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RELIABILITY CONDITIONS IN QUADRATURE ALGORITHMS

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1 Introduction

The existing algorithms for the numerical integration of real valued functions (see, e.g., [1] for details on the available algorithms and a recent review of numerical quadrature) are tailored for specific classes of integrands, with limited possibilities to solve simultaneously families of integrals falling in different classes.

In the attempt to get numerical solution of integrals over ranges of the first Brillouin zone in the two-band singlet-hole Hubbard model of cuprate superconductors [2]–[4], the reliability of the existing numerical algorithms was found to be exceedingly poor to allow straightforward physical insight. The integrals entering this model involve a variable parameter (the hole or electron doping in the high-T_c superconductor) the variation of which results in substantial modification of the behaviour of the involved functions over the Brillouin zone. Thus, in order to make possible the exploration of the predictions of the physical model on the doping, which is fundamental for the acceptance of the proposed mechanism as responsible of the superconducting pairing in cuprates, ways of improving the reliability of the decisions within the automatic adaptive quadrature had to be sought.

To our best knowledge, the $\mathrm{U}(1) \times \mathrm{SU}(2)$ gauge theory model of underdoped cuprate superconductors [5, 6] met similar difficulties.

We may therefore assume that a study able to increase the reliability of the parametric integrals in connection with the solution of physical models is of interest for a large category of users of quadrature algorithms. A recent study [7] addressed a similar problem. However, the proposed solution was found to be too restrictive. In the present paper, we address the reliability problem of the local error estimate e associated to a quadrature sum q on a much general basis.

There are two main reasons why the computed value of e cannot be acceptable: either the occurrence of an *insufficiently resolved integrand profile at the quadrature knots*, or the occurrence of *difficult isolated points* (integrable singularities, turning points, jumps) which result in slow convergence. The identification of both kinds of difficulties can be explicitly done by means of a number of consistency criteria which check whether the integrand profile satisfies or not requirements following from the general definition of the Riemann integral, the fundamental properties of the basis polynomials spanning the approximating linear

space where the interpolatory polynomial of the quadrature rule is defined, the properties of the continuous monotonic functions, and the properties of continuous functions at or near their extremal points.

The occurrence of an insufficiently resolved integrand profile is always superseded under repeated subdivision of the integration range, which eventually results in the fulfillment of all the reliability constraints. The identification of a difficult integrand point may originate both in the occurrence of an insufficiently resolved integrand profile or of a genuine difficult integrand point. In the first case, the diagnostics will no more recover such a point under further subrange subdivision. In the latter case, the diagnostics will remain the same under repeated subrange subdivisions. Therefore, in all the alternatives, the *diagnostics stability under iteration* is achieved. This is the point where the general control routine of an automatic quadrature rule can take safe decisions concerning the best way to continue the solution or to decide that the integral was solved within the input accuracy specifications.

Since the automatic decision processes are all based on diagnostics obtained from the analysis of integrand profiles defined *locally*, we have to consider first the problem of *local quadrature rules* and to establish diagnostics over a single integration range. Thus, while we refer in the sequel to local couples $\{q, e\}$ only, the validation algorithm is formulated such as to be directly applicable to automatic quadrature problems.

The basic definitions and notations of the quantities of interest are given in section 2. The main new results derived within this investigation are summarized in section 3. To assess their practical importance, in section 4 we discuss numerical evidence obtained from the solution of integrals by Gauss-Kronrod 10–21 quadrature rules [8] with improved error estimate [7]. Concluding comments are given in section 5.

2 Definitions and notations

Let I denote the actual value of the integral to be solved numerically,

$$I \equiv I[f] = \int_a^b g(x)f(x)dx \ , \ -\infty < a < b < \infty. \tag{1}$$

Here, the *weight function* $g(x)$ is an analytically integrable function which absorbs a *difficult part* of the integrand (e.g., an oscillatory or a singular factor). In the absence of such factors, $g(x) = 1$. The integrand

function $f(x)$ is assumed to be *continuous almost everywhere* on $[a, b]$, such that (1) exists and is finite.

