Kuwait J. Sci. Eng. **27**(2) 2000

A regularization method for the solution of an integral problem in elastic electron scattering

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PACS numbers: 21.10.Ft, 21.10.Gv, 25.30.Bf

ABSTRACT

The classical problem of deriving the radial distribution of the centre of mass of protons from electric-charge densities is ill-posed in both cases of phenomenological and model-independent descriptions. Solution of the relevant Fredholm's equation can be obtained in numerical form by means of different techniques such as Fourier transform, filter analysis, etc. We propose a theoretical framework based on a regularization procedure which encompasses all these methods and can be applied to all the general cases including those with strong ill-posedness, imposing suitable constraints based on smoothness behavior and boundary conditions. Some realistic examples are shown and discussed.

INTRODUCTION

Traditionally, high-energy electrons are an invaluable tool in probing nuclear structure, even in the innermost region of the nucleus, because of the electromagnetic interaction which is well known and exactly described within the framework of QED theory. In particular, nuclear charge densities can be determined in great detail by electron–nucleus scattering measurements of form factors up to finite maximum momentum transfer due to the high spatial resolution presently achieved in experiments (as shown in the review articles of Frois [1983] and Friar & Negele [1975]). They result from the broad range of momentum transfers available in actual factories, which determine the Fourier–Bessel components of ground-state charge distribution in a model-independent analysis (Dreher *et al.* 1974).

Therefore, a number of nuclear, *model-independent* charge densities extracted from elastic scattering data are now available (de Vries *et al.* 1987), while in the past these distributions were approximated by smooth Fermi-like phenomenological functions. Additional reliable information is supplied by muonic X-ray data which significantly reduces the uncertainty in the lowest-order Fourier–Bessel coefficients of the deduced charge distribution (Friar & Negele 1975).

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As a result, this amount of nuclear data is particularly important in order to check microscopic models of nuclear structure (Friar & Negele 1975, Zverev *et al.* 1987). Recently, relativistic hadron models for finite nuclei have been developed (Furnstahl, Tang & Serot 1995) using effective Lagrangians constrained by the underlying symmetries of QCD, and calculations of bulk properties for a few double-magic nuclei have been carried out. In addition, the proton densities have been evaluated and then folded with phenomenological proton form factors in order to compare the resulting charge densities with the corresponding experimental data. In this work, we follow the inverse procedure, deducing mass densities from charge densities for a direct comparison with measurements.

Moreover, simple algebraic expressions have been proposed for the description of nuclear densities, as performed, for instance, by Gambhir, Ring & de Vries (1989); it is then useful to deduce global nuclear densities from experimental charge densities by means of reliable techniques and to verify the domain of applicability of these semiempirical formulas.

In fact, as pointed out in by Minelli, Pascolini & Villi (1985), meaningful differences could arise between charge and centre-of-mass proton densities even for heavy-mass nuclei, so that comparisons between theoretical calculations and experimental data have to be carefully considered. These quantities are related together by a well-known integral equation of convolution type which, for even–even nuclei, reads as:

$$\rho^{\dagger}(\vec{r}) = \int_{\Re^3} \rho_p(\vec{r} - \vec{s})\rho(\vec{s})\, d\vec{s} \tag{1}$$

where $\rho^{\dagger}(\vec{r})$ and $\rho(\vec{r})$ are the nuclear charge and proton centre-of-mass distributions, respectively, while the proton form factor, $\rho_p(\vec{r})$, is assumed on the basis of a suitable phenomenological nucleon model (Hofstadter 1963). Proton form factors derived in the framework of low-energy QCD (Furnstahl, Tang & Serot 1995) can be also considered and will be treated elsewhere.

