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Analytic calculation of second-order perturbation energy for the one-dimensional Hubbard model in the Hückel limit

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The study of the Hückel limit for the one-dimensional Hubbard model is very complicated. It is necessary to prepare the Lieb–Wu system of equations for expansion and then to initialize the variables which appear in the system, which is not straightforward. However, it is remarkable that, for the second-order contribution to the energy in this limit, it is possible to obtain, after complicated manipulations, quite transparent expressions. The analytical solution is obtained order by order for the variables to β^{-2} which appear in the Lieb–Wu solution and the β^{-1} coefficient in the energy is calculated using these expansions. The energy can be calculated numerically using these analytic results for the variables for increasing values of N.

1. Introduction

The Hubbard model in one dimension is an example of a highly nontrivial model in which the Schrödinger equation can be transformed into a system of transcendental coupled equations which were first obtained by Lieb and Wu [1]. These are referred to as the Lieb–Wu equations [1,2,3]. It is the intention here to examine the general problem of expanding the Lieb–Wu solution for the one-dimensional Hubbard model in the Hückel limit in analytic form, that is, the limit in which the resonance integral coupling β becomes very large. An introduction to this problem has already been presented [4], as well as numerical results for the expansion coefficients in the asymptotic energy series of the energy for a varying number of particles N in the cycle. The asymptotic expansion of the energy for the infinite chain has already been introduced by Misurkin and Ovchinnikov [5].

The one-dimensional Hubbard model is a natural extension of the Heisenberg model. The Hückel limit of the Hubbard model is quite complicated, and we have investigated the ground state as well as the excited states in some detail, to obtain results in numerical as well as analytic form [3,6]. Keeping in mind the complexity of the calculation, it is possible to obtain results for the second order perturbation correction in explicit form. This is possible due to the fact that we are getting considerable decoupling of the Lieb–Wu equations in this limit. Nevertheless, the analytic calculation is not easy, as will be shown in this paper, although the final equations are found to be remarkably transparent. The Hubbard model has a number of physical applications. Of particular importance is the application of the two-dimensional model to describe high temperature superconductors. We have also used the one-dimensional model to construct and investigate interpolant polynomials [6].

There are several reasons for continuing such an investigation from a more analytical point of view. It will be seen that studying the asymptotic limit as β tends to ∞ provides mathematical insights into the model in this limit. In particular, it will provide insight into the structure of the Lieb–Wu equations in this limit. In addition, once these analytical equations have been written down, these equations can be programmed relatively easily. The coefficients for the asymptotic expansions of the variables which appear in the Lieb–Wu equations have been calculated analytically to order β^{-2} in this coupling, and the energy to order β^{-1}. It is found that these analytical expressions yield the required coefficients when evaluated numerically for rings with extremely large numbers of particles in the cycle.

To begin with, the equations written down by Lieb and Wu will be introduced along with the relevant notation. The following system of transcendental equations will describe $4\nu+2$ cycles in terms of the momenta k_i which appear in the wave function and the τ_α which characterize the spin state:

$$Nk_j = 2\pi a_j - 2\sum_{\gamma=1}^{M} \arctan 2(d\sin(k_j) - \tau_\gamma)\,, \quad j = 1,\cdots,N_e\,, \tag{1}$$

$$2\sum_{i=1}^{N_e} \arctan 2(\tau_\sigma - d\sin(k_i)) = 2\pi d_\sigma + 2\sum_{\gamma\neq\sigma} \arctan(\tau_\sigma - \tau_\gamma)\,,$$
$$\sigma = 1,\cdots,M\,, \tag{2}$$

with

$$d = \frac{2\beta}{U}\,.$$

Here, β is the resonance transfer integral, and U is the one center Coulomb repulsion integral in the Hamiltonian [2,3].

In the ground state calculations, cyclic chains with $4\nu+2$ sites with a half-filled band will be considered so that $N_e = N$. The ground state is then a singlet state and the number of down spins is given by $M = 2\nu+1$. The results which are reported are for A_{1g}^{-}, however, similar results for excited states have been obtained.

2. Asymptotic form of variables and equations

The first stage of the calculation is to build the symmetry relations into (1) and (2) directly. From a calculational point of view, this will be seen to be very important because asymptotic series can be calculated out to rather large values of N. Also, some changes can be made which will make the equations more amenable to expansion in this limit.

The Lieb–Wu equations contain $n+\nu$ independent variables. There are $n = 2\nu + 1$ independent momenta k_i and ν spin variables τ_α where $n = N/2$ and all the other variables are related to this basis set by the following system of equations:

$$k_i = -k_{N+1-i}\,, \quad i = 1,\cdots,N\,,$$

$$\tau_\alpha = -\tau_{n+1-\alpha}\,, \quad \alpha = 1,\cdots,\nu\,,$$

$$\tau_{\nu+1} = 0\,.$$

The steps will be described in detail for the first equation (1). It can be found numerically that τ_α in (1) and (2) grow like a linear power of d for large d [4]. Therefore, we replace τ_α by $d\tau_\alpha$ so that the τ_α which will now appear in the equations have been scaled by a linear factor of d. Removing a factor of d from the argument of the arctangent in (1), it is then replaced by B^{-1} so that $d\to\infty$ corresponds to $B\to 0$. Consequently, (1) can be written as

$$Nk_{n+i} = (2i-1)\pi - \sum_{\gamma=1}^{\nu} 2\arctan\left(\frac{2\sin(k_{n+i}) - 2\tau_\gamma}{B}\right) + \sum_{\gamma=\nu+2}^{2\nu+1} 2\arctan\left(\frac{2\sin(k_{n+i}) - 2\tau_\gamma}{B}\right) - 2\arctan\left(\frac{2\sin(k_{n+i})}{B}\right).$$

Setting $\gamma = \nu + 1 + \alpha$ in the second sum, the new limits run from 1 to ν, hence

$$Nk_{n+i} = (2i-1)\pi - \sum_{\gamma=1}^{\nu} 2\arctan\left(\frac{2\sin(k_{n+i}) - 2\tau_\gamma}{B}\right) + \sum_{\alpha=1}^{\nu} 2\arctan\left(\frac{2\sin(k_{n+i}) - 2\tau_{\nu+1+\alpha}}{B}\right) - 2\arctan\left(\frac{2\sin(k_{n+i})}{B}\right).$$

Using the symmetry property $\tau_\alpha = -\tau_{2\nu+2-\alpha}$ on the first sum above and then introducing $2\nu + 2 - \gamma = \nu + 1 + \alpha$ so the limits on α go from ν to 1, we finally obtain

$$Nk_{n+i} = (2i-1)\pi - \sum_{\alpha=1}^{\nu}\left(2\arctan\left(2\frac{\sin(k_{n+i})+\tau_{\nu+1+\alpha}}{B}\right)\right.$$
$$\left.+\,2\arctan\left(2\frac{\sin(k_{n+i})-\tau_{\nu+1+\alpha}}{B}\right)\right) - 2\arctan\left(2\frac{\sin(k_{n+i})}{B}\right), \qquad (3)$$

where $i = 1, \cdots, n$. The remaining k_j are related to these by the antisymmetry constraint.

