Vol. 40 (2009) *ACTA PHYSICA POLONICA B* No 4

FROM GRAM–CHARLIER SERIES TO ORTHOGONAL POLYNOMIALS*

H.C. Eggers

Department of Physics, University of Stellenbosch
Stellenbosch, South Africa

(Received February 4, 2009)

The systematic study of shape in non-Gaussian HBT distributions requires a systematic understanding of the underlying mathematical structures. Gram–Charlier series as the statistics approach to their systematic description have elegant series and good properties but do not converge uniformly. Extensions and relationships to other systems are briefly outlined.

PACS numbers: 13.85.Hd, 13.87.Fh, 13.85.–t, 25.75.Gz

There has been a very successful programme of description of the shape of the two-particle correlation function $R(\boldsymbol{q}) = C(\boldsymbol{q}) - 1$ and the relative source distribution $S(\boldsymbol{r})$ by expansions in terms of spherical harmonics [1,2] and Cartesian harmonics [3], which are couched in the language of orthogonal functions and spherical coordinates $(q, r, \cos\theta_{qr})$. Expansions based on statistical considerations were proposed by Hegyi and Csörgő [4]. Termed "Edgeworth Series" there and more generally "Gram–Charlier Series", they are based on derivatives of a reference probability distribution function (PDF) $f_0(x)$.

Fully three-dimensional expansions for $R(\boldsymbol{q})$ in terms of a Gram–Charlier series (GCS) were calculated in [5]. With $\boldsymbol{q} = (q_1, q_2, q_3)$ the three-momentum difference in the out-side-long system, $R(\boldsymbol{q})$ is normalised to a "data PDF" $f(\boldsymbol{q}) = R(\boldsymbol{q}) / \int R(\boldsymbol{q})\, d\boldsymbol{q}$ with moments $\mu_{n_1 n_2 n_3} = \int f(\boldsymbol{q})\, q_1^{n_1}\, q_2^{n_2}\, q_3^{n_3}\, d\boldsymbol{q}$ and cumulants $\kappa_{n_1 n_2 n_3}$, while the reference PDF $f_0(\boldsymbol{q})$ has moments $\nu_{n_1 n_2 n_3}$ and cumulants $\lambda_{n_1 n_2 n_3}$. In Refs. [5, 6], the Gram–Charlier expansion with

* Presented at the IV Workshop on Particle Correlations and Femtoscopy, Kraków, Poland, September 11–14, 2008.

Gaussian reference $f_0(\boldsymbol{q})$ was calculated in detail, yielding

$$\begin{aligned}\frac{f(\boldsymbol{q})}{f_0(\boldsymbol{q})} &= 1+\tfrac{1}{4!}\left\{\kappa_{400}H_{400}[3]+4\kappa_{310}H_{310}[6]+6\kappa_{220}H_{220}[3]+12\kappa_{211}H_{211}[3]\right\}\\ &\quad+\tfrac{1}{6!}\left\{\kappa_{600}H_{600}[3]+6\kappa_{510}H_{510}[6]+15\kappa_{420}H_{420}[6]+30\kappa_{411}H_{411}[3]\right.\\ &\quad\left.+20\kappa_{330}H_{330}[3]+60\kappa_{321}H_{321}[6]+90\kappa_{222}H_{222}\right\} + \ldots \end{aligned} \tag{1}$$

with square brackets indicating the number of terms of a given type ("Stirling numbers") and where, with $n = n_1 + n_2 + n_3$,

$$H_{n_1 n_2 n_3}(\boldsymbol{q}) = \frac{1}{f_0(\boldsymbol{q})} \frac{(-1)^n \, \partial^n f_0(\boldsymbol{q})}{(\partial q_1)^{n_1}(\partial q_2)^{n_2}(\partial q_3)^{n_3}} \tag{2}$$

are the "hermite tensors" generalising normal hermite polynomials for an arbitrary covariance matrix. Prescriptions for experimental measurement of three-dimensional $\boldsymbol{q}$-cumulants $\kappa_{n_1 n_2 n_3}$ were set out in Ref. [6].