A *local quadrature rule* produces as solution of (1) a couple $\{q,\ e\}$, where the *quadrature sum* q yields an approximate value of the integral I, while the *local error estimate* $e > 0$ provides information on the accuracy of q. If $e > |e_Q|$, where

$$e_Q = I - q \tag{2}$$

is the actual error associated to q, then the couple $\{q,\ e\}$ is *reliable*, otherwise it is *unreliable* and the numerical solution fails.

To get a $(2n + 1)$-knot interpolatory quadrature sum q_{2n}, the integrand $f(x)$ is replaced by an interpolatory polynomial of $2n$-th degree,

$$P_{2n}(x) = \sum_{k=0}^{2n} \alpha_k\ p_k(x), \tag{3}$$

where $\{p_k(x)\}$ is the set of orthogonal polynomials of degree at most $2n$ spanning the approximating space of $P_{2n}(x)$. The coefficients α_k are obtained from the set of conditions of interpolation

$$P_{2n}(x_i) = f(x_i), \tag{4}$$

at a set of $2n + 1$ abscissas inside $[a, b]$, $a \leq x_0 < x_1 < \cdots < x_{2n} \leq b$.

Although most of the following discussion holds true for general quadrature sums, we restrict it to *symmetric* $2n + 1$-knot quadrature sums. In this case, the interpolation abscissas inside $[a, b]$ are given by

$$x_i = c + hy_i;\ c = (b + a)/2;\ h = (b - a)/2;\ i = -n, -n + 1, \cdots, n, \tag{5}$$

where the reduced quadrature knots y_i are defined on $[-1, 1]$, such that $0 = y_0 < y_1 < y_2 < \cdots < y_n \leq 1$, while $y_{-i} = -y_i,\ i = 1, \cdots, n$.

The local quadrature sum q_{2n} is then expressed as a linear combination of the integrand values at the quadrature knots,

$$q_{2n} \equiv Q_{2n}[f] = \sum_{i=-n}^{n} w_i f(x_i)\,, \tag{6}$$

with the quadrature weights showing the symmetry property $w_{-i} = w_i$.

The information provided by the $2n + 1$ integrand values at the quadrature knots, $\{f(x_i) | i = -n, \cdots, n\}$, is insufficient for the derivation of an expression for the error estimate e_{2n} associated to q_{2n}.

Kronrod [9] derived an error estimate (called in what follows *genuine Gauss-Kronrod* kind of error estimate) from an upper bound of the right hand side of

$$e_{ggk} = |q_{2n} - q_n| \,, \tag{7}$$

where q_{2n} is the quadrature sum (6), while q_n is a lower degree quadrature sum derived over the subset of (5),

$$x_{-n+\gamma} < x_{-n+\gamma+2} < \cdots < x_{n-\gamma-2} < x_{n-\gamma} \,, \tag{8}$$

where $\gamma = 1$ for an open quadrature sum (typically, the Gauss-Kronrod (GK) quadrature where the spanning basis $\{p_k(x)\}$ in (4) is given by Legendre polynomials and their orthogonal Kronrod extensions), while $\gamma = 0$ for a closed quadrature sum (typically, the Clenshaw-Curtis (CC) quadrature where the spanning basis $\{p_k(x)\}$ in (4) is given by Chebyshev polynomials).

In the QUADPACK package [8], which has been incorporated in most major program libraries, while maintaining unchanged the above idea in the case of the CC quadrature, the GK error estimate was reformulated as follows. Let $\tilde{f}$ denote the computed value of the average of $f(x)$ over $[a, b]$ at the knots (5),

$$\tilde{f} = q_{2n}/(b-a) \,, \tag{9}$$

and let $\Delta = Q_{2n}\big[|f - \tilde{f}|\big]$ denote the computed value of the integral $\int_a^b |f(x) - \tilde{f}| dx$, which measures the area covered by the deviations of $f(x)$ around $\tilde{f}$.

