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2009 J. Phys. A: Math. Theor. 42 365206

(http://iopscience.iop.org/1751-8121/42/36/365206)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **42** (2009) 365206 (9pp) doi:10.1088/1751-8113/42/36/365206

Terahertz-sideband spectra involving Kapteyn series

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Received 9 February 2009, in final form 24 July 2009
Published 24 August 2009
Online at stacks.iop.org/JPhysA/42/365206

Abstract

Kapteyn series of the second kind appear in models of even- and odd-order sideband spectra in the optical regime of a quantum system modulated by a high-frequency (e.g., terahertz) electromagnetic field (Citrin D S 1999 *Phys. Rev.* B **60** 5659) and in certain time-periodic transport problems in superlattices (Ignatov A A and Romanov Y A 1976 *Phys. Status Solidi* b **73** 327; Feise M W and Citrin D S 1999 *Appl. Phys. Lett.* **75** 3536). This paper shows that both the even- and the odd-order Kapteyn series that appear can be summed in closed form, thereby allowing more transparent insight into the structural dependence of the sideband spectra and also providing an analytic control for the accuracy of numerical procedures designed to evaluate the series. The general method of analysis may also be of interest for other Kapteyn series.

PACS numbers: 02.30.Gp, 42.65.Ky, 78.67.De

1. Introduction

In discussing an optical analogue for phase-sensitive measurements in quantum transport through a quantum dot whose energy levels are modulated periodically in time, Citrin (1999) has considered optical propagation of a monochromatic optical beam at frequency ω (known as the fundamental frequency) transmitted through or reflected from a quantum well modulated by a high-frequency field (henceforth called the terahertz field) at frequency Ω. The transmitted and reflected optical beams are shown to contain new frequencies $\omega + p\Omega$, where p is an integer, known as *terahertz sidebands* (Citrin 1999). The amplitude of such signals as a function of ω is known as *terahertz sideband spectra*. In the case when only one modulated energy level (at time-averaged energy ϵ_0) is relevant and the periodic modulation of that energy level is sinusoidal, a simple and useful model can be obtained that permits considerable analytic progress to be made before numerical methods need to be brought to bear on the problem. Such a model then permits one to study in a straightforward fashion how the terahertz sidebands scale with various parameters such as Ω and the modulation strength (the degree to which the energy level varies with respect to its time average ϵ_0).

A formally similar analytic model also arises in connection with miniband transport in a superlattice subjected to a strong terahertz field (Ignatov and Romanov 1976, Feise and Citrin 1999). The phases of the reflected and transmitted complex electromagnetic amplitudes for each sideband (with respect to the initial optical beam at angular frequency ω) provide information on the quantum system. The detailed development given by Citrin (1999) has its basic underpinning from the calculation of the amplitude of the transmitted optical electric field, $T(\omega', \omega)$, at frequency ω'. Equation (2) of Citrin (1999) provides

$$T(\omega', \omega) = \frac{2\pi}{\zeta}\left[\frac{\omega - \varepsilon_0}{\omega - \varepsilon_0'}\delta_{\omega',\omega} + K_p(\omega)\delta_{\omega'-\omega.p\zeta}\right] \tag{1}$$

with

$$K_p(\omega) = 2\mathrm{i}\Gamma\Delta\,\mathrm{e}^{-\mathrm{i}p\alpha} S, \tag{2}$$

where

$$S = \sum_{k=1}^{\infty}{}' \frac{1}{\Delta^2 - (k\zeta/2)^2} J_{(k+p)/2}\left(k\varepsilon_1/(2\Delta)\right) J_{(k-p)/2}\left(k\varepsilon_1/(2\Delta)\right). \tag{3}$$