In general, the approach usually adopted to obtain the deconvoluted distribution, $\rho(\vec{r})$, makes use of the Fourier transform since it is well known that the Fourier transform, F, of the folding of two convoluted functions is equal to the product of the Fourier transforms of the single functions,

$$F(\rho^{\dagger}) = F(\rho_p) \cdot F(\rho) \tag{2}$$

and $\rho(\vec{r})$ can be formally obtained by an inverse transform,

$$\rho = F^{-1}[F(\rho^{\dagger})/F(\rho_p)]. \tag{3}$$

However, the ill-posedness of Eq. (1) sets stringent limits on the formal validity and numerical reliability of solution (3) relevant to its degree of ill-posedness which depends on the explicit form of the kernel, $\rho_p(\vec{r} - \vec{s})$, and also (see, for instance, Friar & Negele 1975) on the smoothness of $\rho(\vec{s})$. If $\rho^{\dagger}(\vec{r})$ is affected by some source of errors, as necessarily arises in the case of physical measurements and even from numerical approximations, one has to seek a stable or filtered approximation to the unknown solution, $\rho(\vec{s})$.

The inadequacies of Eqs. (2, 3) and the resulting need for improved filtered approaches based on statistical regularization or constrained Fourier extrapolations are extensively discussed in both an experimental framework and mathematical point of view by Bonifazzi, Maino & Tartari (2000). In this paper, we present a complete and exact mathematical treatment of the integral problem given by Eq. (1) in a very general context. Obviously, in many actual cases, Eq. (3) is able to give a satisfactory and simple solution; however, it deserves some attention for development of an algorithm for its solution, valid even in the case of severe ill-posedness.

Previously, analytical solutions have been obtained by Minelli, Pascolini and Villi (1985) for the integral equation (1) in many cases of physical significance, when $\rho^{\dagger}(\vec{r})$ is expressed in closed form, assuming proton models which give a density, $\rho_p^{\dagger}(\vec{r})$ with the following general functional form:

$$\rho_p^{\dagger}(\vec{r}) = \left(\frac{\mu_p^3}{4\pi}\right) f(\mu_p r) \frac{e^{-\mu_p r}}{\mu_p r} + c_p \delta(\vec{r}), \tag{4}$$

where $f(\mu_p r) = a_p - 2b_p + b_p \mu_p r$ and $c_p = 1 - a_p$, while $\delta(\vec{r})$ is the usual Dirac distribution.

The values of a_p, b_p and μ_p for different proton models are summarized in Table 1, where μ_p has been evaluated assuming the experimental value, $R_p = 0.862 \pm 0.012$ fm, of the r.m.s. proton radius (Friar & Negele 1975, Minelli, Pascolini & Villi 1985).

We intend to show on rigorous mathematical grounds that a reliable solution of Eq. (1) always exists and can be easily recovered even if $\rho^{\dagger}(\vec{r})$ is derived in a *model-independent* way from scattering data and hence affected by experimental uncertainties which can be properly considered in the procedure hereafter described. The main result is that in general cases when Eq. (1) represents an ill-posed problem, according to Hadamard's criterion, then a formally rigorous solution can be achieved only by means of a suitable regularization procedure that removes spurious contributions devoid of physical significance. In particular, our method can be applied to the analysis of charge densities expressed as a sum of Gaussian functions centered at different radii, whose widths are constrained to be larger than a minimal width, Γ, of physical significance (Sick 1974, McCarthy, Sick & Whitney 1977) and represent a generalization of the usual adopted procedure based on Fourier transforms, etc.

THE REGULARIZATION PROCEDURE

It is worth noticing that the term involving the Dirac function in Eq. (4)—when different from zero—reduces Eq. (1) to an integral equation of the second kind which, in practice, is of the Fredholm type. In fact, since $\rho(\vec{s})$ vanishes outside a finite region, the (in principle) infinite integral of Eq. (1) can be replaced by a finite one. Moreover, since we are mainly interested in finite nuclei in the neighborhood of major shell closures for which many precise experimental data and also theoretical results are available, spherical shapes can be assumed and—because of the spherical symmetry—the three-dimensional problem of Eq. (1) can be reduced to a monodimensional integral one depending on the radial coordinate only.

Different nuclear shapes, namely nuclei with stable axially-symmetric deformations, can be easily included in the following formalism at the cost of a slightly heavier computational task, in an analogous way to that applied to the stellar image reconstruction of elliptic galaxies by Monnet, Bacon & Emsellem (1992), with respect to spherical (globular) ones, analyzed by Bendinelli (1991).

