

Necklace solid-on-solid models of interfaces and surfaces

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1986 J. Phys. A: Math. Gen. 19 385

(<http://iopscience.iop.org/0305-4470/19/3/020>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 31/05/2010 at 19:26

Please note that [terms and conditions apply](#).

Necklace solid-on-solid models of interfaces and surfaces

D B Abraham[†] and P M Duxbury[‡]

[†] Department of Theoretical Chemistry, University of Oxford, 1 South Parks Road, Oxford OX1 3TG, UK

[‡] Department of Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, UK

Received 12 June 1985

Abstract. Using the exact generating functions for solid-on-solid models, we construct 'necklace' partition functions for wetting and prewetting at a sticky wall in two (bulk) dimensions. Three-component generalisations of these models, constructed to study interfacial wetting, are introduced and solved. Based on these models we discuss the types of interfacial critical behaviour to be expected in three-component systems in two dimensions.

1. Introduction

In two-dimensional systems many surface and interface properties in two-component systems are well approximated by solid-on-solid (sos) models (see Abraham and Smith (1985) and references therein). Recently, Fisher (1984) (see also Huse *et al* 1983) has studied these systems using a combination of random walk arguments and a 'necklace' (see § 2) generating function, and is able to straightforwardly recapture the asymptotic results found in the original sos calculations (Abraham and Smith (1985) and references therein). In this paper we show that the original sos calculations (with a sticky wall potential) can be *exactly* recaptured using necklace generating functions. This assertion is explicitly demonstrated for wetting and prewetting at a sticky wall in two-component systems. The basic ingredients of the necklace generating functions and the subunit partition functions are given in § 2, while the wetting and prewetting cases are elucidated in § 3.

Using the above ideas, a model for interfacial wetting in three-component systems is constructed and solved. This model generalises those considered by Fisher (1984) (an area term is added) and Selke *et al* (1985) (the direct interface is allowed a different string tension from the sum of the two indirect interfaces). As has been suggested before (Selke *et al* 1985), the critical exponents present in sos models of interfaces in three-component systems are the same as those found in depinning transitions at surfaces in two-component systems. This equivalence is explicitly demonstrated in the models studied here.

In § 5 we discuss the various interfacial behaviours possible in real three-component systems. In particular we suggest that the exponent $\frac{1}{3}$ should be observed at the chiral clock ($2D$) wetting line if a single-site anisotropy term is added and the interfacial adsorption is measured as a function of the anisotropy at fixed temperature, in the limit of small single-site anisotropy. In addition we suggest that at a first-order bulk transition, the interface may remain dry up to a certain temperature. There may be a tricritical wetting point present in such cases. This may occur in the Blume-Emery-Griffiths model as the quadratic interaction term is increased in magnitude.

The paper concludes in § 6.

2. sos necklace model components

As discussed by Fisher (1984) (and references therein) and Huse *et al* (1983), a two-subunit necklace partition function of length n can be found from

$$Z_n = \frac{1}{2\pi i} \oint \frac{dt}{t^{n+1}} \frac{Z_x(t)}{1 - v^2 Z_x(t) Z_y(t)} \tag{1}$$

where $Z_x(t)$ and $Z_y(t)$ are the generating functions for the two subunits x and y , and the integration contour is a small circle around the origin. The result (1) may be seen from the following (Fisher 1984).

If one knows the partition function, Z_n , for an n -site system, then the generating function for the system is defined by

$$Z(t) = \sum_{n=1}^{\infty} t^n Z_n \tag{2}$$

where t is a fugacity variable. If one now considers a necklace composed of two types of subunits x and y , as depicted in figure 1, and one can calculate the generating functions, $Z_x(t)$ and $Z_y(t)$, for the two components, then the generating function for the necklace of figure 1 is given by

$$Z(t) = Z_x(t)/(1 - v^2 Z_x(t) Z_y(t)) \tag{3}$$

where $Z(t)$ is the generating function for the necklace and v is an arbitrary vertex factor placed at each junction of the x and y beads. The contour integration in (1) then selects from (3) the necklace with n sites.