The series S is the Kapteyn series of the second kind of interest here. In general, there are two kinds of Kapteyn series (Kapteyn 1893). Kapteyn series of the first kind involve summations over terms containing one Bessel function of the form $J_n(nx)$, while Kapteyn series of the second kind involve terms each of which is proportional to a product of two such Bessel functions. Note that the index of summation k appears both in the order and the argument of the Bessel functions. The notation in equations (1)–(3) is that given by Citrin (1999). In particular, the prime on the summation indicates that only terms where the parity of k is that of p are retained and $\Delta = \omega - \mu\zeta/2 - \epsilon_0$ is the (sideband order μ-dependent) detuning between the average energy $\omega - \mu\zeta/2$ of the fundamental and relevant sideband and the time-average energy of the modulated level ϵ_0. The first term in equation (1) gives the transmitted beam at the input frequency $\omega' = \omega$ in the absence of the modulation field, while the second contains the terahertz sidebands at $\omega' = \omega + p\zeta$. The cardinal point for this paper is the requirement that the sum in equation (3) is the sum over integers with the same parity as p. Thus if $p = 2n$ ($n = 0, 1, 2, \ldots$), then $k = 2r$ ($r = 0, 1, 2, \ldots$), while if $p = 2n + 1$, then $k = 2r + 1$ ($r = 0, 1, 2, \ldots$). Note that due to the form of equation (3), there is no need to consider negative values of p.

Citrin (1999) notes that by expanding equation (3) in powers of $(\varepsilon_1/\zeta^{1/2})$ one can identify the various multi-photon processes contributing to each sideband, and he provides the appropriate expansion. Numerical evaluation at this stage is required and has the consequence that convergence of an infinite product inside an infinite sum must be proven, a less than trivial task.

The purpose of this paper is to show that the Kapteyn series represented in equation (3) can indeed be summed in a closed form, thereby facilitating not only the general understanding of the sideband spectra but also obviating the need to prove convergence of an infinite product inside an infinite sum—a serendipitous result that is definitely a welcome blessing. Moreover, the closed-form expressions found as well as the approach by which they are obtained are likely to be of interest for other areas of physics and applied mathematics.

2. Evaluation of the Kapteyn series

For $p = 2n$ (and so $k = 2r$), i.e. for the even-order sideband spectra, one has to evaluate

$$S_E(n) = \sum_{r=1}^{\infty} \frac{1}{\Delta^2 - (r\zeta)^2} J_{r+n}(ar) J_{r-n}(ar) \tag{4}$$

with $a = \varepsilon_1/(2\Delta)$, for all nonnegative integers n.

For $p = 2n + 1$ ($n = 0, 1, 2, \ldots$) and so $k = 2r + 1$ ($r = 0, 1, 2, \ldots$), i.e. for the odd-order side spectra, one has to evaluate

$$S_O(n) = \sum_{r=0}^{\infty} \frac{1}{\Delta^2 - \left(r + \frac{1}{2}\right)^2 \zeta^2} J_{r+n+1}\left(a\left(r + \frac{1}{2}\right)\right) J_{r-n}\left(a\left(r + \frac{1}{2}\right)\right) \tag{5}$$

with $a = \varepsilon_1/(2\Delta)$, for all integers n including $n = 0$.

It is the closed-form evaluation of the Kapteyn series $S_E(n)$ and $S_O(n)$ that is of concern here. Thus, equations (4) and (5) may be regarded as the starting point of our study.

2.1. The even-order side spectra summation

Consider first the even-order sideband spectrum summation written in the form

$$S_E(n) = -(1/\zeta)^2 \, K_E(a, \, b) \tag{6}$$

with

$$K_E(a, b) = \sum_{r=1}^{\infty} \frac{1}{r^2 - b^2} J_{r+n}\,(ar)\, J_{r-n}\,(ar) \tag{7}$$

and $b = \Delta/\zeta$. Closed-form evaluation of $K_E(a, b)$ proceeds as follows. From Watson (1965, equation (1) in Section 5.43 on page 150), one has

$$J_\mu(z) J_\nu(z) = \frac{2}{\pi} \int_0^{\pi/2} J_{\mu+\nu}(2z\cos\theta)\cos((\mu-\nu)\theta)\,\mathrm{d}\theta, \tag{8}$$

which is valid in general when μ and ν are arbitrary integers, and is otherwise valid so long as $\mathrm{Re}(\mu + \nu) > -1$.

