead that the condition $\phi'=0$ is usually fulfilled close to the location of the source. Qualitatively, this can be justified by noticing that, close to the source, the dynamics of ζ is ruled in Eq. (2) more by the source than by transport if ω is large enough, hence $\zeta \approx iS\omega^{-1}$ and $S'=0$ implies $\phi'=0$.

Physically, transport coefficients are defined even at the singular points $r=r_s$. Throughout this work we conventionally choose λ_0 to be the eigenvalue that vanishes at r_s. Accordingly, the actual value of ζ produced by the source S must align the flux $\mathbf{\Gamma}$ exactly along the $\mathbf{E}_1$ eigenvector:

$$\mathbf{M}\cdot\mathbf{Y} = \lambda_1 y_1\mathbf{E}_1, \qquad \mathbf{\Gamma} = \gamma_1\mathbf{E}_1, \qquad (r=r_s) \quad (7)$$

Because of unavoidable uncertainties arising in the experiment, the estimated $\mathbf{\Gamma}$ takes on a component along $\mathbf{E}_0$ too, thus making the inversion impossible. However, we may solve for the component of $\mathbf{Y}$ along $\mathbf{E}_1$, whereas the component along $\mathbf{E}_0$ remains completely unknown: $\mathbf{Y}(r_s)$ belongs to a straight line parallel to $\mathbf{E}_0$ in the plane (χ, V).

We present now a comprehensive discussion, including both regular and singular points. We label with the subscript m the quantities measured by the experiment: $\mathbf{M}_m$, ζ_m, $\mathbf{\Gamma}_m$. Equation (4) implies $\mathbf{M}_m\cdot\mathbf{Y}_m = \mathbf{\Gamma}_m$. Let the subscript "c" label likewise the same quantities as estimated by transport codes solving Eq. (1) via least squares. Finally, let the asterisk label the "true" (unknown) quantities that the experimental measure is addressing: $\mathbf{M}_*$, ζ_*, $\mathbf{\Gamma}_*$, and $\mathbf{M}_*\cdot\mathbf{Y}_* = \mathbf{\Gamma}_*$. Quantity $\mathbf{\Gamma}_m$ generally contains some arbitrariness due to the lack of precise knowledge about the source term, too. Let $\delta\zeta = \zeta_c - \zeta_m$, $\delta\mathbf{M} = \mathbf{M}_c - \mathbf{M}_m$, $\delta_*\mathbf{Y} = \mathbf{Y}_c - \mathbf{Y}_*$. The target of any transport modeling is $\delta_*\mathbf{Y} = 0$. Finally, we write $\mathbf{\Gamma}_c = \mathbf{\Gamma}_* + \Delta\mathbf{\Gamma}_S + \Delta\mathbf{\Gamma}_m + \Delta\mathbf{\Gamma}_\zeta$. In this expression $\Delta\mathbf{\Gamma}_S$ is the error in the calculation of the flux due to the imperfect knowledge of the source, $\Delta\mathbf{\Gamma}_m$ is the error related to imprecise measurement of ζ: $\zeta_m - \zeta_*$, and the third term comes from the error in the reconstruction of the measured ζ: $\delta\zeta$. For brevity, we set $\mathbf{\Gamma}_\Delta = \mathbf{\Gamma}_* + \Delta\mathbf{\Gamma}_S + \Delta\mathbf{\Gamma}_m$, $\mathbf{\Gamma}_c = \mathbf{\Gamma}_\Delta + \Delta\mathbf{\Gamma}_\zeta$. Since (4) is a first integral of (1), $\mathbf{M}_c\cdot\mathbf{Y}_c = \mathbf{\Gamma}_c$ holds. Using above definitions, we rewrite the latter expression as

$$\mathbf{M_m}\cdot\delta_*\mathbf{Y} = \mathbf{\Gamma_\Delta} - \mathbf{M_m}\cdot\mathbf{Y}_* + \mathbf{\Delta\Gamma}_\zeta - \delta\mathbf{M}\cdot\mathbf{Y}_* - \delta\mathbf{M}\cdot\delta_*\mathbf{Y}. \quad (8)$$

Whenever $\delta\zeta = \zeta_c - \zeta_m = 0$, then $\delta\mathbf{M} = \mathbf{M}_c - \mathbf{M}_m = 0$, $\Delta\mathbf{\Gamma}_m = 0$. Let again λ_0 be the smaller eigenvalue (in absolute value). If $\lambda_0 \neq 0$ it is possible to check that (8) can be fulfilled by setting $\delta\zeta = 0$: for regular points, transport codes can potentially attain a perfect reconstruction of measured value, provided the set of trial profiles includes the solution given by the matricial method.