The local QUADPACK *error estimate* (QDP) is then given by

$$e_{qdp} = \Delta \times \min\{(200 e_{ggk}/\Delta)^{3/2},\ 1\}. \tag{10}$$

The values (7) and (10) are taken for error estimates provided they do not fall below the attainable accuracy limit imposed by the relative machine precision. The latter threshold is defined as the product

$$e_{roff} = \tau_0 \epsilon_0 Q_{2n}\big[|f|\big]. \tag{11}$$

Here τ_0 is an empirical multiplicative factor (following QUADPACK, we have chosen $\tau_0 = 50$) and ϵ_0 denotes the relative machine accuracy.

Using the error estimates (7), (10) and (11), we get the improved error estimate [7]

$$e_{2n} = \max\left[e_{roff},\ \min(e_{ggk}, e_{qdp})\right] \,. \tag{12}$$

For the case study integrals considered below, the value I of (1) is computed from the existing analytical expressions, such that the *exact* error e_Q (2) of the quadrature sum q_{2n} can be defined.

In the graphical presentation of the quadrature errors, the *moduli of the relative errors* (simply called relative errors in the sequel) are useful,

$$\varepsilon_\alpha = |e_\alpha / I| \,, \quad \alpha \in \{2n, Q\}. \tag{13}$$

The derivation of the local error estimate e_{2n} within a subroutine which implements a quadrature rule uses information inferred from the *estimated relative errors*,

$$\rho_{2n} = |e_{2n} / q_{2n}| \,. \tag{14}$$

3 Well-conditioned integrand structures

The set of integrand values at the quadrature knots (5) define the *integrand profile*, the study of which provides the necessary information concerning the output reliability. The derivation of criteria concerning its well-conditioning uses several kinds of consistency arguments which are discussed in separate subsections.

3.1 Insensitivity of the integral sums to discretization details

The very definition of the integral sums in a Riemann integral assumes the fulfillment of the following two features:

(i) The norm of the discretization defined over the integration domain tends to zero.

(ii) The integral sum is insensitive to the the addition or removal of a single discretization abscissa within the defined partition.

These features have straightforward consequences in the numerical quadrature:

(I) A denser discretization of a well-defined integrand $f(x)$ secures better accuracy of the quadrature sums than a sparser one.

(II) The removal of a single knot value from the sampling of a well-defined integrand $f(x)$ does not result in *substantial* modification of the integrand profile.

The quantity

$$d_{av} = 1/n \tag{15}$$

defines the average density of the quadrature knot distribution over the fundamental range $[-1, 1]$.

For the GK and CC quadrature rules mentioned above, the fundamental range $[-1, 1]$ consists of a sparser knot region centered around the origin and two denser knot regions located towards the range ends.

A direct consequence of the well-conditioning criterion (I) is the following enhancement of the opposite of (II):

(IIa) If the sensitivity criterion (II) is infringed over a region of dense discretization, then the integrand profile is ill-conditioned.

3.2 Features of the basis orthogonal polynomials

Since the equations (5) perform the mapping of the original interval $[a, b]$ onto the reduced interval $[-1, 1]$ over which the orthogonal polynomials are usually defined, in this subsection we refer to this reduced interval and use the notation $p_k(y)$ for the basis polynomials. All the properties discussed below hold true over arbitrary interval lengths, hence reference to the expression (3) of the interpolatory polynomial spanned by the basis orthogonal polynomials does not give rise to any confusion.

Within the set of basis polynomials spanning the interpolatory polynomial (3), the following properties hold true:

(iii) $p_0(y) = const.$

(iv) The set of the successive extremal values of a polynomial $p_k(y)$ of degree $k \geq 1$ defines an *alternating sequence* over $[-1, 1]$.

(v) The locations of the extremal values of the polynomials $p_k(y)$ and $p_{k+1}(y)$ are interlaced over the open range $y \in (-1, 1)$.