The GCS expansions are, however, asymptotic series, both in the sense that the magnitude of cumulants as well as some combinatoric factors entering the expansions both rise with order. It is therefore imperative to understand the behaviour of expansions in theory before applying them to experimental data with associated additional complications. At the same time, the use of non-Gaussian reference PDFs opens up significant opportunities, in the same way (but at a higher level) that fitting of non-Gaussian data is augmented by non-Gaussian parametrisations.

In the following, we therefore study the mathematics of underlying expansions while confining ourselves to the one-dimensional case. The reference PDF $f_0(x\,|\,\theta)$ will be a one-dimensional analytic PDF (which may or may not be Gaussian) with a parameter θ. The measured $R(\boldsymbol{q})$ will be modelled by another (definitely non-Gaussian) "test PDF" $f(x\,|\,\alpha)$ whose form and parameter(s) α are "measured experimentally", *i.e.* chosen freely for test purposes. The symmetry $R(-\boldsymbol{q}) = R(\boldsymbol{q})$ for identical particles guides our choice of symmetric toy PDFs, $f(-x) = f(x)$ and $f_0(-x) = f_0(x)$.

A Gram–Charlier series is an expansion of $f(x)$ in derivatives of $f_0(x)$,

$$f(x\,|\,\alpha) = a_0 f_0(x) - a_1 f_0'(x) + \tfrac{1}{2}a_2 f_0''(x) - \ldots = \sum_{j=0}^{\infty} \frac{a_j}{j!} \, (-D_x)^j f_0(x\,|\,\theta)\,, \tag{3}$$

where $D_x = (d/dx)$. Multiplying by e^{itx} and integrating, we find formally

$$\Phi(t\,|\,\alpha) = \sum_{j=0}^{\infty} \frac{a_j}{j!} \int e^{itx}\,(-D_x)^j f_0(x\,|\,\theta)\,dx\,, \tag{4}$$

where $\Phi(t\,|\,\alpha) = \int e^{itx} f(x\,|\,\alpha)\,dx$ is both the characteristic function and proportional to the relative source distribution for noninteracting particles. Assuming that $f_0(x)$ is continuous and that it and its derivatives vanish at the surface of the support of x, *i.e.* assuming that, after j-fold integration by parts

$$\int e^{itx}\,(-D_x)^j f_0(x\,|\,\theta)\,dx = (it)^j \int e^{itx}\,f_0(x\,|\,\theta)\,dx\,, \tag{5}$$

Eq. (4) simplifies to

$$\Phi(t\,|\,\alpha) = \Phi_0(t\,|\,\theta)\sum_{j=0}^{\infty}\frac{a_j}{j!}\,(it)^j\,, \tag{6}$$

where $\Phi_0(t\,|\,\theta) = \int e^{itx}\,f_0(x)\,dx$. Defining $\tau = it$ and $D_\tau = -i\,d/dt$, the a_j are then just the coefficients in the Taylor expansion of Φ/Φ_0 [7],

$$a_j = D_\tau^j \frac{\Phi(t\,|\,\alpha)}{\Phi_0(t\,|\,\theta)}\bigg|_{\tau=0} \tag{7}$$

and therefore functions of both parameter sets (α,θ). The characteristic functions can be expanded in terms of their respective moments or cumulants,

$$\Phi(t\,|\,\alpha) = \sum_{j=0}^{\infty}\frac{\tau^j}{j!}\,\mu_j = \exp\left(\sum_{j=1}^{\infty}\frac{\tau^j}{j!}\,\kappa_j\right), \tag{8}$$

$$\Phi_0(t\,|\,\theta) = \sum_{j=0}^{\infty}\frac{\tau^j}{j!}\,\nu_j = \exp\left(\sum_{j=1}^{\infty}\frac{\tau^j}{j!}\,\lambda_j\right), \tag{9}$$

and so the coefficients a_j can be expressed directly in terms of cumulant differences $\eta_j = \kappa_j - \lambda_j$,

$$a_j = D_\tau^j \exp\left(\sum_\ell \frac{\tau^\ell}{\ell!}\eta_\ell\right)_{\tau=0}\,. \tag{10}$$