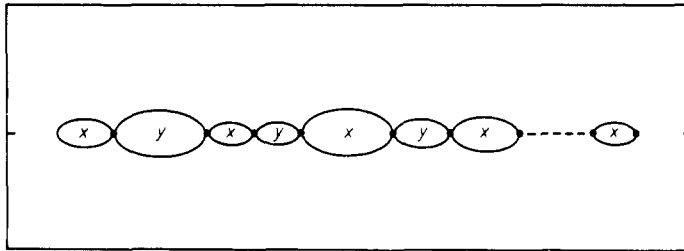


Figure 1. A two-component necklace made up of subunits (beads) of types x and y .

The use of this necklace construction goes back at least as far as Temperley (1956) and has been recently used to study a wide variety of two-dimensional problems (see Fisher (1984) and references therein).

In constructing sos models in two-dimensional systems the evidence suggests that continuous and discrete versions, and all models with weights $P(\Delta h) = \exp(-\beta|\Delta h|^p)$, are in the same universality class, at least for p finite. The most analytic progress has been made on continuous models with $p = 1$ or 2 . In this paper we use models with $p = 1$, as in this case the use of the Green function identity allows us to treat the non-coexistent situation. Considerable analytic progress has also been made in the $p = 2$ case using field theoretical techniques, and for an introduction to this work we refer to Kroll and Lipowsky (1982) and Lipowsky *et al* (1983).

In studying surface properties in two-component systems and interfaces in three-component systems, the appropriate sos models may be formed by various combinations of the following basic string partition functions (see figure 2).

(a) The 'stuck string',

$$Z_n = a^n \tag{4}$$

where a is the surface stickiness.

(b) The Onsager-Temperley string, full-space problem (the string is allowed to take on values $-\infty < h_i < \infty$),

$$Z_n = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(\frac{4K}{4K^2 + \omega^2} \right)^n d\omega \tag{5}$$

where K is the Boltzmann weight for the string tension.

(c) The Onsager-Temperley string, half-space problem (the string is allowed to take on values $0 < h_i < \infty$),

$$Z_n = \frac{1}{\pi} \int_0^{\infty} \left(\frac{4K}{4K^2 + \omega^2} \right)^n \sin^2 \theta(\omega) d\omega \tag{6}$$

where $\tan \theta(\omega) = -\omega/2K$.

(d) The Abraham-Smith string (half-space Onsager-Temperley string in an external field)

$$Z_n = 2H \sum_{j=0}^{\infty} \left(\frac{1}{K\nu_j^2} \right)^n \tag{7}$$

where the ν_j solve $J_{\alpha-1}(\alpha\nu) = 0$ (Abraham and Smith 1982, 1985). $\alpha = 2K/H$, where H is the external field.

The above expressions are found by taking the continuum limit of $p = 1$ sos models (see figure 2), and by using a Green function identity, transforming the eigenvalue problem to that involving a Schrödinger operator. The coexistent situation was first suggested by Abraham (1980) and explicitly presented by several workers (Burckhardt 1981, Chalker 1981, Chui and Weeks 1981, Hilhorst and van Leeuwen 1981, Kroll 1981, Vallade and Lajzierowicz 1981). The non-coexistent calculation leads to a Bessel equation as found by Abraham and Smith (1982).

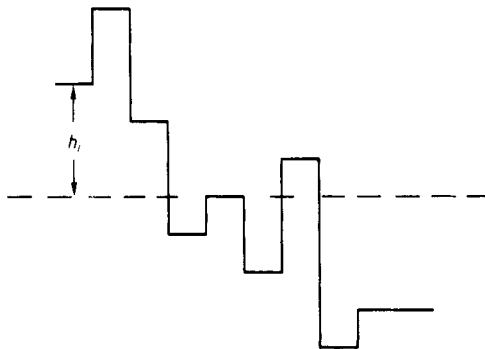


Figure 2. A full-space sos string. The h_i take on integer values in the range $-\infty < h_i < \infty$.