There are several straightforward consequences of these features upon the numerical quadrature rules:

(III) The average value $\tilde{f}$, Eq. (9), of the integrand $f(x)$, which defines its zeroth order moment over the sampling (5), serves as reference value with respect to which the oscillations of the integral profile are counted.

(IV) The deviations from $\tilde{f}$ of the successive extremal values within the quadrature knot sampling of a well-conditioned integrand $f(x)$ define an alternating sequence.

(IVa) If the sampling of a well-conditioned integrand $f(x)$ defined at the abscissas of a symmetric quadrature rule *is folded around the centre c of the integration domain* $[a, b]$, then the well-conditioning property (IV) still holds true.

(V) Over any subdomain length within the regions of dense knot discretizations inside $[a, b]$, the ratio between the number of successive extremal values of the integrand profile over the *fine sampling* (5) and the corresponding number defined over the *coarse sampling* (8) cannot be larger than two.

Over the sparser region around the center, the above ratio is to be counted for the fine sampling value decreased by one.

3.3 Well-conditioning over monotonic subranges

Within any monotonicity subrange of a smooth first order differentiable function f(x), the first order derivative smoothly vary from point to point.

Within numerical quadrature, the fulfillment of this property for well-defined integrands can be checked by making use of first order divided differences. If the integrand profile is monotonic over $[a, b]$, or monotonicity subranges can be defined which extend over three successive knots at least, then a smoothly varying profile will by characterized by the *absence of jumps:*

(VI) Over monotonicity ranges, the ratio of successive first order divided differences cannot exceed a smoothness threshold which depends on the relative accuracy requsted at the input.

If one of the knots involved in the divided differences is an extremal point, or it coincides with one of the end points a or b of the integration domain, then this smoothness condition is to

be checked only one-directionally, skipping the case of vanishingly small divided difference at the extremal point.

3.4 Integrand variations around its isolated extremal points

The lateral first order derivatives of a smooth first order differentiable function vanish at an extremal point, while the curvature of a second order differentiable function (which is given by the second order derivative) keeps constant sign over a nonvanishing neighbourhood of the extremum.

Within the discrete mesh defined by the quadrature knots, inquieries about these properties can be made only at *isolated* extremal points of the integrand.

As it concerns the first order derivatives, the following consistency criterion establishes the normal relationship which should exist within the data:

(VII) Let us assume that an extremal point isolated to the right/left of a well-conditioned integrand was identified over a sufficiently well resolved integrand profile.

Then the approximation of the lateral derivative as defined from data over the fine sampling should be closer to zero as compared to the value estimated from data defined over a coarse sampling with respect to the extremum location.

The following consistency criterion establishes the sign constancy of the curvature of a well-conditioned smooth integrand:

(VIII) Let us assume that an extremal point isolated to the right/left of a well-conditioned integrand was identified over a sufficiently well resolved integrand profile.

Then the approximation of the second order derivative as defined from data over the fine sampling centered at the extremum should have the same sign as compared to the value estimated from data involving the reference extremum as a lateral point to the left/right.

The technical implementation of these consistency requirements needs the definition of the isolated extremal points of the mesh at the quadrature knots.

The following definition allows the analysis of lateral both first and second order derivatives:

Definition # 1: An extremal point is *isolated to the right* if it is separated from the previous extremum to the left by *at least one* intermediate quadrature knot and it is separated from the next extremum to the right by *at least* n_{iso} intermediate quadrature knots.

A similar definition holds for an extremal point which is *isolated to the left.*

The next definition applies only to lateral limits of the first order derivatives:

Definition # 2: An extremal point is *isolated to the right/left* provided it is separated from the next extremum to the right/left by *at least* n_{iso} intermediate quadrature knots.

For practical purposes, a value $n_{iso} = 2$ was chosen for the estimate of the first order derivatives, while a value $n_{iso} = 4$ was chosen for the estimate of second order derivatives. The latter value is necessary to ensure the *absence* of the inflection point from the region of analysis with a sufficiently high probability.

To illustrate how such an analysis works, consider for instance the case of an extremal point isolated to the right in the frame of the first definition.