If $c_p \neq 0$, i.e. $a_p \neq 1$, is not approaching an eigenvalue of the kernel in Eq. (1), the relevant solution, $\rho(\vec{s})$, can be evaluated by means of stable methods, like the direct numerical inversion of the linear algebraic system obtained by discretization of the corresponding monodimensional case of Eq. (1), or the Fourier transform technique of Eqs. (2, 3). This is the most common case, usually dealt with in the literature.

If $a_p = 1$, as for Drell's and Hofstadter's proton models (see Table 1), Eq. (1) becomes an integral equation of the first kind, which gives rise to an ill-posed problem (Tikhonov & Arsenine 1976), whose solution is unstable under arbitrarily small perturbations which are always present because of experimental uncertainties. Naïve techniques for the numerical inversion of Eq. (1), which do not take into account the ill-posedness of the problem, will strongly depend on even small data errors, and be numerically unstable. In fact, from the Riemann–Lebesgue theorem for integrable functions it results that even small perturbations in $\rho^{+}(r)$ produce arbitrarily large perturbations in the solution, $\rho(s)$, and therefore Eq. (1) cannot be directly inverted.

It is worth mentioning that this solution instability originates from kernel properties only and does not arise from the adopted method of inversion. In particular, even if we consider the conjugate space by means of suitable Fourier (or Bessel–Fourier) transforms, the ill-posedness of the problem still holds and any relevant solution is highly unstable. In these cases Eq. (3) represents just a formal result without physical usefulness, which can be—in principle—affected by unpredictable numerical errors.

As an example, in Fig. 1 the nuclear density of ^{40}Ca obtained by direct inversion of Eq. (1) is shown and the ill-posedness of this particular problem is evident from the unphysical fluctuations of the deconvoluted distribution. This fact does not depend, of course, on the adopted method for numerical inversion and, moreover, we have obtained similar results by using different algorithms and computing codes or routines, such as those provided in the main software packages (LINPACK, IMSL, NAG, etc.). Therefore, in order to manage this class of cases which cannot be handled by means of the usual formalism, a suitable regularization procedure (Tikhonov & Arsenine 1976, Davies *et al.* 1983) has to be applied which reduces the problem to a well-posed one admitting stable approximate solutions. According to Tikhonov's regularization method (Tikhonov & Arsenine 1976), Eq. (1) can be transformed into a corresponding variational problem by imposing suitable con-

Table 1. Parameters of different proton models.

Model	a_p	b_p	μ_p (fm^{-1})
Pointlike	0.0	0.0	∞
Drell	1.0	0.0	2.841
Hofstadter	1.0	0.5	4.016
Clementel-Villi	1.2	0.0	3.115

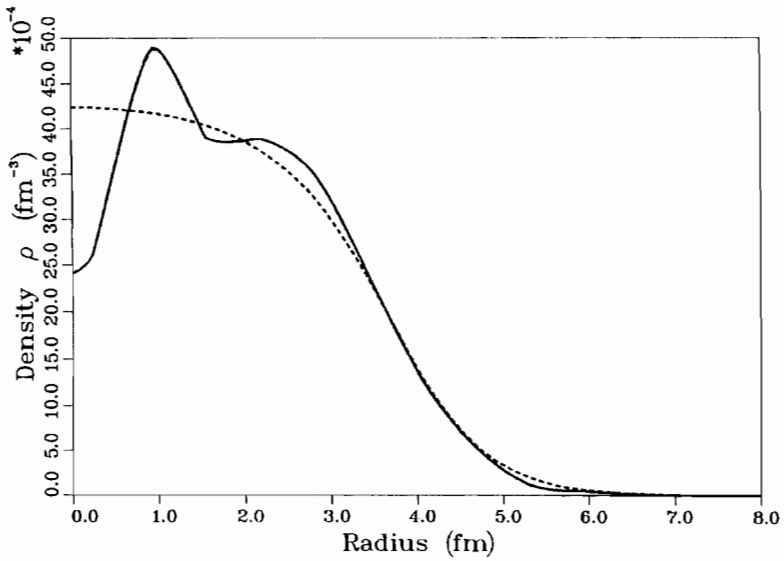

Fig. 1. Nuclear density of ^{40}Ca (solid line), obtained from empirical electric charge density measured by Sinha *et al.* (1973), (dashed line) by direct inversion of Eq. (1) without regularization.