A similar analysis can be done on the second equation (2), and it is possible to write (2) in the equivalent form

$$2\sum_{i=1}^{2\nu+1}\left(\arctan\left(2\frac{\tau_{\nu+1+\alpha}+\sin(k_{n+i})}{B}\right) + \arctan\left(2\frac{\tau_{\nu+1+\alpha}-\sin(k_{n+i})}{B}\right)\right)$$
$$= 2\pi\alpha + 2\arctan\left(\frac{\tau_{\nu+1+\alpha}}{B}\right) + 2\arctan\left(\frac{2\tau_{\nu+1+\alpha}}{B}\right)$$
$$+\,2\sum_{\gamma\neq\alpha}^{\nu}\left(\arctan\left(\frac{\tau_{\nu+1+\alpha}+\tau_{\nu+1+\gamma}}{B}\right) + \arctan\left(\frac{\tau_{\nu+1+\alpha}-\tau_{\nu+1+\gamma}}{B}\right)\right). \qquad (4)$$

The variables in these equations will be expanded out in formal power series. A problem arises in that these series must be initialized in order to be able to solve for the other unknowns at higher orders. Although this problem can be approached numerically, the required quantities are just the Hückel values which arise out of Hückel theory. At $B = 0$, the values of the momenta are given by the Hückel values, which will be designated $k_j^{(0)}$ and are given as follows:

$$k_{n+1}^{(0)} = 0,$$

$$k_{n+2i}^{(0)} = k_{n+2i+1}^{(0)} = \frac{2\pi}{N}i, \qquad (5)$$

where $i = 1, \cdots, \nu$. Further, in the range $0 < B < \infty$, none of the k_j should coincide,

$$0 < k_{n+1} < k_{n+2} < \cdots < k_{N-1} < k_N .$$

The limiting values of the $\tau_{\nu+1+\alpha}$ as B approaches 0 are given by

$$\tau_{\nu+1+\alpha}^{(0)} = \sin\left(\frac{2\pi}{N}\alpha\right). \qquad (6)$$

Consequently, in order that the k_{n+i} go over into their Hückel values as B goes to 0 in the Lieb–Wu equations, the set of functions of the form

$$2\arctan\left(2\frac{\sin(k_{n+i}) \pm \tau_{\nu+1+\alpha}}{B}\right)$$

must approach certain limiting values, namely $\pm\pi$, as the variable B tends to zero.

The asymptotic behaviour of the arctangent functions which is evident from the table suggests that we make the following substitution in the Lieb–Wu system:

$$2\arctan(x) = \pm\pi - 2\,\mathrm{arccot}(x) \tag{7}$$

for $x \gtrless 0$, $x \neq 0$ when $-\pi/2 \leqslant \mathrm{arccot}\, x \leqslant \pi/2$ and $\mathrm{arccot}\, x \to 0$ as $|x| \to \infty$. It is the argument of the arccotangent which becomes large, and in this case, it has the following expansion:

$$\mathrm{arccot}(\chi) = \sum_{m=0}^{\infty} \chi^{-(2m+1)} .$$

However, as far as the formal power series expansions are concerned, the arccotangent can be replaced by arctangent of the reciprocal of the argument in the function. The arctangent is much easier to manipulate symbolically. In this case, the system of equations is

$$\begin{aligned} Nk_{n+i} = Nk_{n+i}^{(0)} &+ \sum_{\alpha=1}^{\nu}\left(2\arctan\left(\frac{B}{2\sin(k_{n+i}) + 2\tau_{\nu+1+\alpha}}\right)\right. \\ &\left. + 2\arctan\left(\frac{B}{2\sin(k_{n+i}) - 2\tau_{\nu+1+\alpha}}\right)\right) + 2\arctan\left(\frac{B}{2\sin(k_{n+i})}\right) \end{aligned} \tag{8}$$

$$\begin{aligned} &\sum_{i=1}^{n}\left(\arctan\left(\frac{B}{2\sin(k_{n+i}) + 2\tau_{\nu+1+\alpha}}\right) - \arctan\left(\frac{B}{2\sin(k_{n+i}) - 2\tau_{\nu+1+\alpha}}\right)\right) \\ &\quad = 2\pi\alpha + \arctan\left(\frac{B}{\tau_{\nu+1+\alpha}}\right) + \arctan\left(\frac{B}{2\tau_{\nu+1+\alpha}}\right) \\ &\qquad + \sum_{\gamma\neq\alpha}\left(\arctan\left(\frac{B}{\tau_{\nu+1+\alpha} + \tau_{\nu+1+\gamma}}\right) + \arctan\left(\frac{B}{\tau_{\nu+1+\alpha} - \tau_{\nu+1+\gamma}}\right)\right). \end{aligned} \tag{9}$$

Formal power series expansions for the variables in the Lieb–Wu equations can be written down. It is found that a new variable must be introduced to carry out the expansions of the k_{n+i}, namely, we introduce the variable

$$s^2 = B .$$

The expansions of the momenta will contain odd powers of s. In terms of the variable s, which is related to B through this equation, the momenta and spin variables τ are to be expanded in powers of s as follows:

$$k_{n+i} = k_{n+i}^{(0)} + \sum_{m=1}^{\infty} a_{n+i}^{(m)} s^m , \tag{10}$$

$$\tau_{\nu+1+\alpha} = \tau_{\nu+1+\alpha}^{(0)} + \sum_{m=1}^{\infty} t_{\nu+1+\alpha}^{(m)} s^m . \tag{11}$$

Substitute these expansions into the Lieb–Wu equations, and then expand the equations out in powers of s. From the expansions, it is found that it is possible to solve for the coefficients $a_{n+i}^{(m)}$ and $t_{\nu+1+\alpha}^{(m)}$ analytically one order at a time in terms of the variables obtained at lower orders. This procedure will give k_{n+i} and $\tau_{\nu+1+\alpha}$ as power series in s. The power series for the k_{n+i} can be used to calculate a series representation for the energy in powers of the variable s.