Let the reference extremum be denoted x_0. Then the available information range over which the analysis may be done extends over the set of abscissas $\{x_{-1}, x_0, x_1, x_2\}$ at which the integrand function takes respectively the values $\{f_{-1}, f_0, f_1, f_2\}$.

To estimate the right lateral approximation of the first order derivative, we define the interpolatory polynomial of the third degree fitting these four data. This yields the following result:

$$f'_{r,fine}(x_0) = d^{(1)}_{1,0} - \frac{h_{1,0}}{h_{2,-1}}\left[h_{0,-1}d^{(2)}_{2,1} + h_{2,0}d^{(2)}_{1,-1}\right]. \tag{16}$$

Here, $h_{i,j} = x_i - x_j$, $d^{(1)}_{i,j} = (f_i - f_j)/h_{i,j}$ denote the first order divided differences at x_i and x_j, while $d^{(2)}_{2,1} = \left(d^{(1)}_{2,0} - d^{(1)}_{1,0}\right)/h_{2,1}$ and $d^{(2)}_{1,-1} = \left(d^{(1)}_{1,0} - d^{(1)}_{0,-1}\right)/h_{1,-1}$ denote specific second order divided differences.

On the other hand, the coarse sampling around x_0 yields:

$$f'_{r,coarse}(x_0) = d^{(1)}_{2,0}. \tag{17}$$

The criterion (VII) then simply requires that the approximations (16) and (17) should satisfy $|f'_{r,fine}(x_0)| < |f'_{r,coarse}(x_0)|$.

Over the same set of data, the condition for the constancy of the sign of the second order derivative writes

$$\left(d^{(1)}_{2,0} - d^{(1)}_{1,0}\right)\left(d^{(1)}_{1,0} - d^{(1)}_{0,-1}\right) > 0\,. \tag{18}$$

3.5 Stability of the diagnostics under subrange subdivision

The existence and finiteness of the Riemann integral (1) guarantees that, for a well-defined integrand, the discretization process will reach, after a *finite* number of subrange subdivisions, a *stable* profile configuration, the refinement of which will result in unessential modifications only.

Under the occurrence of *isolated* difficult points of the integrand, the discretization process will resolve the profile over the well-conditioned subranges within a finite number of subrange subdivisions, and then it will mainly create a dense mesh around the difficult points. In this case, the automatic control subroutine will safely decide upon the activation of a specific convergence acceleration algorithm, such that a reliable numerical solution will be available in the end.

The achievement of the *stability* of the iterative diagnostics emerging from the study of the conditioning properties of the integrand profiles over subranges is the fundamental feature which secures the efficiency of the procedure proposed in this investigation. We formalize it in the final reliability criterion, enabling safe automatic control decisions:

(IX) The iterative integrand profile analyses result in *stable* diagnostics after a finite number of subrange subdivisions.

The occurrence of identical reliability diagnostics under successive subrange subdivisions enables the general control routine to make safe choices among the implemented alternatives.

4 Numerical results

To illustrate the present analysis, numerical data have been obtained from Gauss-Kronrod 10–21 (`GK 10-21`) quadrature rule solutions of the families of elementary integrals considered in ref. [7].

First, we considered the two families involving monotonic integrands:

- Integrals over $[0,1]$ of the terms of the fundamental power series, x^n,

$$\int_0^1 x^n \, dx \; = \frac{1}{n+1}, \quad n = 0, 1, \cdots, 1023. \tag{19}$$

- Integration of a constant integrand (which simulates a centrifugal potential at large x) over ranges of variable length,

$$\int_0^b \frac{1}{x^2+1} \, dx \; = \arctan(b), \quad b = 2^n, \quad n = 0, 1, \cdots, 511. \tag{20}$$

For these two families of integrals, the conclusions drawn from the numerical outputs can be summarized as follows:

- The present analysis correctly identified the upper threshold n_{cr} which separates the outputs carrying at least two most significant figures from the spurious outputs: $n_{cr} = 160$ in the case of the first family of integrals, and $n_{cr} = 8$ in the case of the second family. These figures are to be contrasted with the answers $n_{cr} = 59$ and $n_{cr} = 4$ respectively yielded by the error estimates proposed in [7].

