Static Properties of the One-Dimensional Planar Ferromagnet in an External Field

A. Patkós  
Department of Atomic Physics, Roland Eötvös University, Budapest, Hungary

P. Rujfán  
Institute for Theoretical Physics, Roland Eötvös University, Budapest, Hungary

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The thermodynamic functions and the correlation length of the classical one-dimensional XY model in an external field are calculated by the numerical integration of the transfer matrix equation in both ferro- and antiferromagnetic cases. We show that for a finite but weak magnetic field the low temperature structure of the ferromagnetic partition function consists of a spin-wave part and a factor corresponding to the interaction of topological excitations. The contributions of the soliton like topological objects to the static properties are calculated through a systematic perturbative method. Finally we discuss in detail the regions of validity of different analytical approaches by comparing them with our exact numerical solution.

I. Introduction

In the last decade a large amount of experimental and theoretical work has been done in studying the properties of one-dimensional magnets [1, 2]. In fact there exist magnetic crystals in which the localized spins have a significant one-dimensional behaviour due to the large intrachain per interchain coupling ratio. We mention here CsNiF₃, TMNC and RbFeCl₃ forming ferromagnetic and CsNiCl₃ forming antiferromagnetic chains with an easy magnetisation plane. Generally these materials have a three-dimensional phase transition at very low temperatures (Tc = 2.61 K for CsNiF₃) and show one-dimensional properties above Tc.

The theoretical model describing such materials has the form:

\[ H = -2J_s \sum_i s_i s_{i+1} + A \sum_i (s_i^1)^2, \]

where A represents the action of the crystal field. If s is integer and A > 0 is large enough the s_i = 0 state is favoured (as long as T ∝ (J_s A)^1/3) and one can use instead of (1) an XY model Hamiltonian. For example the s = 1 CsNiF₃ has J_s/k_B ≈ 9 K and A/k_B ≈ 9 K [3].

It is generally accepted that the classical planar model provides the leading contributions to the thermodynamic properties of (1) if s → ∞ [4]. Quantum corrections can be calculated using an 1/s expansion. Therefore if \( A/J_s \cdot s(s+1) ≪ 4\pi^2 \) the classical model represents well the equilibrium behaviour of such materials [5], except that the crystal field anisotropy effect is eventually modified by quantum corrections [3].

In spite of the interesting dynamic properties of the one-dimensional magnets — tested directly by neutron scattering experiments — we will deal only with the equilibrium properties of the classical one-dimensional planar model in an external field. In fact our interest in this model was motivated by recent techniques worked out for the two-dimensional case and leading to vortex-like excitations [6]. The Hamiltonian of the one-dimensional XY model is also periodic and one expects that some kind of topological objects occur also in this simpler case. The presence and the role played by sine-Gordon solitons in the dynamics of the system has been studied recently [7]. Although these solitons start moving around the chain even under an infinitesimal perturbation, they give contributions also to the statics of the system. In fact we show that at low temperatures the partition function factorizes into two parts: one corresponding to the harmonic approximation and the other con-
one can easily calculate the matrix elements of the (asymmetric!) perturbation. For example
\[
\langle \psi^{(o)}_0 | V | \psi^{(o)}_0 \rangle = \sum_k \sum_m I_1(K) \delta_{a,0} \delta_{m+k,0}
\]
\[
\times \left\{ \frac{h^2}{4} \delta_{m,0} + \frac{h^2}{2} (\delta_{m,1} + \delta_{m,-1}) + \frac{h^2}{8} (\delta_{m,2} + \delta_{m,-2}) \right\} = \frac{h^2}{4} I_0(K).
\]

Note that the eigenvalues \( \lambda_x (x > 0) \) are two-fold degenerate and the perturbation theory has to be applied accordingly. The results for small fields are
\[
\lambda_0(K, h \ll 1) = I_0 + \frac{h^2}{4} \frac{I_0 + I_1}{I_0 - I_1} + \frac{h^4}{8} \frac{1 + I_1}{I_0 - I_1}
\]
\[
+ \frac{1}{4 (I_0 - I_1)^2} \left\{ \frac{5 I_1^2}{8} + I_1 (I_0 + I_1) \right\} + \frac{1}{2 (I_0 - I_1)} \left\{ \frac{1}{I_0 + I_1} \right\} + \ldots,
\]

\[
\lambda_1(K, h \ll 1) = I_1 \left[ 1 + \frac{h^2}{8} \frac{I_1 + I_2 + \ldots}{I_1 - I_2} \right].
\]

and for \( |x| > 1 \) the eigenvalues remain degenerate \( O(h^2) \)
\[
\lambda_x(K, h \ll 1) = I_x \left[ 1 + \frac{h^2}{4} \right] + \ldots,
\]

where the argument of \( I_x \)'s is \( K \).