3. First-order analysis for the ground state

In terms of the variable s, the system of equations takes the form

$$Nk_{n+i} = Nk_{n+i}^{(0)} + \sum_{\alpha=1}^{\nu}\left(2\arctan\left(\frac{s^2}{2\sin(k_{n+i}) + 2\tau_{\nu+1+\alpha}}\right) + 2\arctan\left(\frac{s^2}{2\sin(k_{n+i}) - 2\tau_{\nu+1+\alpha}}\right)\right) + 2\arctan\left(\frac{s^2}{2\sin(k_{n+i})}\right), \quad (12)$$

$$\sum_{i=1}^{n}\left(\arctan\left(\frac{s^2}{2\sin(k_{n+i}) + 2\tau_{\nu+1+\alpha}}\right) - \arctan\left(\frac{s^2}{2\sin(k_{n+i}) - 2\tau_{\nu+1+\alpha}}\right)\right)$$
$$= 2\pi\alpha + \arctan\left(\frac{s^2}{\tau_{\nu+1+\alpha}}\right) + \arctan\left(\frac{s^2}{2\tau_{\nu+1+\alpha}}\right) + \sum_{\gamma\neq\alpha}^{\nu}\arctan\left(\frac{s^2}{\tau_{\nu+1+\alpha} + \tau_{\nu+1+\gamma}}\right) + \arctan\left(\frac{s^2}{\tau_{\nu+1+\alpha} - \tau_{\nu+1+\gamma}}\right). \quad (13)$$

To carry out the first-order analysis, we are concerned with the terms which are linear in s which arise from the expansion of the terms in these equations.

For the case in which $i = 1$, we have $k_{n+1}^{(0)} = 0$, and in this case, the term which is linear in s comes from the term

$$2\arctan\left(\frac{s^2}{2\sin(k_{n+1})}\right)$$

and gives the equation

$$-Nk_{n+1}^{(1)} + \frac{1}{k_{n+1}^{(1)}} = 0\,.$$

This has the general solution

$$k_{n+1}^{(1)} = \pm N^{-1/2}\,.$$

On account of this cancellation, the Lieb–Wu system decouples into blocks which can be solved independently of each other. To first order in s, (12) gives the following pair of independent equations

$$-Nk_{n+i}^{(1)} + \frac{1}{-t_{\nu+1+\alpha}^{(1)} + \cos(k_{n+i}^{(0)})k_{n+i}^{(1)}} = 0\,,$$

$$-Nk_{n+i+1}^{(1)} + \frac{1}{-t_{\nu+1+\alpha}^{(1)} + \cos(k_{n+i+1}^{(0)})k_{n+i}^{(1)}} = 0\,,$$

where $i = 2\alpha$ and $2\alpha + 1$ where there are three unknown variables. A third equation comes from the second Lieb–Wu equation (13),

$$-\frac{1}{-2t_{\nu+1+\alpha}^{(1)} + 2\cos(k_{n+i}^{(0)})k_{n+i}^{(1)}} = \frac{1}{-2t_{\nu+1+\alpha}^{(1)} + 2\cos(k_{n+i}^{(0)})k_{n+i+1}^{(1)}}\,.$$

To simplify these equations, let us introduce the notation $t = t_{\nu+1+\alpha}^{(1)}$, $x = k_{n+i}^{(1)}$, $y = k_{n+i+1}^{(1)}$. To summarize, the first-order coefficients in the expansions of the variables for a general $4\nu + 2$ member ring requires that we solve the following simple set of coupled equations,

$$a(x + y) = 2t\,,$$

$$Nax^2 - Nxt = 1\,,$$

$$Nay^2 - Nyt = 1\,,$$

where $a = \cos(k_{n+i}^{(0)})$. If one subtracts the last two equations, one obtains the equation

$$Na(x + y)(x - y) - Nt(x - y) = 0\,,$$

which implies that either $x = y$ or $a(x + y) - t = 0$, and the second equation implies that $t = a(x + y)$. Putting this in the first equation, the following constraint is obtained:

$$x = -y\,;$$

hence, $t = 0$. Setting $t = 0$ in the last equation will give explicit expressions for x and y, that is

$$k_{n+i}^{(1)} = \pm\frac{1}{(N\cos(k_{n+i}^{(0)}))^{1/2}}\,,$$

$$k_{n+i+1}^{(1)} = \mp\frac{1}{(N\cos(k_{n+i}^{(0)}))^{1/2}}\,,$$

and the equation which was derived above, namely $x = -y$, specifies the difference in relative sign between x and y. The other possibility, $x = y$, does not lead to a mathematically consistent solution.

4. General expansion to fourth order in s

It is shown how the Lieb–Wu variables can be expanded consistently to fourth order in the variable s in general for an $N = 4\nu + 2$ member ring, and that these expansions can be used to calculate the β^{-1} contribution to the energy of the system. It will be shown that one can calculate this contribution for the case of very large rings, and these results can be used to calculate an approximation to $\zeta(3)$ by comparing the finite N calculation for the β^{-1} coefficient in the expansion of the energy per particle for the infinite chain [5].

It will be shown first how the coefficients to fourth order in s contribute to the energy, which is given by the expression

$$E = -2\beta \sum_{i=1}^{N} \cos k_i \tag{14}$$

This can be expanded in powers of s once the expansions for the momenta have been obtained.

To calculate an expansion for the energy in terms of s, an expansion for the $\cos(k_i)$ which appear in the energy must be carried out.

Expanding the corresponding cosine term in the energy for k_{n+1}, one has

$$2\cos(k_{n+1}) = 2 - k_{n+1}^{(1)2} s^2 + \left(\frac{1}{12} k_{n+1}^{(1)4} - 2k_{n+1}^{(3)} k_{n+1}^{(1)}\right) s^4 + \cdots .$$