One also has $J_{r\text{-}n}(ar) = (-1)^{r-n} J_{n-r}(ar)$. Thus, with $\mu = n + r$, $\nu = n - r$ and $z = ar$, it follows that

$$J_{n+r}(z) J_{r-n}(z) = (-1)^{r-n} \frac{2}{\pi} \int_0^{\pi/2} J_{2n}(2ar\cos\theta)\cos(2r\theta)\,\mathrm{d}\theta. \tag{9}$$

Now use the representation

$$J_{2n}(x) = \frac{2}{\pi} \int_0^{\pi/2} \cos(x\sin\theta)\cos(2n\theta)\,\mathrm{d}\theta \tag{10}$$

in equation (9) and substitute the result into equation (7) to obtain

$$K_E(a, b) = (-1)^n \left(\frac{2}{\pi}\right)^2 \int_0^{\pi/2} \cos(2n\psi)\,\mathrm{d}\psi \int_0^{\pi/2} A\,\mathrm{d}\theta \tag{11}$$

with

$$A = \sum_{r=1}^{\infty} \frac{(-1)^r}{r^2 - b^2} \cos(2r\theta)\cos(2ar\cos\theta\sin\psi). \tag{12}$$

Use the fact (Gradshteyn and Ryzhik 2000, equation (FI III 545) in section 1.445 on page 47) that

$$\sum_{r=1}^{\infty} \frac{(-1)^r}{r^2 - b^2} \cos(rf) = \frac{1}{2b^2} - \frac{\pi}{2b} \csc(\pi b) \cos(bf) \tag{13}$$

valid in the range $-\pi \leqslant f \leqslant \pi$. In fact, as is readily obtained from equation (13), one shows that

$$\sum_{r=1}^{\infty} \frac{(-1)^r}{r^2 - b^2} \cos(rf) \cos(rg) = \frac{1}{2b^2} - \frac{\pi}{2b} \csc(\pi b) \cos(bf) \cos(bg), \tag{14}$$

which holds for $f, g \in [-\pi, \pi]$. Consequently, we obtain

$$K_E(a, b) = -(-1)^n \frac{2}{\pi} \csc(\pi b) \frac{1}{b} \int_0^{\pi/2} \cos(2n\psi)\, \mathrm{d}\psi \times \int_0^{\pi/2} \cos(2b\theta) \cos(2ab \cos\theta \sin\psi)\, \mathrm{d}\theta. \tag{15}$$

Care must be taken that the relevant ranges of the cosine arguments in equation (15) lie in the appropriate range of modulo (2π) to ensure that one handles the integrals in the correct domain. The bookkeeping associated with values of the cosine arguments outside the range $(0, 2\pi)$ is cumbersome but the general sense of evaluation of the double integral in equation (15) remains unaltered. For ease of exposition here we treat solely the case where the cosine arguments are restricted to the range $(0, 2\pi)$; all other ranges can be dealt with accordingly, *mutatis mutandis*.

There is also a slight restriction on the argument b. As Citrin (1999) has noted, neglect of any imaginary component of b allows one to obtain an optical theorem (Newton 1976). To the same extent, neglect of the imaginary part of b in equation (15) is equally justified. Then use equation (10) to write

$$K_E(a, b) = -(-1)^n \frac{2}{\pi} \csc(\pi b) \frac{1}{b} \int_0^{\pi/2} \cos(2b\theta) J_n(2ab \cos\theta)\, \mathrm{d}\theta. \tag{16}$$

Again use equation (8) with $\mu - \nu = 2b$ and $\mu + \nu = 2n$ to obtain

$$K_E(a, b) = -(-1)^n \frac{\pi}{2b} \csc(\pi b) J_{n+b}(ab) J_{n-b}(ab), \tag{17}$$

which is the summation required and is valid for n, an integer and $n \geqslant 1$, with $0 < a < 1$, $0 < b < 1$.