The correlation length is calculated from (10–11):
\[
\xi^{-1} = \ln \frac{\lambda_0}{\lambda_1} = \ln \left[ \frac{I_0 \left( 1 + \frac{h^2}{4} \frac{I_1 + I_0}{I_1 - I_0} \right)}{I_1 \left( 1 + \frac{h^2}{8} \frac{I_1 + I_2}{I_1 - I_2} \right)} \right].
\]
in second order.

The same procedure applied at high temperatures leads to
\[
\lambda_0(K \ll 1, h) = I_0(h) + K \frac{I_1(h)}{I_0(h)} + \ldots.
\]

Note that the zero field susceptibility calculated from (10) agrees with the results of Stanley [11] while for \( K \rightarrow \infty, h = 0 \) the correlation length (12) goes to the result of Wegner [12]. In the antiferromagnetic case one has to change \( K \) to \( -K \) and then \( I_n(K) \rightarrow (-1)^n I_n(K) \) in Eqs. (10–12).

**Low Temperature Representations**

Two limiting cases are usually studied to determine \( \lambda_0 \) at low temperatures. In an infinitesimal magnetic field \( (K \rightarrow \infty, h K \text{ fixed}) \) the average orientation of the spins is slowly varying from site to site and the width of the single spin distribution (described by \( \psi_0(\phi) \)) is large. The transfer operator eigenvalue problem (5) can be transformed into a Sturm-Liouville eigenvalue equation and one has to calculate the lowest eigenvalue of a Matthieu-type equation [8].

For completeness this result is rederived in a simpler way in the Appendix. Generalizing this mapping to a dynamics with propagating modes Mikeska [7] has recently obtained a sine-Gordon equation of motion and has shown that the soliton solutions give measurable effects in the dynamics of CsNiF3.

We shall discuss in detail here the second case, when one has a finite external field
\[
\left( K \rightarrow \infty, \frac{h}{|K|} = \tau = \left| \frac{\mu B}{J} \right| \text{ fixed} \right).
\]

In that situation the spins are fluctuating with a small angle around their ground state values (spin waves). Our purpose was to go beyond the usual harmonic approximation by taking into account topological excitations (spin configurations where the orientation of the spins changes over several interatomic distances more than \( 2\pi \)).

We rewrite the partition function (3) in Fourier space at low temperatures. We calculate the Fourier transform of the whole kernel \( \exp(h((t, t'))(t', t)) \) after expanding \( h((t, t')) \) around its ground state \( (T=0) \) value up to second order terms. We get for the Fourier transform of the kernel:
\[
T(m, n) = C \exp \{-A(m-n)^2 - B(m+n)^2\},
\]
where
\[
A^{-1} = 8 K \left( 1 + \frac{\tau}{4} \right), \quad B^{-1} = 2 K \tau,
\]
\[
C^{-1} = 2 \pi K (2\tau(T+4))^{1/2} e^{-K-h}.
\]

The partition function can be expressed using (14) and the Poisson resummation formula:

\[
Z(K \gg 1, \tau) = C^N \sum_{(m_i)} \prod_i d \xi_i \cdot \exp (2\pi i \sum_l m_l \xi_l) \prod_l T(\xi_l, \xi_{l+1}).
\]

Integrating over \( \xi_l \)'s, one recovers the product of the spin wave contribution and a factor describing the interaction of integer valued fields \( \{ m_l \} \).
The corresponding correlation length is:
\[ \xi_{(0)}^{-1} = \ln[1 + \frac{1}{2}(\tau + (\tau^2 + 4\tau)^{1/2})]. \] (23)