- For the higher order values of the parameters n entering the two families of integrals, the present analysis predicted the occurrence of jumps, somewhere inside the sparser discretization region.

Fig. 1 illustrates the behaviour of the error estimates with the power n in the case of the family of integrals (19).

Second, we considered two families of integrals showing nonmonotonic (oscillatory) behaviour, written in algebraically equivalent forms:

$$\textbf{(C1)} \qquad \int_{-1}^1 e^{p(x-x_0)} \cos(\omega x) \, dx \; = \tag{21}$$

$$\textbf{(C2)} \qquad \int_0^1 2e^{-px_0} \cosh(px) \cos(\omega x) \, dx \; = \tag{22}$$

$$= 2e^{-px_0}[p \sinh(p) \cos(\omega) + \omega \cosh(p) \sin(\omega)]/(\omega^2 + p^2) \, ; \tag{23}$$

$$\textbf{(S1)} \qquad \int_{-1}^1 e^{p(x-x_0)} \sin(\omega x) \, dx \; = \tag{24}$$

$$\textbf{(S2)} \qquad \int_0^1 2e^{-px_0} \sinh(px) \sin(\omega x) \, dx \; = \tag{25}$$

$$= 2e^{-px_0}[p \cosh(p) \sin(\omega) - \omega \sinh(p) \cos(\omega)]/(\omega^2 + p^2) \, . \tag{26}$$

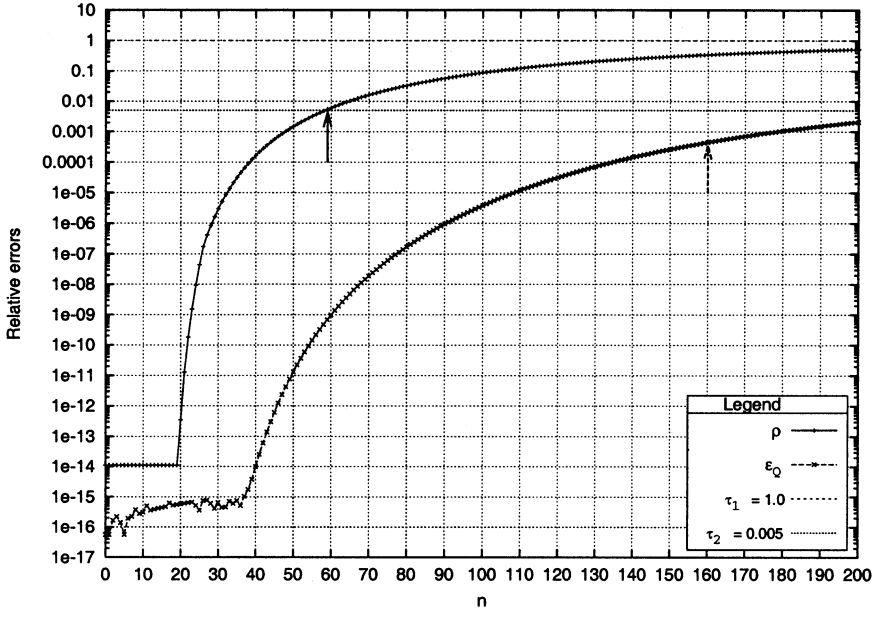

Fig. 1: Relative errors of the GK 10-21 outputs for the family of integrals (19) at exponents $n \leq 200$.

The parameter ω was chosen to run over the set of values

$$\omega_n = n\pi/60, \quad n \in \{0, 6000\}, \tag{27}$$

while constant values $p = 1$ and $x_0 = -1$ have been chosen on the ground that they are typical for the description of the behaviour of the numerical results.