Outside of these ranges for a and b one must proceed with the evaluation using the argument given above for validation of the cosine integrals with considerably more bookkeeping as a and b increase systematically. In principle, there is no difficulty in completing the evaluations because the method is precise as given above, but the resulting expressions become increasingly unwieldy compared to equation (17).

2.2. The odd-order side spectra summation

Consider equation (5) written in the form

$$S_O(n) = -(1/\zeta)^2 K_O(a,\ b) \tag{18}$$

with

$$K_O(a, b) = \sum_{r=0}^{\infty} \frac{(-1)^{n-r}}{\left(r + \frac{1}{2}\right)^2 - b^2} J_{n+r+1}\left(a\left(r + \frac{1}{2}\right)\right) J_{n-r}\left(a\left(r + \frac{1}{2}\right)\right). \tag{19}$$

By a procedure similar to that followed for the even-order series, one replaces the product of the Bessel functions in equation (19) by an integral over one Bessel function using equation (8), then one replaces the single Bessel function occurring under the integral by

$$J_{2n+1}\left(a\left(r+\frac{1}{2}\right)\cos\theta\right)=\frac{2}{\pi}\int_0^{\pi/2}\sin((2n+1)\psi)\sin\left(a\left(r+\frac{1}{2}\right)\cos\theta\sin\psi\right)\mathrm{d}\psi, \quad (20)$$

and finally one performs the summation over r from $r = 0$ to ∞. Then the reversal of the integral representations is undertaken, just as for the even-order spectra, with the result that one finds

$$2K_O(a,\ b)=(-1)^n(\pi/2)b^{-1}\ \sec(\pi b)\ J_{n+1/2+b}(ab)J_{n+1/2-b}(ab), \quad (21)$$

which is the summation sought, and is valid in $0 < b < 1/2$ and $0 < a < 1$. For values of a and b outside these ranges one has to ensure that the arguments of the various cosine and sine terms in the relevant integrals lie in the appropriate ranges—just as is required for the even-order series.

It is noteworthy that the forms of the results for both the even- and odd-order sideband spectra are similar. It is also immediately evident that the given sideband spectrum will vanish if ab is chosen such that it is a zero of the relevant Bessel function.

Fortunately, as Citrin (1999) has discussed, the parameter b is directly proportional to the detuning frequency and so is considered in some sense as small; this smallness allowed Citrin (1999) to expand the Kapteyn sums in ascending powers of b.

The suggestion then is that $b \ll 1$ so that there will be little need to include the higher argument ranges. However, the evaluation of the Kapteyn series for such higher range values for a and b is not complicated, rather fraught with bookkeeping and so is tedious. For this reason only the outline of the procedure has been given here for such ranges. For the ranges most appropriate for the quantum optics and transport experiments discussed by Citrin (1999), the closed-form detailed evaluations have been given here of the even- and odd-order Kapteyn series.

3. Numerical comparison

To illustrate the degree of agreement between the analytical closed-form solutions and the direct evaluation of the Kapteyn series summations within the ranges chosen, this section provides a few illuminating cases for both the even- and the odd-order summations.

3.1. Even-order numerical results

Start with the even-order representations. As shown in figure 1 for the case of $n = 1$, $b = 0.5$, the agreement between direct computation of the value of K_E from the series (solid) and the analytic closed-form expression for K_E (dashed) is so close that there is no discernable difference between the two curves when plotted as a function of the parameter a in $a < 1$, as is evident also from the inset, which shows the relative deviation between the two curves.