The \( m \neq 0 \) terms give exponentially small contributions to the \( \lambda \) and therefore can be calculated perturbatively using the expansion of \( \Psi(z) \) in terms of the \( \psi_n(z) \) functions. The first order corrections to the spin-spin correlation length can be readily derived
\[ \xi^{-1} = \xi_{(0)}^{-1} - \ln \left[ 1 - \frac{\sum \pi^2 (AB)^{-1} m^2 \exp \left( -\pi^2 m^2 / 2(AB)^{3/2} \right)}{\sum \exp \left( -\pi^2 m^2 / 2(AB)^{3/2} \right)} \right] \] (24)

The sums in (24) converge very fast for \( K \gg 1 \) and only the few first terms have to be calculated. The presence of solitons, as expected, decreases the mean size of fluctuations.

**Antiferromagnetic Coupling**

At the end of this Section we make a few comments on the generalization of the above method to antiferromagnetic coupling (\( J < 0 \)).

The ground state of the system is easily determined minimizing the transfer-Hamiltonian:
\[ h(\varphi, \varphi') = |J| \cos(\varphi - \varphi') - \frac{\mu B}{2} (\cos \varphi + \cos \varphi'). \]

The result is:
\[ E_0/N = -|J| \left( 1 + \frac{\tau^2}{8} \right), \]
\[ \varphi_o = -\varphi'_o = \arccos \frac{\tau}{4}, \quad \text{if } \tau < 4, \] (25a)
\[ E_0/N = -|J| (\tau - 1), \]
\[ \varphi_o = -\varphi'_o = 0, \quad \text{if } \tau > 4. \] (25b)

The corresponding spin configurations are shown in Fig. 2.

Let us point out that in the absence of an external staggered field the antiferromagnetic order parameter (the sublattice magnetisation) \( m_s \) has zero average value if \( T = 0 \) but at \( T = 0, m_s = \sqrt{1 - m_s^2} = 0 \) if \( 0 \leq \tau \leq 4 \) \((J < 0)\). Therefore one expects diverging sublattice susceptibility and order parameter correlation length in the whole \( 0 \leq \tau \leq 4 \) \((J < 0)\) region due to the non-analytic behaviour of \( m_s \) near \( T = 0 \).

As a consequence the spin-wave theory can be applied only when one introduces also an external staggered field ensuring the analytical behaviour of the sublattice magnetisation near \( T = 0 \). Although one can formally apply the spin-wave theory without including a staggered field \([9, 13]\) the resulting order parameter correlation length is always finite, a false result, if \( \xi_{(0)} \approx 4 \) \((J < 0)\). However, in the \( \tau > 4 \) \((J < 0)\) region \( m_s = 0 \) even at \( T = 0 \) and the procedure (14) leads to the same kind of results as (22) with the following constants \((K \gg 1)\):

\[ A^{-1} = 8K \tau; \quad B^{-1} = 2K \left( \frac{\tau}{4} - 1 \right); \]
\[ C^{-1} = e^{\kappa - k} 2\pi K \left[ \frac{\tau}{4} - 1 \right]^{1/2} \]
and
\[ \xi_{A.F.}^{-1} = \ln \left[ \frac{2 + \frac{2}{\sqrt{\tau - 4 - 2\sqrt{\tau}}}}{2 + \frac{1}{\sqrt{\tau - 4 - 2\sqrt{\tau}}}} \right], \quad \tau > 4, \quad K \gg 1. \] (26)

**III. The Numerical Solution**

Let us turn back to the transfer operator eigenvalue problem in the \( \varphi \)-space (4-5). We solve numerically this equation using a 16-point Gauss quadrature \([9]\). In this way one expects to obtain an approximate representation of the first 16 eigenvectors and eigenvalues of (5). The diagonalisation of the \( 16 \times 16 \) kernel matrix is further reduced to the diagonalisation of two \( 8 \times 8 \) matrices, corresponding to the even, and to the odd eigenvectors, respectively.