For the conjugate pair $k_{n+2\alpha}$, $k_{n+2\alpha+1}$ where $\alpha = 1, \cdots, \nu$, it is useful to group the terms in pairs and expand to take advantage of sign cancellations on account of the symmetry conditions:

$$\begin{aligned}
&2(\cos(k_{n+2\alpha}) + \cos(k_{n+2\alpha+1})) \\
&\quad = 4\cos(k_{n+2\alpha}^{(0)}) + (-4\sin(k_{n+2\alpha}^{(0)}) k_{n+2\alpha}^{(2)} - 2\cos(k_{n+2\alpha}^{(0)}) k_{n+2\alpha}^{(1)2}) s^2 \\
&\quad\quad + (2\sin(k_{n+2\alpha}^{(0)}) k_{n+2\alpha}^{(2)} k_{n+2\alpha}^{(1)2} - 4\sin(k_{n+2\alpha}^{(0)}) k_{n+2\alpha}^{(4)} + \tfrac{1}{6}\cos(k_{n+2\alpha}^{(0)}) k_{n+2\alpha}^{(1)4} \\
&\quad\quad - 2\cos(k_{n+2\alpha}^{(0)}) k_{n+2\alpha}^{(2)2} - 4\cos(k_{n+2\alpha}^{(0)}) k_{n+2\alpha}^{(3)} k_{n+2\alpha}^{(1)}) s^4 + \cdots ,
\end{aligned}$$

where we have just kept terms out to order s^4. If this equation is summed over α from 1 to ν, and the expansion for $2\cos(k_{n+1})$ is added to the result, the energy to fourth order in s can be calculated. Summing the geometric series in the cosine gives

$$\sum_{\alpha=1}^{\nu} \cos\left(\frac{2\pi}{N}\alpha\right) = \frac{1 - \sin(\frac{\pi}{N})}{\sin(\frac{\pi}{N})} .$$

Collecting terms, it is found that

$$\frac{E^{(4)}}{-2\beta}=\frac{2}{\sin(\frac{\pi}{N})}+\Bigg(-k_{n+1}^{(1)}+\sum_{\alpha=1}^{\nu}(4\cos(k_{n+2\alpha}^{(0)})-4\sin(k_{n+2\alpha}^{(0)})$$
$$-2\cos(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(1)2})\Bigg)s^2+\Bigg((\tfrac{1}{12}k_{n+1}^{(1)4}-2k_{n+1}^{(3)}k_{n+1}^{(1)})$$
$$+\sum_{\alpha=1}^{\nu}(2\sin(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(2)}k_{n+2\alpha}^{(1)2}-4\sin(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(4)}+\tfrac{1}{6}\cos(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(1)4}$$
$$-2\cos(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(2)2}-4\cos(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(3)}k_{n+2\alpha}^{(1)})\Bigg)s^4\,.$$

Notice that if we divide both sides of this equation by N, the limit of the first term as N goes to infinity is just $2/\pi$ and then multiplying by -2β, one obtains the first term in the expansion of the energy for the infinite chain. It is noted that (14) is equivalent to the results of perturbation theory, as will be shown by explicit calculation in a forthcoming paper.

5. Solution of equation for arbitrary N

The equations for the general case rapidly become more complicated. However, by considering each term individually, the contribution at each order in s which is made by a specific term in the set of equations can be written down, and then programmed [7,8].

The expansions are carried out in powers of s by first writing down the Lieb–Wu equations in the form given below and substituting the series (10) and (11). Consider the first set of equations (12). Suppose $i=2\alpha$ is not equal to one. Then there is a term in the sum in which $\gamma=\alpha$, and the resulting term can be taken out of the sum on its own. Dropping the unimportant constant, the first system of equations becomes

$$Nk_{n+2\alpha}=2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha})+2\tau_{\nu+1+\alpha}}\right)$$
$$+2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha})-2\tau_{\nu+1+\alpha}}\right)$$
$$+\sum_{\substack{\gamma=1\\ \gamma\neq\alpha}}^{\nu}\left(2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha})+2\tau_{\nu+1+\gamma}}\right)\right.$$
$$\left.+2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha})-2\tau_{\nu+1+\gamma}}\right)\right)+2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha})}\right)\,. \tag{15}$$

Since the Hückel variables are given by (5) and (6), important cancellations occur when the second term on the right is expanded out in powers of s,

$$2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha})+2\tau_{\nu+1+\alpha}}\right)$$

$$=\frac{s^2}{2\sin(k^{(0)}_{n+2\alpha})}-\frac{\cos(k^{(0)}_{n+2\alpha})k^{(1)}_{n+2\alpha}+t^{(1)}_{\nu+1+\alpha}}{\sin^2(k^{(0)}_{n+2\alpha})}s^3+\cdots.$$

The other term is

$$2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha})-2\tau_{\nu+1+\alpha}}\right)=-\frac{s}{(t^{(1)}_{\nu+1+\alpha}-\cos(k^{(0)}_{n+2\alpha})k^{(1)}_{n+2\alpha})}$$

$$+\frac{2t^{(2)}_{\nu+1+\alpha}+\sin(k^{(0)}_{n+2\alpha})k^{(1)2}_{n+2\alpha}-2\cos(k^{(0)}_{n+2\alpha})k^{(2)}_{n+2\alpha}}{(t^{(1)}_{\nu+1+\alpha}-\cos(k^{(0)}_{n+2\alpha})k^{(1)}_{n+2\alpha})^2}s^2+\cdots.$$

On the other hand, when $\gamma\neq\alpha$, the expansions are given as

$$2\arctan\left(\frac{s^2}{2\sin(k^{(0)}_{n+2\alpha})+2\tau_{\nu+1+\gamma}}\right)$$

$$=\frac{s^2}{\sin(k_{n+2\alpha})+\tau^{(0)}_{\nu+1+\gamma}}-\frac{\cos(k^{(0)}_{n+2\alpha})k^{(1)}_{n+2\alpha}+t^{(1)}_{\nu+1+\gamma}}{(\sin(k^{(0)}_{n+2\alpha})+\tau^{(0)}_{\nu+1+\gamma})^2}s^3+\cdots$$

and

$$2\arctan\left(\frac{s^2}{2\sin(k^{(0)}_{n+2\alpha})-2\tau_{\nu+1+\gamma}}\right)$$

$$=\frac{s^2}{\sin(k^{(0)}_{n+2\alpha})-\tau^{(0)}_{\nu+1+\gamma}}+\frac{t^{(1)}_{\nu+1+\gamma}-\cos(k^{(0)}_{n+2\alpha})k^{(1)}_{n+2\alpha}}{(\sin(k^{(0)}_{n+2\alpha})-\tau^{(0)}_{\nu+1+\gamma})^2}s^3+\cdots.$$

It has been pointed out that a linear term in s appears on account of the cancellation noted above. The first-order contributions have already been derived, and so we use the results obtained to go to higher orders.

