



8-1992

A Study of the Transfer Matrix Method for the Classical Statistical Mechanics of One Dimensional Systems

Dietmar R.A. Johlen

Follow this and additional works at: https://scholarworks.wmich.edu/masters_theses



Part of the Condensed Matter Physics Commons

Recommended Citation

Johlen, Dietmar R.A., "A Study of the Transfer Matrix Method for the Classical Statistical Mechanics of One Dimensional Systems" (1992). *Master's Theses*. 873.

https://scholarworks.wmich.edu/masters_theses/873

This Masters Thesis-Open Access is brought to you for free and open access by the Graduate College at ScholarWorks at WMU. It has been accepted for inclusion in Master's Theses by an authorized administrator of ScholarWorks at WMU. For more information, please contact wmu-scholarworks@wmich.edu.



**A STUDY OF THE TRANSFER MATRIX METHOD FOR THE
CLASSICAL STATISTICAL MECHANICS OF
ONE DIMENSIONAL SYSTEMS**

by

Dietmar R. A. Johlen

**A Thesis
Submitted to the
Faculty of The Graduate College
in partial fulfillment of the
requirements for the
Degree of Master of Arts
Department of Physics**

**Western Michigan University
Kalamazoo, Michigan
August 1992**

**A STUDY OF THE TRANSFER MATRIX METHOD FOR THE
CLASSICAL STATISTICAL MECHANICS OF
ONE DIMENSIONAL SYSTEMS**

Dietmar R. A. Johlen, M.A.

Western Michigan University, 1992

Two formalisms using the transfer matrix technique, the first one by Gupta and Sutherland (1976) and the second one by Guyer and Miller (1979), are investigated and a proof is given for their equivalence.

Furthermore, it is pointed out that previous studies neglected the difficulties that arise from nonhermitian pseudo Hamiltonian. This work proves that the same results are obtained by taking into account the nonhermiticity of the pseudo Hamiltonian.

Thus, the transfer integral technique is extended to nonhermitian pseudo Hamiltonians.

ACKNOWLEDGEMENTS

I would like to express my appreciation of the patient guidance and instruction of my research adviser Dr. Sung Chung during this course of work. I also wish to thank Dr. Alvin Rosenthal and Dr. Michitoshi Soga for their constructive criticism.

Furthermore, thanks are due to the Department of Physics and the faculty members for the sustained interest and encouragement during my time as a student at Western Michigan University, Kalamazoo.

I also want to acknowledge the financial support provided by the Konrad-Adenauer-Stiftung that enabled me to participate in this exchange program.

Dietmar R. A. Johlen

INFORMATION TO USERS

This manuscript has been reproduced from the microfilm master. UMI films the text directly from the original or copy submitted. Thus, some thesis and dissertation copies are in typewriter face, while others may be from any type of computer printer.

The quality of this reproduction is dependent upon the quality of the copy submitted. Broken or indistinct print, colored or poor quality illustrations and photographs, print bleedthrough, substandard margins, and improper alignment can adversely affect reproduction.

In the unlikely event that the author did not send UMI a complete manuscript and there are missing pages, these will be noted. Also, if unauthorized copyright material had to be removed, a note will indicate the deletion.

Oversize materials (e.g., maps, drawings, charts) are reproduced by sectioning the original, beginning at the upper left-hand corner and continuing from left to right in equal sections with small overlaps. Each original is also photographed in one exposure and is included in reduced form at the back of the book.

Photographs included in the original manuscript have been reproduced xerographically in this copy. Higher quality 6" x 9" black and white photographic prints are available for any photographs or illustrations appearing in this copy for an additional charge. Contact UMI directly to order.

U·M·I

University Microfilms International
A Bell & Howell Information Company
300 North Zeeb Road, Ann Arbor, MI 48106-1346 USA
313/761-4700 800/521-0600

Order Number 1349103

**A study of the transfer matrix method for the classical
statistical mechanics of one dimensional systems**

Johlen, Dietmar Robert Aloysius, M.A.

Western Michigan University, 1992

U·M·I
300 N. Zeeb Rd.
Ann Arbor, MI 48106

TABLE OF CONTENTS

ACKNOWLEDGEMENTS	ii
CHAPTER	
I. INTRODUCTION	1
II. EQUIVALENCE OF THE GUPTA AND SUTHERLAND FORMALISM AND GUYER AND MILLER FORMALISM	4
Gupta and Sutherland Formalism	4
Guyer and Miller Formalism	10
Equivalence of the Two Formulations	12
III. NONHERMITIAN PSEUDO HAMILTONIAN	14
IV. CONCLUSION	20
BIBLIOGRAPHY	21

CHAPTER I

INTRODUCTION

This thesis is concerned with the investigation of one dimensional fields with symmetric and periodic self-interactions. The field equation has the form:

$$a \frac{\partial^2 \phi}{\partial x^2} - b \frac{\partial^2 \phi}{\partial t^2} - \frac{V'(\phi)}{2} . \quad (1)$$

This field equation is derived from the following Hamiltonian density:

$$H(x) = a \phi_x^2 + b (\phi_x + c)^2 + V(\phi) . \quad (2)$$

The most prominent member of this family of functions is the case where the potential is given by

$$V(\phi) = 1 - \cos(\phi) \quad (3)$$

and is called the sine-Gordon equation.