The accuracy of the method was tested in the \( h = 0 \) case, where the exact solution is known \([10, 11]\). It turns out that the largest even and odd eigenvalue, respectively, are very accurate, however, the higher eigenvalues are less reliable due to the fact that the...
happens in the 1D Heisenberg model [13] the susceptibility goes to a non-zero value for \( J < 0, \tau \leq 4 \), but tends to zero if \( J < 0, \tau > 4 \) at \( T \to 0 \) (Fig. 7). In Fig. 8 we have displayed the order parameter correlation length (30) vs. \( K \). The behaviour of the correlation length in the antiferromagnetic regime supports the physical picture presented in the previous Section.

**IV. Discussion and Conclusions**

The regions of validity of the different analytic approaches are drawn schematically on Fig. 9 for ferromagnetic coupling. The functional integral methods at infinitesimal [8] and finite external fields are valid in the adjacent regions III and IV. Therefore the low temperature behaviour of the spin-chain is
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A. Patkós
P. Ruján
Department of Atomic Physics
Institute for Theoretical Physics
Roland Eötvös University
Puskin u. 5–7
H-1088 Budapest
Hungary
In this Appendix we rederive in a simple way the low temperature form of the transfer matrix equation for an infinitesimal field, that is when
\[ K \to \infty, \quad hK = \text{fixed}. \]

One starts from the asymmetric form of the transfer operator eigenvalue problem:
\[
\int_{-\pi}^{\pi} \frac{d\varphi}{2\pi} \exp[K \cos(\varphi - \varphi') + h \cos \varphi'] \psi(\varphi) = \lambda \psi(\varphi').
\]
(A.1)

(A.1) is transformed into the form
\[
(2\pi K)^{-\frac{1}{2}} \exp[K + h \cos \varphi'] \sum_{m} \exp \left[ -\frac{m^2}{2K} - im \varphi \right] \Psi(m) = \lambda \psi(\varphi').
\]
(A.2)

using the character expansion (6) and the asymptotic representation of the Bessel-functions \((K \to \infty)\). The same left hand side is obtained when acting on \(\psi(\varphi')\) with the operator
\[
(2\pi K)^{-\frac{1}{2}} \exp(K + h \cos \varphi') \exp \left( \frac{1}{2K} \frac{d^2}{d\varphi^2} \right).
\]
(A.3)

Linearising (A.3) in the above limit one has to solve a Matthieu type eigenvalue problem:
\[
\left( \frac{1}{2} \frac{d^2}{d\varphi^2} + hK \cos \varphi \right) \psi(\varphi) = \lambda \psi(\varphi),
\]
\[
\lambda = (2\pi K)^{-\frac{1}{2}} \exp(K + h/K).
\]
(A.4)

The largest eigenvalue of the transfer matrix for small \(hK\) (to be compared with (10)) is the following [8]:
\[
\lambda_0 = (2\pi K)^{-\frac{1}{2}} \exp \left[ K + \frac{h^2}{2} K - \frac{h^4}{4} K^3 + \ldots \right], \quad 4hK \ll 1.
\]
(A.5)

For large \(hK\) (A.4) goes over into an oscillator problem:
\[
\lambda_0 = (2\pi K)^{-\frac{1}{2}} \exp \left[ K + h - \frac{1}{2} \sqrt{h/K} + \ldots \right], \quad hK \gg 1.
\]
(A.6)

References
discrete eigenvectors can hardly imitate functions with many nodes.
Formal expressions for thermodynamical functions and correlations are given in [9] and we do not reproduce them here. Using the largest eigenvalue $\lambda_0$ and its associated eigenvector $\psi_0$ we have calculated the free energy per spin,

$$\frac{F}{Nk_B T} + \ln 2\pi = f(K, \tau) = \ln \lambda_0,$$

(27)

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the magnetisation per spin

$$\frac{M}{\mu N} = m(K, \tau) = \langle s_z \rangle,$$

(28)

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and the spin pair correlation function $\langle s_z s_{z+1} \rangle$. The

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specific heat

$$C_B(K, \tau) = \frac{k_B N}{k_B N} = K^2 \left( \frac{\partial^2 f}{\partial T^2} \right)_T,$$

(29)

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and the susceptibility

$$\chi(K, \tau) = \left( \frac{\mu^2}{k_B T} \right) \left( \frac{\partial^2 f}{\partial h^2} \right)_K = \frac{\mu^2}{J} \chi,$$

(30)