This is no longer true when $\lambda_0 = 0$, since in this case the left-hand side of (8) is aligned along the other eigenvector $\mathbf{E}_1$, whereas the right-hand side has generically components along both directions. At a singular point a transport code provides a natural regularization because of the limited flexibility of the set of $\mathbf{Y}$ profiles available for the minimization. In terms of Eq. (8) the code generates the minimum finite value of $\delta\zeta(r_s)$ over the set of trial profiles providing a finite value of $\delta\mathbf{M}_\zeta(r_s)$ which cancels the $\mathbf{E}_0$ component of $\delta\mathbf{\Gamma}(r_s)$, that exists for $\delta\zeta(r_s)=0$. More precisely the choice of all the $\delta\zeta(r_s)$'s is done simultaneously, because of the global norm used by the codes. Therefore this optimized finite value of $\delta\zeta(r_s)$ may not be the smallest one. It is independent of $\delta\mathbf{Y}(r_s)$ if $\delta\mathbf{M}\delta\zeta(r_s)$ is small. Therefore $\delta\zeta(r_s)$ does not measure the accuracy of the calculation of $\mathbf{Y}(r_s)$. Since $\delta\mathbf{M}\delta\zeta(r_s)$ has a random sign, it does not improve this accuracy, even if it is not negligible. Finally the finite value of $\delta\zeta(r_s)$ also modifies the component of $\mathbf{Y}(r_s)$ along $\mathbf{E}_1$, which increases the uncertainty of the calculation.

Summarizing, the matricial approach: (i) highlights that the source term plays a critical role for profile calculation; the best situation is obtained when the source is localized at the plasma outer edge: then, the inverse problem is well-conditioned and the error on the source estimate does not enter the calculation of the profile for smaller radii. The worst case is conversely expected to be when the source is spread radially. Then the calculated profile may be strongly influenced by the somewhat arbitrary regularization. (ii) Points out that the common strategy of least-squares minimization performed by transport codes actually hides some subtle practicalities.

So far, we have implicitly assumed that measurements are performed on a very fine mesh of points, such that ζ may be treated as a continuous variable. In real cases, measurements are taken on a discrete and often quite coarse mesh, $r = r_j,\ j = 1, \ldots, N$. This raises issues of interpolation and extrapolation, needed to compute the derivatives and the integrals involved in Eq. (4), and emphasizes the intrinsic reverse character of our approach with respect to transport codes solving Eq. (1): the matricial approach computes $\mathbf{Y}$ only at the discrete set of measurement points r_j, but needs a continuous interpolation of the data A and ϕ in order to compute the derivatives involved in Eq. (4). Conversely, transport codes do need continuous profiles for (χ, V) and only the knowledge of A, ϕ at discrete points. From Eq. (5) one can estimate the uncertainty associated to the calculation of $\mathbf{Y}(r)$. $\mathbf{Y}$ depends on $3 \times N$ experimental quantities $\{A_i\}, \{\phi_i\}, \{S_i\}$. We label collectively these quantities as $\vartheta_k, k = 1, \ldots, 3N$. Let $\delta\vartheta_k$ be an estimate of the associated uncertainty and $\partial_k \equiv \frac{\partial}{\partial \vartheta_k}$. Thus,

$$\delta\mathbf{Y} = \sum_{k,l} \delta\vartheta_k \left[\frac{\mathbf{\Gamma}\cdot\mathbf{E}_l}{\lambda_l}\partial_k\mathbf{E}_l + \mathbf{E}_l\left(\frac{\partial_k\mathbf{\Gamma}\cdot\mathbf{E}_l}{\lambda_l} + \frac{\mathbf{\Gamma}\cdot\partial_k\mathbf{E}_l}{\lambda_l} - \frac{\mathbf{\Gamma}\cdot\mathbf{E}_l}{\lambda_l^2}\partial_k\lambda_l\right)\right]. \quad (9)$$