straints on the solution, based on *a priori* knowledge about its smoothness and boundary conditions. It must be noticed that the regularization method depends only on very general conditions on differentiability and boundary at infinity, which do not constrain the resulting distribution from a physical point of view.

We write Eq. (1) in the L_2 space of square summable functions defined in the real interval $S = [0, r_0]$, where r_0 is the upper bound for nuclear and charge densities, namely $\rho(r) = 0$ for $r \geq r_0$. Equation (1) can then be put in the following form:

$$f^{\dagger} = Kf, \tag{5}$$

where

$$f^{\dagger}(x) = f_0^{\dagger}(\mu_p r) = \frac{4\pi r}{\mu_p^2}\rho^{\dagger}(r) = \frac{4\pi}{\mu_p}\int_0^{r_0} K(\mu_p r, \mu_p r')\rho(r')\, r'\, dr'. \tag{6}$$

The L_2-setting is suggested by the smoothness conditions for $f^{\dagger}$ dictated by physical assumptions (the nuclear density and its first derivative are continuous and bounded functions) and by the properties of the kernel, so defined:

$$Kf = \int_0^{r_0} k(x, y) f(y)\, dy, \tag{7}$$

with $f(y)$ as given in Eqs. (5, 6) and $k(x, y)$ defined as follows:

$$k(x, y) = \begin{cases} \bar{k}(x, y), & \text{if } y \leq x, \\ \bar{k}(y, x), & \text{otherwise} \end{cases}$$

$$\bar{k}(x, y) = \mu_p e^{-x}[(1 - b_p + b_p x)\sinh y - b_p y \cosh y]. \tag{8}$$

Some assumptions also have to be made about the searched function, f. Without loss of generality, we assume that f is differentiable up to the fourth order and vanishes at zero and r_0, together with its first derivative. Then, a regularized solution of Eq. (5) can be easily obtained by minimizing in the considered subspace of L_2 the following quadratic functional:

$$\Phi_\alpha(f) = \|Kf - f^\dagger\|^2 + \alpha\|Lf\|^2, \tag{9}$$

where symbol $\| \bullet \|$ denotes the L_2 norm, Lf is the stabilizing functional where L is a linear operator inclusive of constrained conditions on the solution (Davies *et al.* 1983, Bonifazzi, Maino & Tartari 2000), while α is the so-called regularization parameter. It can be shown (see, for instance, Tikhonov & Arsenine 1976) that the variational equation (9) admits a unique solution for $\alpha > 0$ which is stable against perturbations on $f^\dagger(x)$ and converges uniformly to the solution, $f(y)$ of Eq. (5) when $\alpha \to 0$, depending in an appropriate way from the norm of the error, and simultaneously the data error vanishes.

In this way a correspondence is set between the ill-posed problem of Eqs. (1, 5) and the well-posed one represented by the minimization of functional (9). This can be accomplished by solving the relevant Euler equation once a discretization procedure has been applied to Eq. (9). The detailed derivation of the discrete analogue of Eq. (9) and the description of the relevant numerical algorithm are given by Bonifazzi, Maino & Tartari (2000).

It is worth pointing out that the suitable value of the regularization parameter, α, depends on both the stabilizing functional (9) and the uncertainties on the experimental data, represented by function $f^\dagger$. In practice, it is determined by a numerical iteration procedure, essentially based on an *a posteriori* choice strategy and stopping rule (Turchin, Kozlov & Malkevich 1971, Engl & Gfrerer 1988, Landl *et al.* 1991, Bonifazzi, Maino, & Tartari 2000), that lead to an optimal convergence setting between accuracy and stability of the searched solution.