The analysis of the families of integrals (21–25) shows that the identification of a well-conditioned nonmonotonic integrand profile needs testing the *complete set* of consistency criteria established in Sec. 3. Therefore, the analysis is long. However, it is straightforward and can be easily implemented in a computer program.

The main reward of the detection of a reliable output is the identification of its occurrence at a much earlier stage than within the standard qudrature programs. Fig. 2 provides supplementary support to the results reported in Fig 1.

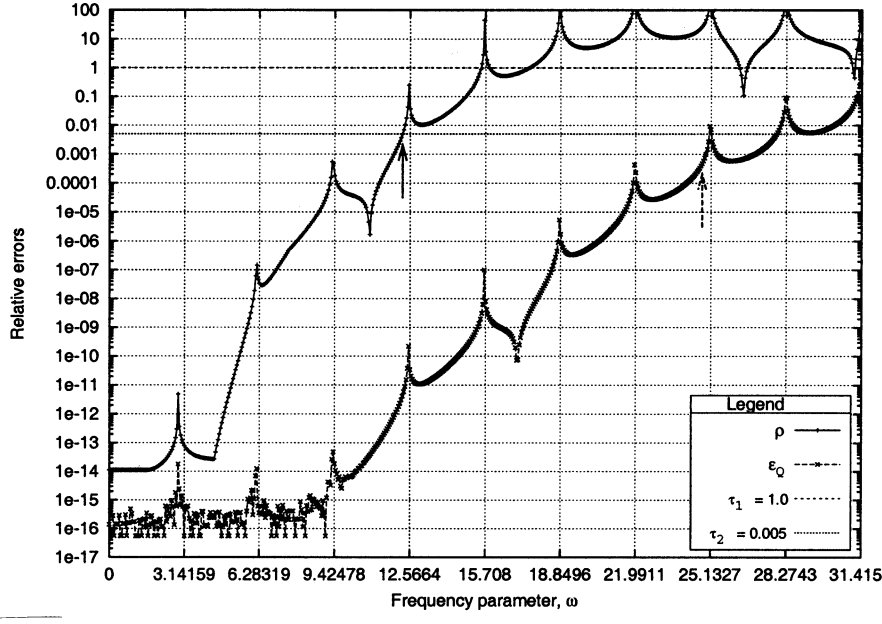

Fig. 2: Outputs of the GK 10-21 quadrature rule for the family of integrals (21) at $p = 1$. The left arrow points to the frequency parameter value up to which the improved error estimator proposed in ref. [7] shows that the output is reliable. The right arrow points to the result of the present analysis.

Fig. 3, presents integrand profiles for the four integrals (21–22) and (24–25) at an arbitrarily chosen large value $\omega = (1612\pi/60)$.

The analysis of the profile established their ill-conditionings due to the infringement of the following criteria:

- *The integral* **(C1)**: Criterion (IV) (four times, marked by solid line arrows) and criterion (II) (at knot label +5).

- *The integral* **(C2)**: Criterion (II) (five times, -8, -7, -6, +6, and +7) and criterion (VIII) (-4 (right) and +4 (left)).

- *The integral* **(S1)**: Criterion (II), once, in a dense region (+7) and criterion (VIII) [-3 (right) and +3 (left)].