Generally, the $\delta\vartheta_k$'s should be treated as stochastic variables picked up from some statistical distribution. Accordingly the vector $\delta\mathbf{Y}(r_j)$ spans an area W around the point $\mathbf{Y}(r_j)$: the uncertainty on this quantity is geometrically displayed as a roughly elliptic region with low eccentricity if $\lambda_0/\lambda_1 \approx O(1)$. Near the points where λ_0 is small the term proportional to λ_0^{-2} dominates:

$$\delta\mathbf{Y} \approx -\mathbf{E}_0\frac{\mathbf{\Gamma}\cdot\mathbf{E}_0}{\lambda_0^2}\sum_k d\vartheta_k(\partial_k\lambda_0) + \mathbf{E}_1 O\left(\frac{1}{\lambda_0}\right). \quad (10)$$

Thus W is stretched along $\mathbf{E}_0$, as qualitatively assessed earlier.

Till now we considered a single experimental setup endowed with a single modulation frequency and source. However, it is easy to generalize to experiments where—under the same transport conditions—multiple harmonics are measured, or the location of sources is changed. Then, the above procedure may be repeated, and the independent domains of uncertainty W compared. If for all points they have a nonvanishing intersection, this should provide a smaller global uncertainty, and thus improve the accuracy of the profile calculation. If one of the intersections vanishes, the assumptions of the calculation must be questioned. In particular, one may wonder whether (i) the uncertainties have been underestimated and whether the correct W's are larger than estimated; (ii) some source terms have not been computed correctly or are missing; (iii) it is not true that the independent measurements correspond to the same $(\chi(r), V(r))$ profile; (iv) Eq. (1) fails: transport is not of the advection-diffusion type. Whenever the modulated source has several harmonic components, by virtue of the linearity of Eq. (2), each harmonic can be treated as a separate measurement. This may improve the accuracy in the regions where λ_0 is not small. If λ_0 is small, since $\mathbf{E}_0$ has almost the same orientation for all harmonics, the precision of the calculation cannot be improved.

In order to make visual the above statements we propose below a check using synthetic data. Spatial profiles of transport coefficients and sources are given in advance [Figs. 1(a) and 1(b)] and used in Eq. (2) to produce synthetic $(A,\ \phi)$ data sets [Figs. 1(c) and 1(d)]. Notice that the central source S_2 produces a singular point close to half radius (i.e., near the location of its peak), whereas the edge source S_1 does not. The matricial method is then employed on these data to check that the original transport coefficients are correctly recovered back [Figs. 1(e) and 1(f)]. Finally, we add a finite uncertainty to the "measurements" in order to mimic experimental error: to each point is added a random contribution taken from a normal distribution with a mean amplitude equal to 1% (both in the amplitude and the phase). The new data sets have been then smoothed using a moving average, in order to avoid too brusque variations, that would deteriorate the quality of the derivatives, and were interpolated using third-order splines. Then the coefficients (χ, V) are recomputed, repeating the whole procedure for a total of 400 independent statistical runs at $x = 0.41$, i.e., close to the singularity for the source S_2. Figures 1(g) and 1(h) show how the different estimates spread around the true value. For the "regular" case S_1 all the estimates have a relatively small spread, unlike S_2, whose data align along the eigenvector $\mathbf{E}_0$, as predicted earlier, when $\lambda_0 \to 0$. The width of the spread is remarkable, which stresses again the ill-posed nature of the problem.