Similarly, if we set $i=2\alpha+1$, again not equal to 1, and remove the $\gamma=\alpha$ term from the sum, one has

$$Nk_{n+2\alpha+1} = 2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha+1}) + 2\tau_{\nu+1+\alpha}}\right) + 2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha+1}) - 2\tau_{\nu+1+\alpha}}\right) + \sum_{\substack{\gamma=1\\ \gamma\neq\alpha}}^{\nu}\left(2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha+1}) + 2\tau_{\nu+1+\gamma}}\right) + 2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha+1}) - 2\tau_{\nu+1+\gamma}}\right)\right) + 2\arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha+1})}\right). \tag{16}$$

The final set of equations is

$$\arctan\left(\frac{s^2}{2\sin(k_{n+1}) + 2\tau_{\nu+1+\alpha}}\right) - \arctan\left(\frac{s^2}{2\sin(k_{n+1}) - 2\tau_{\nu+1+\alpha}}\right) + \arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha}) + 2\tau_{\nu+1+\alpha}}\right) - \arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha}) - 2\tau_{\nu+1+\alpha}}\right) + \arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha+1}) + 2\tau_{\nu+1+\alpha}}\right) - \arctan\left(\frac{s^2}{2\sin(k_{n+2\alpha+1}) - 2\tau_{\nu+1+\alpha}}\right) \sum_{\substack{i=2\\ i\neq 2\alpha,2\alpha+1}}^{\nu}\left(\arctan\left(\frac{s^2}{2\sin(k_{n+i}) + 2\tau_{\nu+1+\alpha}}\right) - \arctan\left(\frac{s^2}{2\sin(k_{n+i}) - 2\tau_{\nu+1+\alpha}}\right)\right)$$
$$= \arctan\left(\frac{s^2}{\tau_{\nu+1+\alpha}}\right) + \arctan\left(\frac{s^2}{2\tau_{\nu+1+\alpha}}\right) + \sum_{\gamma\neq\alpha}^{\nu}\left(\arctan\left(\frac{s^2}{\tau_{\nu+1+\alpha} + \tau_{\nu+1+\gamma}}\right) + \arctan\left(\frac{s^2}{\tau_{\nu+1+\alpha} - \tau_{\nu+1+\gamma}}\right)\right). \tag{17}$$

The required terms are collected together in tables 3 and 4 for the third-order and in tables 5 and 6 for the fourth-order terms for the expansion in s. The second-order calculation will be treated in detail, and the contribution to $k_{n+2\alpha}$ is given by the following equation:

$$Nk^{(2)}_{n+2\alpha} = \left(\frac{1}{2\sin(k^{(0)}_{n+2\alpha})} + \frac{2t^{(2)}_{\nu+1+\alpha} + \sin(k^{(0)}_{n+2\alpha})k^{(1)2}_{n+2\alpha} - 2\cos(k^{(0)}_{n+2\alpha})k^{(2)}_{n+2\alpha}}{2(t^{(1)}_{\nu+1+\alpha} - \cos(k^{(0)}_{n+2\alpha})k^{(1)}_{n+2\alpha})^2}\right) + \sum_{\substack{\gamma=1\\ \gamma\neq\alpha}}^{\nu}\left(\frac{1}{\sin(k^{(0)}_{n+2\alpha}) + \tau^{(0)}_{\nu+1+\gamma}} + \frac{1}{\sin(k^{(0)}_{n+2\alpha}) - \tau^{(0)}_{\nu+1+\gamma}}\right) + \frac{1}{\sin(k^{(0)}_{n+2\alpha})},$$

Table 1
Definition of quantities which appear in contributions at fourth order in s from Lieb–Wu equations.

$$A_{n+2\alpha} = -2c_\alpha^3 k_{n+2\alpha}^{(1)4} k_{n+2\alpha}^{(2)}$$

$$B_{n+2\alpha} = 6c_\alpha k_{n+2\alpha}^{(1)4} k_{n+2\alpha}^{(2)}$$

$$C_{n+2\alpha} = 48c_\alpha^3 k_{n+2\alpha}^{(1)} k_{n+2\alpha}^{(2)} k_{n+2\alpha}^{(3)}$$

$$D_{n+2\alpha} = 3k_{n+2\alpha}^{(1)6} s_\alpha$$

$$E_{n+2\alpha} = -24c_\alpha^3 k_{n+2\alpha}^{(2)3}$$

$$F_{n+2\alpha} = -3s_\alpha k_{n+2\alpha}^{(1)2}$$

$$G_{n+2\alpha} = 6c_\alpha k_{n+2\alpha}^{(2)}$$

$$c_\alpha = \cos(k_{n+2\alpha}^{(0)})$$

$$s_\alpha = \sin(k_{n+2\alpha}^{(0)})$$

where $\alpha = 1, \cdots, \nu$. A second equation which also contains the variable $t_{\nu+1+\alpha}^{(2)}$ comes out by setting $i = 2\alpha + 1$ and since $k_{n+2\alpha}^{(0)} = k_{n+2\alpha+1}^{(0)}$ the same value of $\beta = \alpha$ in the sum provides the same cancellation. There is then another equation identical with the above but with $k_{n+2\alpha}^{(2)}$ replaced by $k_{n+2\alpha+1}^{(2)}$ everywhere. The first-order analysis yields the conditions $t_{\nu+1+\alpha}^{(1)} = 0$ and $k_{n+2\alpha}^{(1)} = -k_{n+2\alpha+1}^{(1)}$. Therefore, it follows easily from the equation above and its $k_{n+2\alpha+1}^{(2)}$ companion that

$$k_{n+2\alpha}^{(2)} = k_{n+2\alpha+1}^{(2)} .$$

Table 2
Numerical values for $|f_N^2|$ and approximations to $\zeta(3)$ for rings with $N = 6$ to $N = 8738$. The approximate $z_N(3)$ is calculated using $f_N^{(2)}$. The absolute errors $\Gamma = |z_N(3) - \zeta(3)|/\zeta(3)$ are also given.

N	$\lvert f_N^2\rvert$	$z_N(3)$	Γ
6	0.03356481481	1.189394212	1.3×10^{-2}
10	0.03379101966	1.197409948	4.7×10^{-3}
14	0.03385488195	1.199672957	2.4×10^{-3}
30	0.03310743938	1.201535368	4.3×10^{-4}
34	0.03391069544	1.201650749	4.1×10^{-4}
102	0.03392088250	1.202011735	3.7×10^{-5}
514	0.03392210695	1.202055124	1.5×10^{-6}
2570	0.03392215514	1.202056832	5.9×10^{-8}
8738	0.03392215697	1.202056897	5.0×10^{-9}

Table 3
Third order in s with symmetry conditions applied to k_{n+i} and $\tau_{\nu+1+\alpha}$.