DISCUSSION OF THE NUMERICAL RESULTS

In Figs. 2, 3 and 4, numerical results for ^{40}Ca and ^{60}Ni are shown, obtained by means of the procedure described in the previous section. We recall that these cases cannot be solved by means of the usual approaches developed in the literature, since they represent severely ill-posed problems. However, the deduced nuclear mass densities can be safely compared with the corresponding quantities obtained by Minelli, Pascolini & Villi (1985), resorting to different proton models such as that of Clementel-Villi, for instance. Results obtained with use of different proton models and inversion procedures show an overall agreement, with some discrepancies

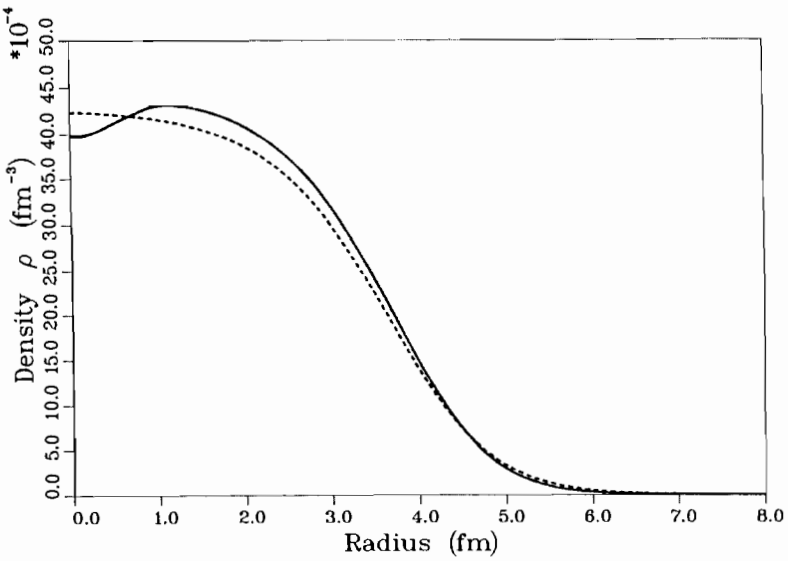

Fig. 2. Nuclear density of ^{40}Ca (solid line), obtained from empirical electric charge density measured by Sinha *et al.* (1973), (dashed line) by means of Tikhonov's regularization procedure as described in the text. Hofstadter's proton model has been considered.

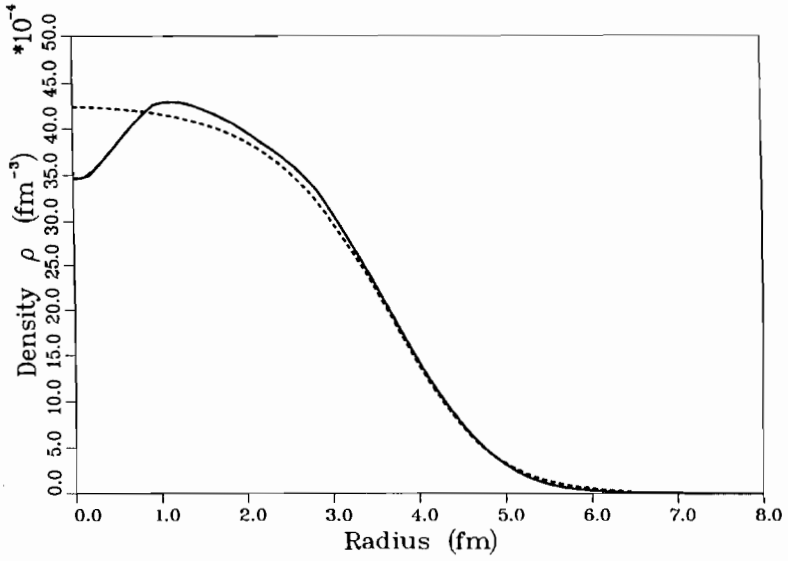

Fig. 3. Same caption as for Fig. 2. In addition, an uncertainty of 10% on the experimental charge-density distribution has been included in the calculations for the nuclear density.