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were determined by numerical derivation.
The order parameter correlation length is defined from the large distance behaviour of the $\langle s_z s_{z+r} \rangle$ correlation function and equals to

$$\xi^{-1} = \ln \left| \frac{\lambda_0}{\lambda_1} \right|^{-1},$$

(31)

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Taking into account the symmetries of the kernel (4) one easily sees that

$$f(K, h) = f(-K, h),$$

(32)

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where $h_\mu$ denotes a staggered field. Therefore the numerical results presented below apply also to a ferro- or an antiferromagnet in a staggered external field (note that $m\rightarrow m_\mu$, $X\rightarrow X_\mu$, $C_\tau\rightarrow C_\tau_\mu$).

In Fig. 3 we have plotted the spin pair correlation function $\langle s_z s_{z+1} \rangle$ vs. $K$ for several values of $\tau$. Using the $T=0$ values of the internal energy and of the magnetisation per spin one obtains the limiting values for $\langle s_z s_{z+1} \rangle$ which are equal to 1 for $J>0$, 1 $-\tau^2/8$ for $J<0$, 0 $\leq \tau \leq 4$ and -1 for $J<0$, $\tau \geq 4$.

The magnetisation per spin is shown in Fig. 4. We note that in the $J<0$, $\tau \leq 4$ region (see Fig. 2) the magnetization is not saturated at $T=0$ and according to (25a) equals $\tau/4$. However in the $J<0$, $\tau \leq 1$ region the perturbative calculation (Eq. (10)) leads to the asymptotic value $\tau/8 (K \rightarrow -\infty)$, a fact confirmed by the numerical results. At higher $\tau$ values, however, ($\tau>1$) the magnetisation goes to its ground state value.

The specific heat is presented in Fig. 5 and has the limiting value $Nk_B/2$, as expected from general principles [11]. The maximum appearing at low temperatures represents clearly a transition between the 1D Ising and the 1D Heisenberg specific heat (see [9, 11–13]).

The same observation can be made in the case of the susceptibility (Fig. 6). Note that similarly to what
In our case the Villain-Hamiltonian is defined as
\[ \beta H_V((\phi_i, m_i, l_i)) = -\frac{K}{2} \sum_i (\phi_i - \phi_{i-1} - 2\pi m_i)^2 - \frac{\hbar}{2} \sum_i (\phi_i - 2\pi l_i)^2, \]
where \( m_i \) and \( l_i \) are integers.

Applying again the Poisson formula and performing the arising Gaussian integrals we have for the partition function
\[ Z_V = \text{const.} \times \sum_{|a_i, p_i|} \prod_i \left[ \int \frac{d\phi_i}{2\pi} \exp \left\{ -\frac{q_i^2}{2K} \right\} - i q_i (\phi_i - \phi_{i-1}) - \frac{p_i^2}{2\hbar} - i p_i \phi_i \right]. \]
The \( \varphi_i \)-integrals give the constraints \( p_i = q_{i+1} - q_i \), so the final form is
\[ Z_V = \text{const.} \times \sum_{|a_i|} \exp \left\{ -\frac{\sum_i q_i^2}{2K} - \frac{\sum_i (q_{i+1} - q_i)^2}{2\hbar} \right\}, \]
which apart from a constant term represents just the low temperature form of (7).

Therefore in the \( \tau \to 0 \) limit, if \( |l-j| \) is finite, \( V_{ij} \) tends to the one-dimensional Coulomb potential. The absence of the neutrality condition for this “plasma” is related to the fact that \( V_{ii} \) is finite, so that the excitation of a single soliton (charge) requires a finite (although large) amount of energy.

The interpretation of the \( m \)-excitations (see Fig. 1) cannot be given directly, because – as emphasized by Savit [14] – the Fourier space objects can hardly be identified with configurations in the \( \varphi \)-space. A convincing argument would be the construction of a Villain-type model, where the multiple \( 2\pi \) rotations between neighbouring spins are introduced as independent degrees of freedom [15] having the same low-temperature behaviour as (3).

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taining the interaction between integer valued fields. These latter have a simple physical meaning as can be recognized when using a Villain type model corresponding to the low-temperature limit of the XY chain in an external field.