Insertion of expressions obtained for the lowest orders leads to the GCS in terms of cumulant differences. Setting cumulants of odd order to zero due to the symmetry, we have

$$\begin{aligned} f(x) &= f_0(x) + \tfrac{1}{2!}\,\eta_2 f_0^{(2)} + \tfrac{1}{4!}\,(\eta_4 + 3\eta_2^2) f_0^{(4)} + \tfrac{1}{6!}\,(\eta_6 + 15\eta_4\eta_2 + 15\eta_2^3) f_0^{(6)} \\ &\quad + \tfrac{1}{8!}\,(\eta_8 + 35\eta_4^2 + 28\eta_6\eta_2 + 210\eta_4\eta_2^2 + 105\eta_2^4) f_0^{(8)} + \dots\,, \end{aligned} \tag{11}$$

with $f_0^{(j)} = D_x^j f_0(x\,|\,\theta)$. Define the functions

$$h_j(x\,|\,\theta) = \frac{(-D_x)^j f_0(x\,|\,\theta)}{f_0(x\,|\,\theta)}\,, \tag{12}$$

which for Gaussian f_0 are the usual hermite polynomials but will take on other forms for other choices of f_0. In terms of the $h_j(x)$, Eq. (11) can be expressed as

$$\begin{aligned}\frac{f(x)}{f_0(x)} &= 1 + \tfrac{1}{2!}\,\eta_2\,h_2(x) + \tfrac{1}{4!}(\eta_4 + 3\eta_2^2)\,h_4(x) + \tfrac{1}{6!}(\eta_6 + 15\eta_4\eta_2 + 15\eta_2^3)\,h_6(x)\\ &\quad + \tfrac{1}{8!}\,(\eta_8 + 35\eta_4^2 + 28\eta_6\eta_2 + 210\eta_4\eta_2^2 + 105\eta_2^4)\,h_8(x) + \dots \,. \end{aligned} \tag{13}$$

The textbook Gram–Charlier series, which we shall call the "fixed GCS" is the special case where f_0 is chosen to be Gaussian $f_0(x\,|\,\sigma) = e^{-x^2/2\sigma^2}/\sqrt{2\pi\sigma^2}$ with the free parameter $\theta^2 \equiv \sigma^2 = \lambda_2$ set equal to κ_2, the measured cumulant of $f(x)$, so that $\eta_2 = 0$ and (13) simplifies to

$$\frac{f(x)}{f_0(x)} = 1 + \tfrac{1}{4!}\,\eta_4 h_4(x) + \tfrac{1}{6!}\,\eta_6 h_6(x) + \tfrac{1}{8!}\,(\eta_8 + 35\eta_4^2)h_8(x) + \dots\,. \tag{14}$$

The same series can be expressed also in terms of moments, either by direct application of Eq. (7) and using $\mu_j = D_\tau^j \Phi(t)|_{\tau=0}$ and $\nu_j = D_\tau^j \Phi_0(t)|_{\tau=0}$, or multiplying both sides of (3) by x^k and integrating.

The above infinite sums are, of course, never implemented experimentally. Inevitably, a partial sum up to a maximum order k is used

$$f_k(x\,|\,\alpha) = \sum_{j=0}^{k} \frac{a_j}{j!}\,(-D_x)^j f_0(x\,|\,\theta)\,, \tag{15}$$

so that all formulae following from it will also be truncated at order k as experiments probably cannot measure cumulants beyond $k = 6$ or 8.

The textbook formalism for GCS which culminates in (14) is instructive and elegant, but it does not automatically yield a convergent series or even a partial sum which approximates $f(x)$ reasonably well. In Fig. 1, we show an example: take for the test PDF the "logistic distribution", $f(x\,|\,\alpha) = [4\alpha\cosh^2(x/2\alpha)]^{-1}$ which has cumulant $\kappa_2 = \alpha^2\pi^2/3$ and for the reference PDF a Gaussian $f_0(x\,|\,\sigma) = (2\pi\sigma^2)^{-1/2}e^{-x^2/2\sigma^2}$, choosing $\alpha = 1$ and $\sigma = \pi/\sqrt{3}$ to ensure $\eta_2 = 0$, we find that the successive partial sums improve from 2nd to 4th order but deteriorate for higher orders. The partial sums may also develop slightly negative tails, which would be unphysical.