3. Wetting and prewetting

In the wetting case, the subunit partition functions are given by the components (a) and (c) of § 2. The subunit generating functions are then given by

$$Z(t) = \sum_{n=1}^{\infty} t^n Z_n. \tag{8}$$

Assuming the series is convergent, for subunit (a) we get

$$Z_a(t) = at/(1 - at). \tag{9}$$

For subunit (c) one has

$$Z_c(t) = \frac{2t^2}{\pi} \int_0^{\infty} \frac{u^2 du}{(1 + u^2)^2(K - t + Ku^2)} \tag{10}$$

where the summation in (8) has been started at $n = 2$ in this case (the $n = 1$ string has no meaning), and the summation and integration have been interchanged (this is valid if the series is convergent). The integration in (10) may be performed to obtain

$$Z_c(t) = t[A - (A^2 - 1)^{1/2}] \tag{11}$$

where

$$A = -1 + 2K/t. \tag{12}$$

The thermodynamics of the composite system is determined by the closest (to the origin) real singularity in the contour integration (1). There are two competing singularities in the composite generating function formed by combining $Z_a(t)$ and $Z_c(t)$ in (1). They are a pole at

$$Z_a(t)Z_c(t)/t = 1 \tag{13}$$

(the extra factor of $1/t$ is a vertex factor arising from the fact that the sum in the generating function $Z_c(t)$ began at $n = 2$) and a branch point at

$$A^2 = 1. \tag{14}$$

The critical point is determined when the dominant contribution crosses over from one to the other. Carrying the calculation through using (9), (11) and (12) gives $a_c = 1/2K$ as expected (Abraham and Smith 1985).

In the case of prewetting at a sticky wall, the appropriate subunits are (a) and (d). The generating function for (d) is

$$Z_d(t) = 2H \sum_{j=0}^{\infty} \left(\frac{1}{K\nu_j^2} \right) \frac{t^2}{K\nu_j^2 - t^2}. \tag{15}$$

Using the Mittag-Leffler expansion (Watson 1966), this becomes

$$Z_d(t) = -K\nu^2 + 2K\nu J_{\alpha}(\alpha\nu)/J_{\alpha-1}(\alpha\nu) \tag{16}$$

where $\nu^2 = t/K$. Combining (15) and (9) gives the problem studied by Abraham and Smith (1982, 1985). The dominant singularity in the composite generating function is always given by the smallest root (in absolute value) of

$$Z_a(t)Z_d(t)/t = 1. \tag{17}$$

Again a vertex factor of $1/t$ is required. Using (9), (16) and (17) we find

$$J_{\alpha-1}(\alpha\nu) = 2K_{\alpha\nu}J_{\alpha}(\alpha\nu) \tag{18}$$

in agreement with the known result (Abraham and Smith 1982, 1985). There is no finite-temperature phase transition in this case as there is no crossover in the dominant singularity at a finite temperature, as long as H is finite.

4. sos models of interfacial adsorption

To construct an sos model of interfacial wetting in three-component mixtures, the two subunits that need to be considered in (1) are a simple string (modelling a direct interface between the two coexistent phases on either side of the interface) and a bubble (modelling a region where the third component of the mixture lies between the two coexistent bulk phases). To be completely general, it is also necessary to include a fugacity transverse to the interface. This allows the strings and bubbles to have a degree of freedom transverse to the direction of the interface. The model is pictorially represented in figure 3. Mathematically it is straightforward to introduce this extra fugacity. One merely introduces another fugacity variable in (1) and performs another contour integration to impose the constraint that the start and end of the interface are at the same height. The introduction of another fugacity variable in the string partition functions (a) to (c) of § 2 is effected by removing the integrations. We then have

$$Z_n = \frac{-1}{4\pi^2} \int_{-\infty}^{\infty} \oint d\omega \frac{dt Z_x(t, \omega)}{t^{n+1}(1 - Z_x(t, \omega)Z_y(t, \omega))}. \tag{19}$$

The generating function for the string parts of the model depicted in figure 3 is

$$Z_b(t, \omega) = \frac{4K_1 t}{4K_1^2 + \omega^2 - 4tK_1} \tag{20}$$

where $K_1 (= J_1/k_b T)$ is the string tension. Equation (20) is found by putting (5) (without the integration) in (8).