  It is perhaps important to observe that the three apparent

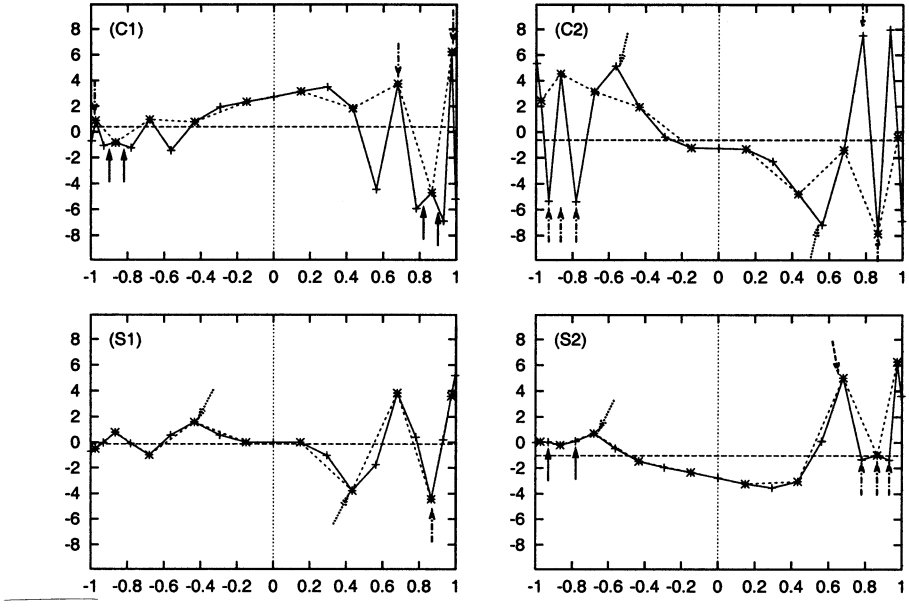

Fig. 3: Ill-conditioned integrand features in the family of integrals (21–25) at $\omega = 1612$.

infringements of criterion (VII) [-7 (left), -3 (right), and 3 (left)] which are suggested by the crudest approximations of the first order derivatives over the fine sampling are denied by the more accurate formula (16).

- *The integral* **(S2)**: Criterion (IV) (three times, marked by solid line arrows), criterion (II) (+6, +7, +8), criterion (VII) [+5 (left)], and criterion (VIII) [-5 (right)].

5 Comments and conclusions

The present investigation started from the need to get reliable numerical solutions of some difficult integrals occurring in theoretical models devoted to the study of the mechanism of the high-T_c superconductivity in cuprates [2]-[6]. An important prerequisite to be satisfied by the

automatic quadrature algorithm was the substantial increase of the reliability of the local error estimates.

We have found that the study of the conditioning of the integrand profile enables the formulation of validation criteria (consistency conditions for a well-conditioned profile) able to identify insufficient profile resolution or the occurrence of isolated difficult points of the integrand. The analysis is simple, it is intuitive, it is easily implemented in a computer program and it is easily done.

An important supplementary bonus offered by this analysis was the identification of output reliability ranges which are substantially larger as compared to those obtained within the usual implementations of quadrature routines. The unsatisfactory features noticed in the validation criteria developed in ref. [7] have been fully removed.

The subroutine doing the profile analysis described in this paper is documented and described in a separate document [10].

We conclude this study with the observation that the validation analysis described in the present paper is *not* intended to replace the existing quadrature algorithms. When the estimated accuracy exceeds a critical threshold (tentatively set to six decimal figures), then the present procedure is skipped altoghether. However, if this threshold is not attained, it is automatically activated by the general control routine. Its results prove to be invaluable in the analysis of complex integrands, where it is able to discover the overwhelming fraction of peculiar integrand profiles at early stages of the analysis.

Acknowledgments

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Условия достоверности алгоритмов вычисления квадратур

Для получения достоверных результатов при вычислении квадратур критическое значение имеет выявление плохо разрешенных или нерегулярных структур в подынтегральных функциях. Сформулированы критерии, налагаемые на профиль подынтегральной функции в узлах квадратурных сумм, выполнение которых позволяет повысить надежность вычислений до значений, близких к теоретически достижимому пределу 100 %, при одновременном улучшении оценки погрешности. Предлагаемый метод представляет наибольший интерес при вычислении интегралов, зависящих от параметров, в сложных физических моделях.

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Reliability Conditions in Quadrature Algorithms

The detection of insufficiently resolved or ill-conditioned integrand structures are critical for the reliability of the quadrature rule outputs. We show that the reliability can be raised towards the theoretical 100 % rate of success, under error estimate sharpening, provided the study of the profile of the integrand at the quadrature knots shows the fulfillment of several validation criteria. The proposed procedure is of the highest interest for the solution of parametric integrals arising in complex physical models.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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