Nevertheless, it is desirable to develop GCS-based systematic expansions as they have some good properties. For example, if the underlying variables (q_1, q_2, q_3) are statistically independent and a factorised reference PDF is

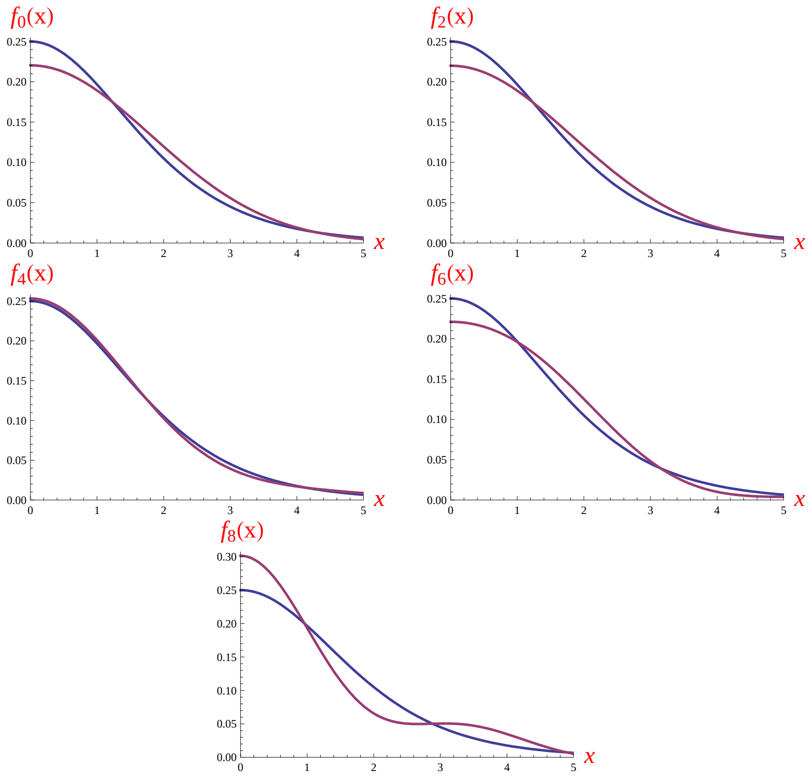

Fig. 1. Fixed GCS example. Partial sums of order beyond $k = 4$ do not improve as approximations of the non-Gaussian $f(x)$, the curve peaking at 0.25.

chosen, a three-dimensional GCS-based series will factorise into products of three one-dimensional series. Depending on the choice of series and reference PDF, the derivative functions $h_j(x)$ can be orthogonal and/or polynomial in form. The cumulant coefficients are highly sensitive measures of correlation, and the prescriptions to measure them exist. For nonsymmetric cases with "offsets", the formalism remains essentially unchanged. And there is flexibility in choice of reference PDF.

A first and immediate improvement over fixed GCS can be obtained with the "free GCS" with $\eta_2 \neq 0$ and expansion (13). The value of free parameter σ is in this case determined by a separate fit for each partial sum. For illustrative purposes, we approximate the experimental goodness-of-fit $\chi^2 = \sum_i [f(x_i) - f_k(x_i \,|\, \sigma)]^2/(\text{error})_i^2$ of a "parametrisation" $f_k(x)$ to "data" $f(x)$ by $\int f_0(x \,|\, \sigma)\, [f(x \,|\, \alpha) - f_k(x \,|\, \sigma)]^2\, dx$, where the f_0 weight mimics larger relative errors in the tails. (The point is not the detail of the fitting procedure *per se*, but the behaviour of the partial sums.) With $f(x)$ again the logistic distribution with $\alpha = 1$ and $f_0(x)$ the Gauss with variable σ, we obtain results shown in Fig. 2 with best-fit values $\sigma = \{1.62, 1.81, 1.86, 2.10, 2.11\} \pm 0.01$ for partial sums of order 0 to 8. While there is visible improvement over the fixed-GCS case, the approximation again does not improve uniformly with the order of the partial sum.