$2\arctan\dfrac{s^2}{2\sin k_{n+i}+2\tau_{\nu+1+\alpha}}$	$-\dfrac{\cos(k^{(0)}_{n+i})k^{(1)}_{n+i}}{(\sin(k^{(0)}_{n+i})+\tau_{\nu+1+\alpha})^2}$
$2\arctan\dfrac{s^2}{2\sin k_{n+i}-2\tau_{\nu+1+\alpha}}$	$-\dfrac{\cos(k^{(0)}_{n+i})k^{(1)}_{n+i}}{(\sin(k^{(0)}_{n+i})-\tau^{(0)}_{\nu+1+\alpha})^2}$
$2\arctan\dfrac{s^2}{2\sin(k_{n+i})}$	$-\dfrac{\cos(k^{(0)}_{n+i})k^{(1)}_{n+i}}{\sin^2(k^{(0)}_{n+i})}$
$\tau^{(0)}_{\nu+1+\alpha}=\sin(k^{(0)}_{n+i})$	
$2\arctan\dfrac{s^2}{(2\sin(k_{n+i})+2\tau_{\nu+1+\alpha})}$	$-\dfrac{\cos(k^{(0)}_{n+i})k^{(1)}_{n+i}}{4\sin^2(k^{(0)}_{n+i})}$
$2\arctan\dfrac{s^2}{(2\sin(k_{n+i})-2\tau_{\nu+1+\alpha})}$	$-\dfrac{\cos(k^{(0)}_{n+i})(k^{(3)}_{n+i}-k^{(1)3}_{n+i}/6)-\sin(k^{(0)}_{n+i})k^{(2)}_{n+i}k^{(1)}_{n+i}}{2\cos^2(k^{(0)}_{n+i})k^{(1)2}_{n+i}}$
	$-\dfrac{(2\cos(k^{(0)}_{n+i})k^{(2)}_{n+i}-\sin(k^{(0)}_{n+i})k^{(1)2}_{n+i})^2}{4\cos^3(k^{(0)}_{n+i})k^{(1)3}_{n+i}}$
	$-\dfrac{1}{12\cos^3(k^{(0)}_{n+i})k^{(1)3}_{n+i}}$

Solving the first equation above for $k^{(2)}_{n+2\alpha}$, one obtains

$$2Nk^{(2)}_{n+2\alpha}=\frac{3}{2\tau^{(0)}_{\nu+1+\alpha}}+N\,\frac{2t^{(2)}_{\nu+1+\alpha}+\sin(k^{(0)}_{n+2\alpha})k^{(1)2}_{n+2\alpha}}{2\cos(k^{(0)}_{n+2\alpha})}$$

$$+\sum_{\gamma\neq\alpha}\left(\frac{1}{\tau^{(0)}_{\nu+1+\alpha}+\tau^{(0)}_{\nu+1+\gamma}}+\frac{1}{\tau^{(0)}_{\nu+1+\alpha}-\tau^{(0)}_{\nu+1+\gamma}}\right).$$

The last equation which relates $k^{(2)}_{n+2\alpha}$ and $t^{(2)}_{\nu+1+\alpha}$ comes from the second Lieb–Wu equation, and it is given by

Table 4
Third order in s from Lieb–Wu continued.

$2\arctan\dfrac{s^2}{2\sin k_{n+i}}$	$-\dfrac{\cos(k_{n+i}^{(0)})k_{n+i}^{(1)}}{\sin^2(k_{n+i}^{(0)})}$
$\arctan\dfrac{s^2}{\tau_{\nu+1+\alpha}}$	0
$\arctan\dfrac{s^2}{2\tau_{\nu+1+\alpha}}$	0
$\arctan\dfrac{s^2}{\tau_{\nu+1+\alpha}+\tau_{\nu+1+\gamma}}$	0
$\arctan\dfrac{s^2}{\tau_{\nu+1+\alpha}-\tau_{\nu+1+\gamma}}$	0
$k_{n+1}^{(0)}=0$	
$2\arctan\dfrac{s^2}{2\sin(k_{n+1})+2\tau_{\nu+1+\alpha}}$	$-\dfrac{k_{n+1}^{(1)}}{\tau_{\nu+1+\alpha}^{(0)2}}$
$2\arctan\dfrac{s^2}{2\sin(k_{n+1})-2\tau_{\nu+1+\alpha}}$	$-\dfrac{k_{n+1}^{(1)}}{\tau_{\nu+1+\alpha}^{(0)2}}$
$2\arctan\dfrac{s^2}{2\sin(k_{n+1})}$	$-\dfrac{(k_{n+1}^{(3)}-k_{n+1}^{(1)3}/6)}{k_{n+1}^{(1)2}}-\dfrac{1}{12k_{n+1}^{(1)3}}$

$$\frac{1}{\tau_{\nu+1+\alpha}^{(0)}}+\frac{1}{4\sin(k_{n+2\alpha}^{(0)})}+\frac{2t_{\nu+1+\alpha}^{(2)}+\sin(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(1)2}-2\cos(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(2)}}{4\cos^2(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(1)2}}$$
$$+\frac{1}{4\sin(k_{n+2\alpha}^{(0)})}+\frac{2t_{\nu+1+\alpha}^{(2)}+\sin(k_{n+2\alpha}^{(0)})k_{n+2\alpha+1}^{(1)2}-2\cos(k_{n+2\alpha}^{(0)})k_{n+2\alpha+1}^{(2)}}{4\cos^2(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(1)2}}$$
$$+\frac{1}{2}\sum_{\substack{i=2\\ i\neq 2\alpha,2\alpha+1}}^{n}\left(\frac{1}{\sin(k_{n+i}^{(0)})+\tau_{\nu+1+\alpha}^{(0)}}-\frac{1}{\sin(k_{n+i}^{(0)})-\tau_{\nu+1+\alpha}^{(0)}}\right)$$
$$=\frac{1}{\tau_{\nu+1+\alpha}^{(0)}}+\frac{1}{2\tau_{\nu+1+\alpha}^{(0)}}+\sum_{\gamma\neq\alpha}^{\nu}\left(\frac{1}{\tau_{\nu+1+\alpha}^{(0)}+\tau_{\nu+1+\gamma}^{(0)}}+\frac{1}{\tau_{\nu+1+\alpha}^{(0)}-\tau_{\nu+1+\gamma}^{(0)}}\right).$$

The sum over i can be turned into a sum over γ by setting $i=2\gamma$ and $2\gamma+1$ consecutively. A factor of 2 must now be included since γ goes from 1 to ν and $\gamma\neq\alpha$.

Table 5
Fourth order contributions from terms in Lieb–Wu equations.