Consider now the value of K_E at a fixed parameter value $a = \pi/6$ as the parameter b varies, again for $n = 1$, the lowest even-order sideband, in figure 2. The inset clearly shows that there is no discernable difference between the series and the closed-form expression for $b < 1$. Indeed, the inset indicates an accuracy of about a part in 10^{16} throughout most of the range of $b < 1$ and even at $b = 1$ the inaccuracy is still only a part in 10^{14}, thus showing the appropriateness of the closed-form analytic expression.

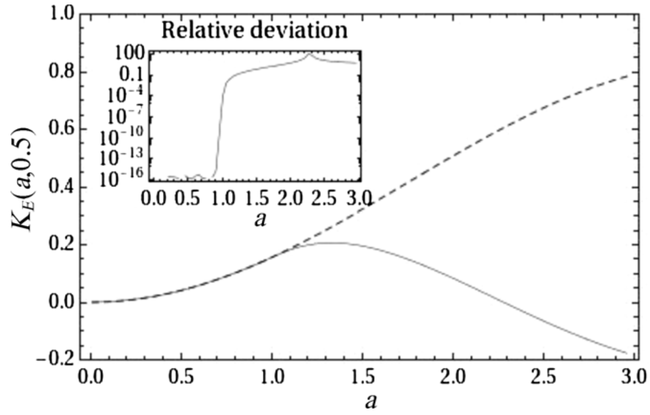

Figure 1. Comparison of the direct series evaluation (solid) and the analytic representation (dashed) for the even-order spectra $K_E\,(a, b)$ with $n = 1$, $b = 0.5$ as a is varied. The inset shows the relative difference between the direct series evaluation and the analytic representation.

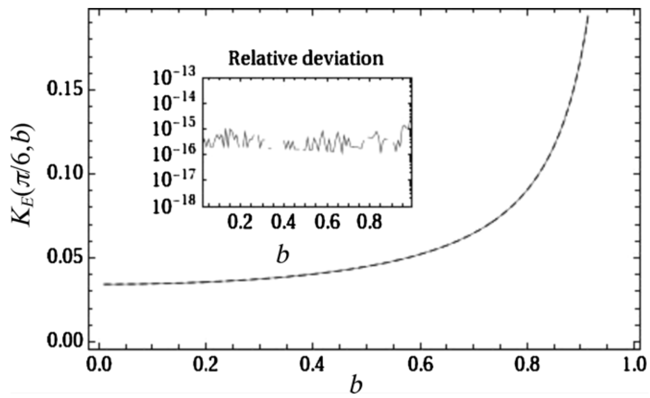

Figure 2. Comparison of the direct series evaluation (solid) and the analytic representation (dashed) for the even-order spectra K_E with $n = 1$, $a = \pi/6$ as b is varied. The inset shows the relative difference between the direct series evaluation and the analytic representation.

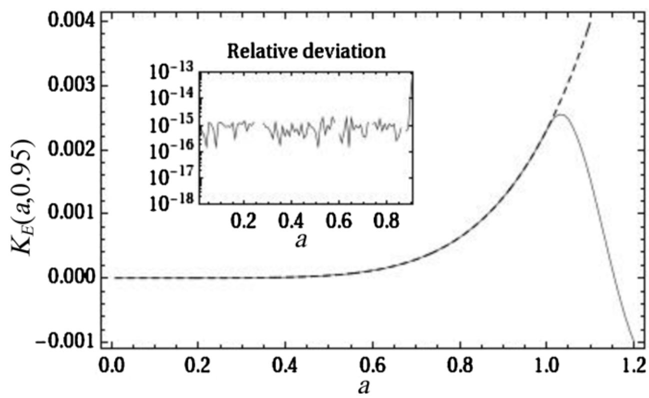

Figure 3. Comparison between the direct series evaluation (solid) and the analytic representation (dashed) for the even-order spectra K_E with $n = 3$, $b = 0.95$ as a is varied. The inset shows the relative difference between the direct series evaluation and the analytic representation.