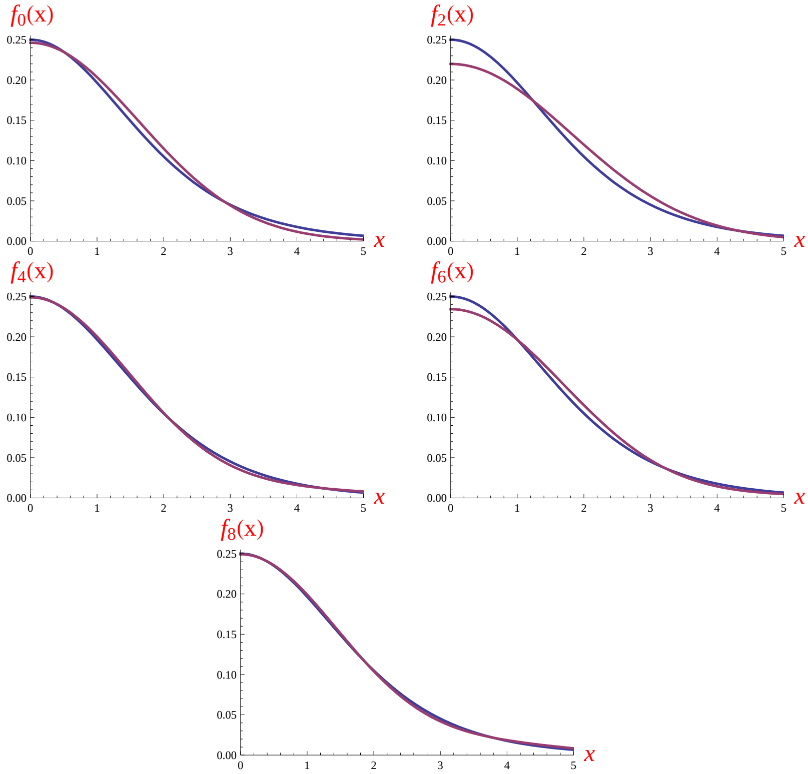

Fig. 2. Free-GCS example. The σ parameter of f_0 is adjusted for each order for a best fit. Approximations do not improve uniformly with increasing order of the partial sum.

Several generalisations of the basic GCS formalism are possible, the most immediate being the use of non-Gaussian reference PDFs. As in the above example, the available parameter can be either fixed from the data to ensure that $\eta_2 = 0$ or determined from fits.

Opening the door to non-Gaussian reference PDFs in the GCS formalism raises the question of the relationship to systems of orthogonal polynomials $\{\phi_r(x)\}_{r=0}^{\infty}$. Eq. (12) is a simplified form of a Rodrigues formula $\phi_r(x) = [e_r f_0(x)]^{-1} D_x^r [f_0(x) g(x)^r]$ with $g(x) = 1$. Indeed, GCS expansions with $g(x) \neq 1$ have been developed for those PDFs which are part of the Pearson system [8], but the resulting functions are not necessarily polynomial. There is also a close connection between the Pearson differential equation

$$\frac{df_0}{dx} = \frac{(x-a)f_0(x)}{b_0 + b_1 x + b_2 x^2} \tag{16}$$

with a, b_0, b_1, b_2 constants, and the second-order differential equations governing the usual orthogonal polynomial systems. So far, it seems that there is no single system having both the good statistical properties of Gram–Charlier series on the one hand, and the good convergence properties of orthogonal polynomials on the other.

REFERENCES

[1] D.A. Brown, P. Danielewicz, *Phys. Rev.* **C57**, 2474 (1998) [nucl-th/9712066].

[2] D.A. Brown *et al.*, *Phys. Rev.* **C72**, 054902 (2005) [nucl-th/0507015].

[3] P. Danielewicz, S. Pratt, *Phys. Lett.* **B618**, 60 (2005) [nucl-th/0501003].

[4] S. Hegyi, T. Csörgő, Proc. Budapest Workshop on Relativistic Heavy Ion Collisions, preprint KFKI–1993-11; *Phys. Lett.* **B489**, 15 (2000).

[5] H.C. Eggers, P. Lipa, *Braz. J. Phys.* **37**, 877 (2007) [nucl-th/0611105].

[6] H.C. Eggers, P. Lipa, *Int. J. Mod. Phys.* **E16**, 3205 (2007).

[7] P. Lipa, H.C. Eggers, B. Buschbeck, *Phys. Rev.* **D53**, 4711 (1996); [hep-ph/9604373].

[8] A. Stuart, J.K. Ord, *Kendall's Advanced Theory of Statistics*, 5th edition Vol. 1, Oxford University Press, New York 1987.