$2\arctan\dfrac{s^2}{2\sin(k_{n+i})+2\tau_{\nu+1+\alpha}}$	$-\dfrac{2\cos(k^{(0)}_{n+i})k^{(2)}_{n+i}-\sin(k^{(0)}_{n+i})k^{(1)2}_{n+i}}{2(\sin(k^{(0)}_{n+i})+\tau^{(0)}_{\nu+1+\alpha})^2}$
	$+\dfrac{\cos^2(k^{(0)}_{n+i})k^{(1)2}_{n+i}}{(\sin(k^{(0)}_{n+i})+\tau^{(0)}_{\nu+1+\alpha})^3}$
$2\arctan\dfrac{s^2}{2\sin(k_{n+i})-2\tau_{\nu+1+\alpha}}$	$-\dfrac{2\cos(k^{(0)}_{n+i})k^{(2)}_{n+i}-\sin(k^{(0)}_{n+i})k^{(1)2}_{n+i}}{2(\sin(k^{(0)}_{n+i})-\tau^{(0)}_{\nu+1+\alpha})^2}$
	$+\dfrac{\cos^2(k^{(0)}_{n+i})k^{(1)2}_{n+i}}{(\sin(k^{(0)}_{n+i})-\tau^{(0)}_{\nu+1+\alpha})^3}$
$2\arctan\dfrac{s^2}{2\sin(k_{n+i})}$	$-\dfrac{(\cos(k^{(0)}_{n+i})k^{(2)}_{n+i}-\sin(k^{(0)}_{n+i})k^{(1)2}_{n+i}/2)}{\sin^2(k^{(0)}_{n+i})}$
	$+\dfrac{\cos^2(k^{(0)}_{n+i})k^{(1)2}_{n+i}}{\sin^3(k^{(0)}_{n+i})}$
$\tau=\sin(k^{(0)})+\tau^{(4)}s^4$	
$2\arctan\dfrac{s^2}{2\sin(k_{n+i})+2\tau_{\nu+1+\alpha}}$	$-\dfrac{2\cos(k^{(0)}_{n+i})k^{(2)}_{n+i}-\sin(k^{(0)}_{n+i})k^{(1)2}_{n+i}}{8\sin^2(k^{(0)}_{n+i})}$
	$+\dfrac{\cos^2(k^{(0)}_{n+i})k^{(1)2}_{n+i}}{8\sin^3(k^{(0)}_{n+i})}$
$2\arctan\dfrac{s^2}{2\sin(k_{n+i})-2\tau_{\nu+1+\alpha}}$	$\dfrac{A_{n+i}-24c^3_{n+i}k^{(1)2}_{n+i}k^{(4)}_{n+i}+24c^2_{n+i}k^{(1)}_{n+i}\tau^{(4)}_{\nu+1+\alpha}}{24c_i^4k^{(1)4}_{n+i}}$
	$+\dfrac{B_{n+i}+C_{n+i}+D_{n+i}+E_{n+i}+F_{n+i}+G_{n+i}}{24c_i^4k^{(1)4}_{n+i}}$
$2\arctan\dfrac{s^2}{2\sin(k_{n+i})}$	$-\dfrac{\cos(k^{(0)}_{n+i})k^{(2)}_{n+i}-\sin(k^{(0)}_{n+i})k^{(1)2}_{n+i}}{\sin^2(k^{(0)}_{n+i})}$
	$+\dfrac{\cos^2(k^{(0)}_{n+i})k^{(1)2}_{n+i}}{\sin^3(k^{(0)}_{n+i})}$
$2\arctan\dfrac{s^2}{\tau_{\nu+1+\alpha}}$	0
$\arctan\dfrac{s^2}{2\tau_{\nu+1+\alpha}}$	0

Table 6
Fourth order contributions from terms in Lieb–Wu equations.

$\arctan \dfrac{s^2}{\tau_{\nu+1+\alpha} + \tau_{\nu+1+\gamma}}$	0
$\arctan \dfrac{s^2}{\tau_{\nu+1+\alpha} - \tau_{\nu+1+\gamma}}$	0
$k_{n+1}^{(0)} = 0$	
$2\arctan \dfrac{s^2}{2\sin(k_{n+1}) + 2\tau_{\nu+1+\alpha}}$	$\dfrac{k_{n+1}^{(1)2}}{\tau_{\nu+1+\alpha}^{(0)3}}$
$2\arctan \dfrac{s^2}{2\sin(k_{n+1}) - 2\tau_{\nu+1+\alpha}}$	$-\dfrac{k_{n+1}^{(1)2}}{\tau_{\nu+1+\alpha}^{(0)3}}$
$2\arctan \dfrac{s^2}{2\sin(k_{n+1})}$	0

Moreover, using the previous results $k_{n+2\alpha}^{(1)} = -k_{n+2\alpha+1}^{(1)}$ and $k_{n+2\alpha}^{(2)} = k_{n+2\alpha+1}^{(2)}$, we obtain the equation which relates $t_{\nu+1+\alpha}^{(2)}$ to $k_{n+2\alpha}^{(2)}$ as follows:

$$t_{\nu+1+\alpha}^{(2)} = \cos(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(2)} - \tfrac{1}{2}\sin(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(1)2}\,.$$

Substituting this into (15), we obtain the following simple equation for $k_{n+2\alpha}^{(2)}$ in terms of known quantities,

$$Nk_{n+2\alpha}^{(2)} = \frac{3}{2\tau_{\nu+1+\alpha}^{(0)}} + \sum_{\gamma\neq\alpha}^{\nu}\left(\frac{1}{\tau_{\nu+1+\alpha}^{(0)} + \tau_{\nu+1+\gamma}^{(0)}} + \frac{1}{\tau_{\nu+1+\alpha}^{(0)} - \tau_{\nu+1+\gamma}^{(0)}}\right).$$

Substituting into the equation above, one obtains an expression for $t_{\nu+1+\alpha}^{(2)}$. There is one final case to be treated, namely the case $i = 1$, which determines k_{n+1}. The equation which results to second order in s is given by

$$Nk_{n+1}^{(2)} = -\frac{k_{n+1}^{(2)}}{k_{n+1}^{(1)2}}$$

and this implies that, for any N-chain, the general solution is

$$k_{n+1}^{(2)} = 0\,.$$

That is, the second order coefficient of the variable k_{n+1} is always zero.

6. Calculation of third- and fourth-order variables

In order to calculate higher-order coefficients in the expansions of the variables, the function terms in the Lieb–Wu equations are expanded out. The required equations which must be solved at each order can be constructed from these tables by taking the corresponding terms from the given table and replacing the term in the Lieb–Wu equation as formulated in the last section to which the term corresponds. These equations can be solved for the coefficients of the variables at that particular order. In calculating the elements in the tables, it should be pointed out that the constraints on the coefficients given previously have been used in order to make the presentation more compact.