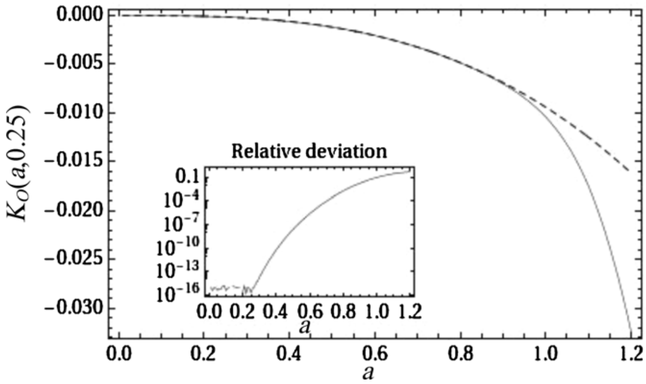

Figure 4. Comparison of the direct series evaluation (solid) and the analytic representation (dashed) for the odd-order spectra K_O with $n = 1$, $b = 0.25$ as a is varied. The inset shows the relative difference between the direct series evaluation and the analytic representation.

Many other values of n have been checked and all curves show marked agreement. For instance, the case of $n = 3$, shown in figure 3, indicates no discernable difference between the analytic and series representations in the range $a < 1$, for $b = 0.95$. As seen in the inset, the mismatch is around a part in 10^{16} throughout most of the range of b and increasing only to about a part in 10^2 at the end of the range $b = 1$.

3.2. Odd-order numerical results

Similar to the even-order spectra, here we present some illustrative examples of the odd-order spectra results for direct summation of the series in comparison to the analytical results. Figure 4 shows the behaviour of K_O as a function of the parameter a for $n = 1$ and $b = 0.25$. Note that while the analytic result is justified for $a < 1/2$ and $b < 0.5$, the numerical evaluation shows that there is a high degree of overlap beyond the limit for a. Indeed, from figure 4 one sees that the two results are in agreement to about $a = 0.9$—perhaps indicative of the larger domain of correctness of the analytic result than is derivable from the arguments given above.

This point can be further extended by considering the case of $n = 0$ and $b = 0.95$, as shown in figure 5—well beyond the range—where analytic justification can be given without inclusion of the additional terms arising from the arduous bookkeeping. Note that as a function of a, there is virtually no difference between the direct series evaluation and the analytic results for the odd-order K_O as far as $a = 1$. This point is further underscored by the inset where agreement to better than a part in 10^{10} is obtained for $a < 0.5$ and, even at $a = 1$, the disagreement is still only about a part in 10^2. Rugged stability is again seen.

Considering the variation of K_O as a function of the parameter b for fixed values of a (exhibited in figure 6 is the case of $a = 0.2$ and $n = 1$, although all other cases yield similar results) one sees that there is almost perfect agreement to $b = 0.5$ and the relative degree of mismatch shown in the inset indicates agreement to better than a part in about 10^{15} throughout this range of b.

In short, the analytic evaluations of both the even- and odd-order spectra presented are numerically accurate outside of the ranges where one needs to include extra terms from the phase variation of the various cosine and sine factors appearing under the integral signs. To

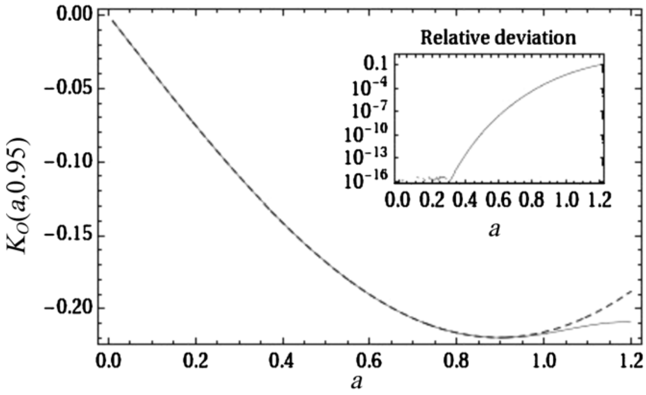

Figure 5. Comparison of the direct series evaluation (solid) and the analytic representation (dashed) for the odd-order spectra K_O with $n = 0$, $b = 0.95$ as a is varied. The inset shows the relative difference between the direct series evaluation and the analytic representation.