One has at hand four different analytical approaches: the high temperature and the low field series, respectively, and two different low temperature functional integral methods, one for an infinitesimal external field [8], another one for finite field values. These approximations are commonly used in higher dimensions and it would be of interest to have an idea on their region of validity. To this end we have solved numerically the transfer matrix eigenvalue problem. We present in a graphical form the results of an extended numerical calculation for the thermodynamics and the correlation length for both ferro- and antiferromagnetic couplings.

Our paper is organized as follows: in Sect. II the analytical approaches are presented. The partition function is reformulated in the Fourier-space and the corresponding transfer matrix form is demonstrated to be a very fruitful starting base for both perturbative and functional integral methods. In Sect. III the numerical method first applied by Blume et al. [9] is shortly discussed. The largest eigenvalue and the corresponding eigenvector of the transfer matrix is used for the calculation of spin-pair correlation function and of magnetisation. The specific heat and the susceptibility are calculated by numerical derivation. The correlation length is also displayed. The regions of validity of the different analytic approximations are determined in Sect. IV through a direct comparison with our exact numerical results. It turns out that they cover together practically the entire \((K, h)\) plane.

Throughout the paper we use the ferromagnetic system. Comments on the antiferromagnetic results are included when needed.

II. Analytical Approximations

The classical Hamiltonian under study is:

\[
-\beta H = K \sum_i \cos(\varphi_i - \varphi_{i+1}) + \frac{1}{2} h \sum_i \left( \cos \varphi_i + \cos \varphi_{i+1} \right),
\]

(2)

where \(\beta = 1/k_B T\), \(K = \beta J\), \(h = \beta \mu B\) and \(\varphi_i\) describes the orientation of the \(i\)-th spin. The canonical partition function is then

\[
Z(T, B) = \frac{\pi}{\pi} \left( \prod_i \frac{d\varphi_i}{2\pi} \right) \prod_j \exp \left( h(\varphi_j, \varphi_{j+1}) \right),
\]

(3)

where

\[
h(\varphi, \varphi') = K \cos(\varphi - \varphi') + \frac{h}{2} \left( \cos \varphi + \cos \varphi' \right).
\]

(4)

The macroscopic properties of the model can be calculated using the transfer operator formalism (for a detailed presentation see, e.g. [9]). The transfer operator eigenvalue problem corresponding to (3) is simply

\[
\int_{-\pi}^{\pi} \frac{d\varphi}{2\pi} \exp(h(\varphi, \varphi')) \psi_n(\varphi) = \lambda_n \psi_n(\varphi).
\]

(5)

Using the character expansion

\[
e^{x \cos \varphi} = \sum_{m=-\infty}^{\infty} I_m(x) e^{im\varphi}
\]

(6)

one can obtain a different form of the partition function, namely

\[
Z(T, B) = \prod_{\{m\}} \prod_i \left[ I_{m_i}(K) I_{m_i-\ldots-1}(h) \right],
\]

(7)

where \(I_m(x)\) is the \(n\)-th modified Bessel function of imaginary argument. The corresponding transfer-matrix eigenvalue problem

\[
I_k(K) \sum_{m=-\infty}^{\infty} I_m(h) \Psi_n(m+k) = \lambda_n \Psi_n(k)
\]

(8)

is essentially the Fourier transform of the Eq. (5). Now we are in the position to show that the expressions (7–8) are extremely useful in deriving analytical approximations.

Perturbative Calculations

First of all let us remark that the matrix eigenvalue problem (8) is trivial for either \(h = 0\) or \(K = 0\) since the matrix is diagonal and one has the exact solution [10]:

\[
\lambda_n(h = 0) = I_n(K), \quad \Psi_n(0)(k) = \delta_{n, k}.
\]

(9)

Therefore it is easy to apply the standard Rayleigh-Schrödinger perturbation theory at small fields or at high temperatures. Using the small argument expansion of \(I_n(x)\)

\[
I_n(x) = \left( \frac{x}{2} \right)^n \sum_{m=0}^{\infty} \frac{(x/2)^{2m}}{m! (m+n)!}
\]

where

\[
h(\varphi, \varphi') = K \cos(\varphi - \varphi') + \frac{h}{2} \left( \cos \varphi + \cos \varphi' \right).
\]

(4)