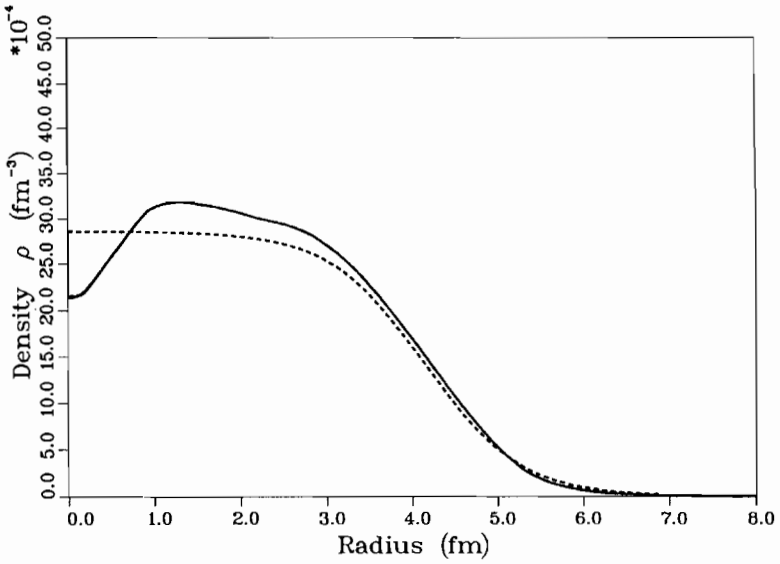

Fig. 4. Nuclear density of ^{60}Ni (solid line), obtained from empirical electric charge density measured by Litvinenko *et al.* (1972), (dashed line), affected by a 10% uncertainty, by means of the proposed regularization procedure. Use has been made of Drell's proton model.

arising in the innermost nuclear region where experimental charge densities are determined with less precision than in outer regions since high-momentum transfers are concerned.

As for the error related to the reconstruction procedure starting from the estimated uncertainties on the experimental data, it is possible to yield an estimate of the error on f, whose explicit form will be given elsewhere. Therefore, the formalism here described can take into account error propagation on deduced quantities and give confidence limits on the calculated nuclear mass densities, to be compared with model predictions. Moreover, our technique is so manageable that electric-charge densities can be supplied in Fourier–Bessel expansions (Dreher *et al.* 1974, de Vries *et al.* 1987), as a sum of Gaussians (Dreher *et al.* 1974, Sick 1974, McCarthy, Sick & Whitney 1977) or by discrete points (not only in closed analytical forms as those considered in the examples of Figs. 2–4), and both microscopic and phenomenological proton form factors can be accounted for.

Finally, the proposed approach provides a general theoretical framework to deal with reconstruction procedures in electron scattering experiments, which includes the usual techniques as particular cases corresponding to special forms of the stabilizing functionals in Eq. (9).

ACKNOWLEDGEMENT

This work has been performed in the frame of the MURST-ENEA research program, QWAA.01, on *Nonlinear and Complex Systems*, and the MURST-UE international project GIANO, funded by 488/92 law.

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(Accepted 23 April 2000)

مشكلة تكاملية في تشتت الإلكترون المرن

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خلاصة

المشكلة الكلاسيكية لاستنتاج التوزيع القطري لمركز كتلة بروتونات من كثافات شحنة كهربائية تعد غير مكتملة ، وذلك بالنسبة لكل من حالتي منطقية الظاهرة ووصفية استقلالية النموذج . يمكن الحصول على حلول موافقة لمعادلة فريدهولم بصيغة عددية ، وذلك بواسطة تقنيات مختلفة مثل تحويل فوريور ، التحليل المرشح ...الخ . نقدم إطاراً نظرياً مبني على طريقة للتنظيم ، والتي تحاصر كل هذه الطرق ، ويمكن استخدامها في الحالات العامة بما فيها حالات عدم الاكتمال القوية مما يلزم بشروط مناسبة تعتمد على السلوك الأملس ، والشروط الحدودية . وقد عرضت ونوقشت بعض الأمثلة الواقعية.