To summarize, the matricial approach (MA) is very light computationally. Indeed, it avoids the heavy spatiotemporal integration of Eqs. (1) and (2) and the iterative least-squares minimization procedure over the set of trial functions. The MA provides a clear geometrical foundation to the nature and size of uncertainties in profile reconstruction. The reconstruction radius-by-radius enables to see how different are the uncertainties over $\mathbf{Y}$ as a function

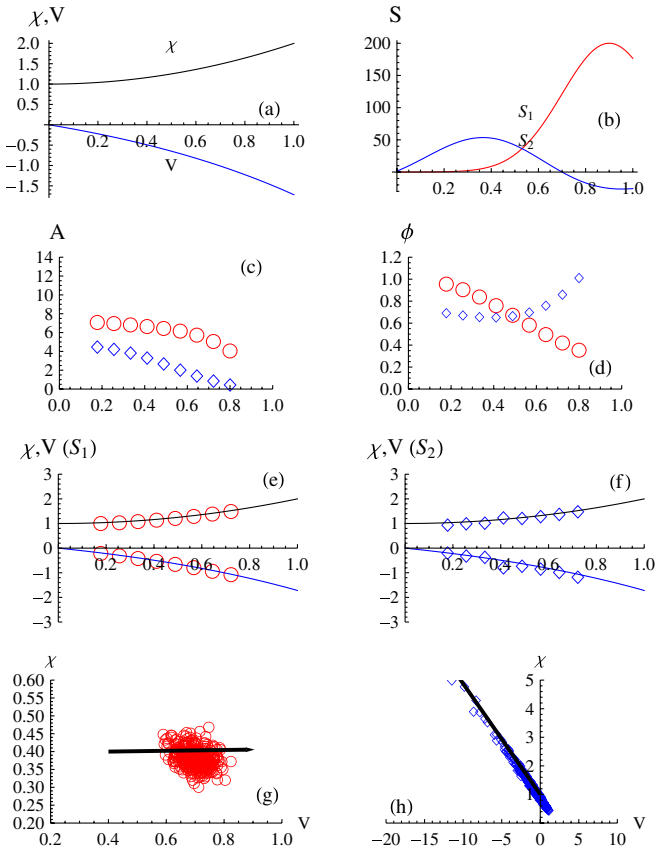

FIG. 1 (color online). (a) Profiles of χ and V. (b) Profiles of the two sources, S_1, S_2. Both sources are modulated with frequency $\nu = 1$. (c) Amplitude A of the signal produced by solving Eq. (2). Circles refer to source S_1, diamonds to S_2. (d) Phase ϕ of the same signal. (e) Symbols are the transport coefficients computed backwards from Eq. (4), superimposed to the true transport coefficients, for the simulation with source S_1. (f) The same for source S_2. (g) Scatter of (χ, V) from Monte Carlo simulation using source S_1 at $x = 0.41$. The black segment is parallel to the local eigenvector E_0. (h) The same as figure (g) for data from source S_2.

of r and to correlate them with the presence of a source. The MA yields a higher precision in the reconstruction of transport profiles than transport codes, provided the uncertainty on the estimate of the derivatives of A and ϕ is not high. Indeed, the MA is not restricted by the *a priori* guess of the trial profiles, but by that of these derivatives, which is much more reliable and controllable. It may provide an assessment of profile predictions already done with transport codes. *A posteriori* some regularization may be applied to MA results. When λ_0 is small at a given radius r_s, the regularization needed to provide a reasonable estimate of $\mathbf{Y}(r_s)$ can be defined in an explicit way, while this is only implicit in the transport code approach. For instance, if a singular point r_s is in between two nearby regular ones r_i and r_{i+1}, one may require $\mathbf{Y}(r_s)$ to be on the straight line joining $\mathbf{Y}(r_i)$ and $\mathbf{Y}(r_{i+1})$. Overlapping the uncertainty intervals for various experiments where the same transport is assumed to hold, provides either a way to improve the precision of the reconstruction (case of a nonvanishing overlap) or to prove the set of initial assumptions in the reconstruction to be wrong (case of a vanishing overlap). The MA can help designing *a priori* the combination of perturbation measurements susceptible of improving the precision of the reconstruction of transport profiles. The MA requires a single boundary condition only: the vanishing flux at $r = 0$, which is a rigorous constraint. In contrast the calculation via Fokker-Planck equation of the $\zeta_i(t)$'s requires a second outer boundary condition which is generally known with some uncertainty. Very often this condition is provided by the data of the outermost chord. Then the matricial approach has the benefit of keeping the outermost chord data available for the profile calculation. It also avoids the uncertainty included in this data to contaminate the profile calculation at smaller radii.

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