The bubble partition function is constructed by forming a bubble from two simple strings, then transforming to centre-of-mass and relative coordinates (Abraham 1983). This transformation is exact for $p=2$ (see § 2) string models with equal tensions on

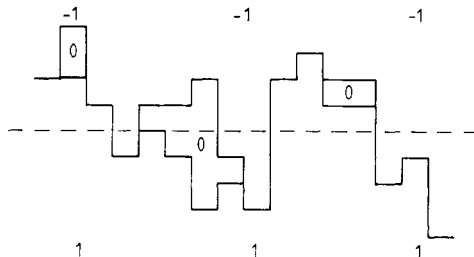


Figure 3. An sos model of interfacial adsorption in three-component systems. The $-1/1$ interfaces are modelled by a full-space sos string. The 0 bubbles are modelled by a combination of two sos strings (see text).

the two strings making up the bubble. Due to the presumed universality of models of the class studied here, the transformation is almost certainly valid for $p = 1$ and for equal string tensions. This is the bubble construction we use. The bubble partition function is then a combination of the strings (b), for the centre-of-mass motion, and (c), for the relative motion. The transverse fugacity is introduced in the centre-of-mass part, and we construct the bubble generating function,

$$Z_c(t, \omega) = \frac{2}{\pi} \int_0^\infty d\omega_2 \sum_{n=2}^\infty t^n \left(\frac{4K_2}{4K_2^2 + \omega^2} \frac{4K_2}{4K_2^2 + \omega_2^2} \right)^n \sin^2 \theta(\omega_2), \quad (21)$$

where $K_2 (= J_2/k_b T)$ is the string tension (the relative and centre-of-mass tensions are the same). The integration may be performed to give

$$Z_c(t, \omega) = \frac{2K_2 s}{1+u^2} [A - (A^2 - 1)^{1/2}] \quad (22)$$

where

$$s = t/K_2^2, \quad u = \omega/2K_2, \quad A = -1 + 2(1+u^2)/s. \quad (23)$$

Combining (20) and (22) in (19) gives the partition function of the sos model of the interface depicted in figure 3. It is possible to evaluate the asymptotic properties of the resulting integrals. Performing the t integration first, there are two singularities that may dominate in the integration. There is a pole at $Z_b(t, \omega)Z_c(t, \omega) = 1$, and a branch point at $A^2 = 1$. The second integration in either of these cases may be performed by steepest descents. The steepest descents calculation shows that the maximum in the ω integration is always at $\omega = 0$. This in fact may have been guessed at the beginning, as it reflects the fact that the transverse degree of freedom makes a negligible contribution to the entropy of the interface configurations, in the thermodynamic limit. The critical condition is determined by when the dominant singularity crosses over from the branch point to the pole. This leads to a phase boundary defined by

$$K_c = K_1 = K_2(K_2 + 1) \quad (24)$$

and the free energies in the two regions are

$$F(K_1, K_2) = \begin{cases} -2k_b T \ln(K_2) - F_{\text{sing}}, & K_1 < K_c, \\ -2k_b T \ln(K_2), & K_1 > K_c, \end{cases} \quad (25)$$

where

$$F_{\text{sing}} = -k_b T \ln \left(\frac{K_1 K_2 - K_1 - 2K_2^2 + 2(K_2^4 + K_1 K_2 - K_1 K_2^2)^{1/2}}{K_2(K_2 - 1)^2} \right).$$

On approaching the phase boundary from the pole side, the singular part of the free energy goes to zero as $F_{\text{sing}} \approx a|K - K_c|^2$. This is the same form of singularity as found for wetting at a wall, and we conclude that the interfacial wetting transition found in this model is in the same universality class as wetting at a wall at coexistence (see § 3). The interfacial adsorption is then expected to diverge with exponent 1 on approaching the phase boundary. The calculation may be easily carried through in the case of different centre-of-mass and relative string tensions. The phase boundary in this case is

$$K_1 = K_3(K_2 + 1) \quad (26)$$

where K_3 is the centre-of-mass tension and K_2 is the relative tension. There is no change in universality class in this generalisation.

We now wish to consider a model which includes an area term in the bubble partition function. The appropriate bubble generating function includes a field term in the centre-of-mass part and we find

$$Z_f(t) = 2H \sum_{n=2}^{\infty} \sum_{j=0}^{\infty} \left(\frac{1}{K_2 \nu_j^2} \frac{4K_2}{4K_2^2 + \omega^2} \right)^n t^n. \tag{27}$$

The dominant singularity for $H \neq 0$ is given by the composite pole. Upon combining (27) and (20) this gives (using the Mittag-Leffler expansion again)

$$(K_1 - K_2^2 \nu^2 + K_2 \nu^2) J_{\alpha-1}(\alpha \nu) - 2K_2 \nu J_{\alpha}(\alpha \nu) = 0 \tag{28}$$

where $\nu = [4t/(4K_2^2 + \omega^2)]^{1/2}$ and $\alpha = 2K_2/H$.