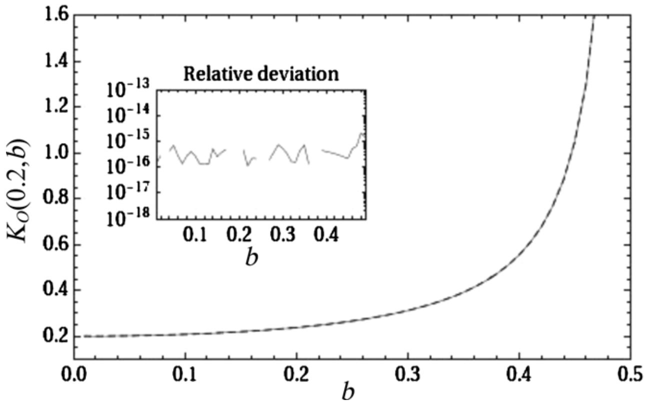

Figure 6. Comparison of the direct series evaluation (solid) and the analytic representation (dashed) for the odd-order spectra K_O with $n = 0$, $b = 0.95$ as the parameter b is varied. The inset shows the relative difference between the direct series evaluation and the analytic representation.

what extent this general pattern persists for all n, a, and b values is not known at the present time but is likely worth exploring at some point in future.

4. Discussion and conclusion

In Feise and Citrin (1999) the *approximate* vanishing of the transport at zeros of the Bessel functions was noted based on the approximate formula. Here, we see that this result is *exact* in the model. If there is loss (b complex), one can also find ab (for a real) that are (complex) zeros of the relevant Bessel functions, but then the index of the Bessel functions is also complex so that one would have to work through the problem *de novo* allowing for a complex value of b from the onset. This is, regrettably, necessary in order to take into account the complex values of b in summing the series to obtain analytic representations. However, it is also possible to obtain the approximate representation of such values because one notes that the original series are even functions of b, whether b is real or complex. As such the series are meromorphic functions of b and so can be analytically continued into the complex plane. Such a detailed investigation is beyond the scope of the present paper, but the point is noted here for future investigation.

It is also opportune to note here that the infinite product representation given by Citrin (1999) (obtained by the expansion of the infinite Kapteyn series in powers of b) enables one to obtain simply useful expressions for the infinite products by the expansion of the analytic results presented for the even- and odd-order series also in powers of b. Such a development is a bit trickier than it appears at first glance because of the presence of the parameter b in both the order and argument of the analytic representations of the series but poses no fundamental difficulties in principle. Such a development would, however, make for a very long paper indeed and so is deferred to the future.

Perhaps one of the most interesting points to be made is that the Kapteyn series arising in the sideband spectra can be given in closed form, enabling more insight to be gained into the response of such quantum systems, as illustrated by the vanishing of the sideband spectrum at selected values of ab. The other point to make is that the ability to produce closed-form expressions for the Kapteyn series is of considerable benefit when one attempts to perform numerical computations because such closed-form expressions act as strong controls on the accuracy determination of any numerical scheme. In addition, the general procedure for summing such Kapteyn series may be of use in other problems where similar Kapteyn series arise.

Acknowledgments

This work was partially supported (RCT) by the Deutsche Forschungsgemeinschaft (DFG) through grant Schl. 201/19-1. The work of DSC was supported in part by the National Science Foundation under grant ECCS 0523923 and by the CNRS, France.

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