To third order in s, the equation which determines $k_{n+1}^{(3)}$ is given by

$$Nk_{n+1}^{(3)} = \sum_{\alpha=1}^{\nu}\left(-\frac{k_{n+1}^{(1)}}{\tau_{\nu+1+\alpha}^{(0)2}} - \frac{k_{n+1}^{(1)}}{\tau_{\nu+1+\alpha}^{(0)2}}\right) - \frac{6k_{n+1}^{(3)} - k_{n+1}^{(1)3}}{6k_{n+1}^{(1)2}} - \frac{1}{12k_{n+1}^{(1)3}} .$$

Solving this for $k_{n+1}^{(3)}$, it is found that

$$k_{n+1}^{(3)} = -k_{n+1}^{(1)3}\sum_{\alpha=1}^{\nu}\frac{1}{\tau_{\nu+1+\alpha}^{(0)2}} + \frac{1}{12}k_{n+1}^{(1)3} - \frac{1}{24k_{n+1}^{(1)}} .$$

To third order in s, there is one independent equation in $k_{n+2\alpha}^{(3)}$ given the symmetry conditions, and we simply present the result after some simplifications,

$$k_{n+2\alpha}^{(3)} = \frac{1}{2N}\sum_{\substack{\gamma=1\\ \gamma\neq\alpha}}^{\nu}\left(\frac{-\cos(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(1)}}{(\sin(k_{n+2\alpha}^{(0)}) + \tau_{\nu+1+\gamma}^{(0)})^2} - \frac{\cos(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(1)}}{(\sin(k_{k+2\alpha}^{(0)}) - \tau_{\nu+1+\gamma}^{(0)})^2}\right)$$
$$- \frac{5\cos(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(1)}}{8N\sin^2(k_{n+2\alpha}^{(0)})} - \frac{1}{24}\left(k_{n+2\alpha}^{(1)3} - \frac{12k_{n+2\alpha}^{(2)2}}{k_{n+2\alpha}^{(1)}} + \frac{-3k_{n+2\alpha}^{(1)4} + 1}{\cos^2(k_{n+2\alpha}^{(0)})k_{n+2\alpha}^{(1)}}\right) . \tag{18}$$

The fourth-order contributions can be extracted from each of the terms in the Lieb–Wu equations in the same way that the third-order contributions were handled. The terms which yield cancellations have already been separated out to give eqs. (15) to (17). To obtain the equations for the fourth-order variables it is necessary to extract the corresponding terms from tables 5 and 6 and then substitute into these two equations, exactly as for the case of the third-order analysis. The details are mode tedious, and will be omitted here.

From eqs. (15), (16) and (17), a system of three linear equations in the three unknowns $k_{n+2\alpha}^{(4)}$, $k_{n+2\alpha+1}^{(4)}$, and $\tau_{\nu+1+\alpha}^{(4)}$ is obtained for each α from 1 to ν. The symmetry constraint $k_{n+2\alpha+1}^{(4)} = k_{n+2\alpha}^{(4)}$ derives from solving these. It is quite useful in terms of programming to implement this constraint directly, and to work with two variables. A set of $\alpha = 1, \cdots, \nu$ structurally equivalent blocks of equations results, such that each block depends only on these three variables. Notice that these equations which give the fourth-order variables depend only on the variables at lower orders which have already been calculated, and one may assume are known, since the calculation proceeds order by order.

At this point, expressions for all of the terms on the right-hand side of the expression $E^{(4)}$ have been obtained, and by straightforward back substitution, an expression for the energy to the required order is obtained.

It has been shown here that the Lieb–Wu system decouples into blocks of three equations each, which contain only three unknown variables at a time $k^{(i)}_{n+2\alpha}$, $k^{(i)}_{n+2\alpha+1}$, $t^{(i)}_{\nu+1+\alpha}$ as well as the variables determined at lower orders, and so we are free to solve at order i by simply solving each of the $\alpha = 1, \cdots, \nu$ blocks separately. This allows for the complete solution to order four of the Lieb–Wu equations in this limit.

It has been shown by explicit calculation of individual terms that this decoupling holds to fourth order in s, in the sense that at any order in s, there are three independent equations in the variables $k^{(i)}_{n+2\alpha}$, $k^{(i)}_{n+2\alpha+1}$, $t^{(i)}_{\nu+1+\alpha}$ which depend only on the variables from only lower orders. These have already been calculated and are assumed known. None of the unknown variables from higher orders appear in this set. This decoupling is closely connected with the cancellation that takes place upon expanding the functions. Although we have no formal proof at the moment, it is conjectured that this decoupling persists to arbitrarily high orders in s. Finally, these results have applications to the interpolation problem which is introduced and discussed in [9,10].

Appendix

NUMERICAL APPROXIMATION OF $\zeta(3)$

It has been shown that by expanding the momentum variables to fourth order in s, the cosine terms which appear in the energy can be consistently expanded to fourth order in s. Since s is proportional to $\beta^{-1/2}$, this represents a contribution of β^{-2} in the expansion of the cosines, and when the factor β outside the cosine terms is included, this analysis leads to the β^{-1} contribution to the energy. It should be emphasized again that this analysis was carried out for arbitrary $N = 4\nu + 2$, and so the β^{-1} contribution can be calculated for very large ring sizes. The values of N considered have relevance to the constructability of a regular N-gon with a straightedge and compass.

Since the contribution can be evaluated numerically for very large N values using this analysis, this leads to the possibility of estimating the Riemann zeta function $\zeta(3)$. This is done by comparing and equating coefficients of powers of β between the energy per particle of the finite system, and the energy per particle in the expansion for the infinite chain. If we represent the corresponding coefficient from the finite ring expansion of the energy per particle in powers of β^{-1} by $a_{N,-2}$, then equating coefficients gives the following simple equation:

$$\frac{25}{32\pi^3} 7\zeta(3) = |a_{N,-2}| .$$

Solving this equation for $\zeta(3)$ and scaling $a_{N,-2}$ to go from β back to s, one obtains

$$\zeta(3) = \frac{32\pi^3}{175} |a_{N,-2}| = \frac{8\pi^3}{7} |f_N^{(2)}| ,$$

where $f_N^{(2)}$ is the coefficient of s^4 in the expansion for the energy per particle. As N becomes large, the values of $f_N^{(2)}$ obtained by calculating $a_{N,-2}$ ought to yield an approximate value of $\zeta(3)$ which tends to the exact value of

$$\zeta(3) = 1.202056903159594285 .$$

By using this technique, the coefficient $f_N^{(2)}$ has been calculated for extremely large but finite particle numbers N. The calculation has been done for rings with $N = 6$ particles all the way out to $N = 8738$ particles, and these results are collected together in table 2.

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