This equation has a similar structure to that occurring in the prewetting case (equation (18)). The behaviour of interest occurs in the limit $H \rightarrow 0$. The asymptotic solution to (28) can then be deduced from the properties of Airy functions (Abraham and Smith 1982, 1985). Using the Bessel recursion relations, one has (where primes denote derivatives with respect to argument)

$$\frac{J'_{\alpha}(\alpha \nu)}{J_{\alpha}(\alpha \nu)} = \frac{(K_2 + K_2^2) \nu^2 - K_1}{\nu [K_1 + (K_2 - K_2^2) \nu^2]}. \tag{29}$$

Now let

$$\nu = 1 + \gamma \alpha^{-2/3} \tag{30}$$

which is the most useful form for the discussion of the asymptotics. Putting (30) in (29), and using the asymptotic expansions of Bessel functions for α large (Abramowitz and Stegun 1970, equations 9.3.23 and 9.3.27), one finds

$$\begin{aligned} \frac{\text{Ai}'(-2^{1/3} \gamma)}{\text{Ai}(-2^{1/3} \gamma)} &= 2^{-1/3} \alpha^{1/3} \left(\frac{K_1 - (K_2 + K_2^2)}{K_1 + K_2 - K_2^2} \right) \\ &+ 2^{-1/3} \alpha^{-1/3} \gamma \left(\frac{K_1 - 2(K_2 + K_2^2)}{K_1 + K_2 - K_2^2} \right) + O(1/\alpha). \end{aligned} \tag{31}$$

In the thermodynamic limit it is the smallest ν which solves (31) that dominates. The nature of the solution is determined by the sign of the leading term in (31). The zero-field critical point is reflected in this term changing sign and the point where this occurs is $K_1 = K_2 + K_2^2$, in agreement with (24) (there is a higher temperature where the sign changes again; however, this is not physically relevant). At the critical point (24), the smallest value of γ which solves (31) occurs very close to (asymptotically at) the first zero of $\text{Ai}'(-2^{1/3} \gamma)$. This occurs at a finite γ (Abramowitz and Stegun 1970), and so the leading scaling behaviour in ν is determined by (30) with γ constant. Above the critical point, the smallest γ which solves (31) is asymptotically at the first zero of the function $\text{Ai}(-2^{1/3} \gamma)$, which again occurs at a finite γ . In both cases, the interfacial adsorption is then given by

$$\frac{1}{\nu_0} \frac{d\nu_0}{dH} = K_2^{-2/3} H^{-1/3} \tag{32}$$

as found in the two-component wall wetting case (Abraham and Smith 1982, 1985). Here ν_0 is the smallest (in absolute value) solution to (31).

For $K_1 < K_c$, the asymptotic behaviour of (31) changes and we find that the solution which minimises ν_0 in this case is (to leading order)

$$\gamma = |K_1 - K_c|^2 2^{-2/3} \alpha^{2/3}. \quad (33)$$

To leading order, ν_0 is then

$$\nu_0 = 1 - |K_1 - K_c|^2 2^{-2/3}. \quad (34)$$

The singular part of the free energy on approaching K_c has the quadratic form found earlier (see equation (25)).

Finally, it is possible to perform the scaling limit on the full integral representation of the partition function. One then finds to leading order the scaling function

$$Z(X) = \frac{1}{2\pi i} \oint \frac{d\nu}{\nu^{2n+1}} \frac{\text{Ai}(-\gamma 2^{1/3})}{\text{Ai}'(-\gamma 2^{1/3}) - 2^{-1/3} X \text{Ai}(-\gamma 2^{1/3})} \quad (35)$$

where $X = (|K_1 - K_c| \alpha^{1/3}) / (K_1 + K_2 - K_3^2)$ is the scaling variable. The formula is valid for any non-zero X . In the case $X = 0$ one must consider the next term in the Bessel function expansion.

5. Interfacial critical behaviour in three-component systems

We consider the interfacial critical behaviour to be expected in two (bulk)-dimensional three-component systems in three cases.

(a) On approaching an interfacial wetting line which lies inside a bulk ordered phase: the interfacial adsorption may then diverge with exponents 1 or $\frac{1}{3}$. The exponent 1 (Selke and Huse 1983, Huse *et al* 1983, Fisher 1984, Derrida and Yeomans 1985) has been observed in the chiral clock model. The exponent $\frac{1}{3}$ should also be observed in the chiral clock model if a DS^2 term is added and the interfacial adsorption is measured at constant T in the limit as D goes to zero.

(b) On approaching a bulk first-order transition from the ordered side: the interfacial adsorption may then diverge with exponents 1 or $\frac{1}{3}$, or if the temperature is low enough, remain dry (that is, the interfacial adsorption exhibits a first-order transition on crossing the bulk phase boundary). The exponent $\frac{1}{3}$ has been observed in the Blume-Capel model above the bulk tricritical point (Selke and Yeomans 1983, Selke *et al* 1985). One may observe a dry interface at the first-order transition in the Blume-Emery-Griffiths model, as the addition of the quadratic spin interaction term changes the relative strengths of the three types of interfaces present in the model. An interface tricritical point may be present in such a system. This tricritical point may not be very interesting, however, as the SOS model presented here suggests that the critical exponents (on approaching the wet region from the finite field region) at the tricritical point are the same as those away from the tricritical point.

(c) On approaching a bulk second-order transition from the bulk ordered side: the interface behaviour is then modified by the bulk fluctuations. The interfacial adsorption may exhibit a first-order transition, as observed in the Blume-Capel model below its tricritical point (Selke *et al* 1985), or diverge with exponent x_r or exponent $x_r/3$. Here x_r is the exponent renormalisation due to bulk fluctuations. The exponent x_r has been observed in the three-state Potts model (Selke and Huse 1983), where the bulk renormalisation is found to be $\nu - \beta$. The behaviour $x_r/3$ should also be observed in the three-state Potts model if one adds a DS^2 and measures the interfacial adsorption at fixed temperature as D is taken to zero.

6. Conclusions

We have shown that the models of wetting and prewetting at a sticky surface, previously solved using transfer integral operator methods, may be solved using necklace generating function methods. The mechanism for a phase transition in this method is a crossover in the dominant singularity in the asymptotic evaluation of a contour integral.

An sos model for interfacial adsorption is introduced and solved using this technique. The model shows interface wetting behaviour in the same universality class as surface wetting in two-component systems. Based on these models, a discussion is given on the interfacial critical behaviour to be expected in three-component systems.

Acknowledgments

PMD thanks the SERC and Trinity College Oxford for financial support. We thank M Fisher and J Yeomans for useful discussion.

References

- Abraham D B 1980 *Phys. Rev. Lett.* **44** 1165
 — 1983 *Phys. Rev. Lett.* **50** 291
 Abraham D B and Smith E R 1982 *Phys. Rev. B* **26** 1480
 — 1985 to be published
 Abramowitz M and Stegun I A 1970 *Handbook of Mathematical Functions* 9th edn (New York: Dover)
 Burckhardt T W 1981 *J. Phys. A: Math. Gen.* **14** L63
 Chalker J T 1981 *J. Phys. A: Math. Gen.* **14** 2431
 Chui S T and Weeks J D 1981 *Phys. Rev. B* **23** 2438
 Derrida B and Yeomans J 1985 *Preprint*
 Fisher M E 1984 *J. Stat. Phys.* **34** 667
 Hilhorst H and van Leeuwen J M J 1981 *Physica* **107A** 319
 Huse D A, Szpilka A M and Fisher M E 1983 *Physica* **121A** 363
 Kroll D M 1981 *Z. Phys. B* **41** 345
 Kroll D M and Lipowsky R 1982 *Phys. Rev. B* **26** 5289
 Lipowsky R, Kroll D M and Zia R K P 1983 *Phys. Rev. B* **27** 4499
 Selke W and Huse D A 1983 *Z. Phys. B* **50** 113
 Selke W, Huse D A and Kroll D M 1985 *Preprint*
 Selke W and Yeomans J 1983 *J. Phys. A: Math. Gen.* **16** 2789
 Temperley H N V 1956 *Phys. Rev.* **103** 1
 Vallade M and Lajzierowicz J 1981 *J. Physique* **42** 1505
 Watson G N 1966 *A Treatise on the Theory of Bessel Functions* 2nd edn (Cambridge: Cambridge University Press)