These equations model a variety of problems which are characterized by two different length scales. The first natural length is given by the background system itself and is, for example, the lattice spacing. The other natural length can describe a property of the system in question, for example, a charge density wave. There would be a competition between different forces trying to establish one of the natural lengths. In the

example of charge density waves described by (2) the second term prefers a wavevector c , whereas the interaction potential would in such a case describe a "lock-in" term with minimal energy for a charge density wave vector having a magnitude somehow proportional to the reciprocal lattice vector.

The crucial part in the investigation of equilibrium properties is the evaluation of the partition function. This thesis concerns a theoretical study of the partition function.

The standard technique for the evaluation of the partition function is the transfer integral operator formalism. Chapter II reviews two different approaches to this problem. The first approach was suggested by Gupta and Sutherland (1976) and uses an analytic continuation of the chemical potential into complex space in the evaluation of the grand partition function. The second approach goes back on Guyer and Miller (1979). They introduce an external force acting on the system.

In Chapter II both approaches are discussed and it is proven that these formulations result eventually in the same partition function. It means that these formulations are equivalent to each other.

Chapter III focuses on the transfer matrix equation that is often also referred to as the pseudo Schrödinger equation. In many cases, the pseudo Hamiltonian operator is nonhermitian. The consequence is that the eigenfunctions of the pseudo Schrödinger equation are not orthogonal. But

in the previous analyses, the non-orthogonality was simply ignored and eigenfunctions were treated as if they are orthogonal, thus casting serious question on the previous results. Using the Schmidt orthonormalization method, however, it can be shown that the same result as before holds for the partition function. Thus we have proved that the transfer integral technique is also applicable to systems with nonhermitian pseudo Hamiltonians.

Chapter IV gives a conclusion.

CHAPTER II

EQUIVALENCE OF THE GUPTA AND SUTHERLAND FORMALISM AND GUYER AND MILLER FORMALISM

Gupta and Sutherland Formalism

The Hamiltonian under consideration is of the form

$$H = \int_0^L dx \{ a \phi_x^2 + b (\phi_x + c)^2 + V(\phi) \} . \quad (4)$$

The discrete version of (4) is obtained by splitting the interval into M parts and replacing the integral by a sum. Therefore

$$H = \sum_{i=1}^M \Delta x \{ a \phi_i^2 + b \left(\frac{\phi_{i+1} - \phi_i}{\Delta x} + c \right)^2 + V(\phi_{i+1}) \} . \quad (5)$$

The boundary condition of particular interest is

$$\phi(L) - \phi(0) = c L = c \Delta x M . \quad (6)$$

To study statistical mechanical properties of the system it is necessary to calculate the partition function.

$$Q = \int \delta \phi_t \int \delta \phi_x e^{-\beta H} \quad (7)$$

The partition function can be split into a momentum factor and a spatial factor. Hence $Q = Q_\pi Q_\phi$. It is trivial to carry out the momentum integration.

$$Q_\pi = \int d\phi_1 \dots \int d\phi_M e^{-\beta \sum_{i=1}^M \Delta x a \phi_i^2} = \left(\frac{\pi}{\beta \Delta x a} \right)^{\frac{M}{2}} \quad (8)$$

The spatial integration is of the form

$$Q_\phi = \int d\phi_M \dots \int d\phi_1 e^{-\beta H_\phi} . \quad (9)$$

We define $K(\phi_i, \phi_{i+1})$ to be the integral kernel

$$K(\phi_i, \phi_{i+1}) = e^{-\beta \Delta x \left(b \left(\frac{\phi_{i+1} - \phi_i}{\Delta x} + c \right)^2 + V(\phi_{i+1}) \right)} . \quad (10)$$

The boundary condition (6) is implemented in the form of a δ -function.

Hence

$$Q_\phi = \int d\phi_{M+1} \dots \int d\phi_1 \delta(\phi_{M+1} - \phi_1 - cL) \prod_{i=1}^M K(\phi_i, \phi_{i+1}) . \quad (11)$$

The δ -function is expanded in a complete set of eigenfunctions Φ_n .

$$\delta(\phi_{M+1} - \phi_1 - cL) = \sum_n \Phi_n^*(\phi_{M+1} - cL) \Phi_n(\phi_1) \quad (12)$$

Thus (11) reads

$$Q_\phi = \sum_n \int d\phi_{M+1} \dots \int d\phi_1 \Phi_n^*(\phi_{M+1} - cL) \prod_{i=1}^M K(\phi_i, \phi_{i+1}) \Phi_n(\phi_1) . \quad (13)$$

A technique to evaluate this path integral is to introduce the transfer matrix equation

$$\int d\phi_i K(\phi_i, \phi_{i+1}) \Phi_n(\phi_i) \sqrt{\frac{\pi \Delta x}{\beta b}} e^{-\beta \Delta x \epsilon_n} \Phi_n(\phi_{i+1}) . \quad (14)$$

The transfer matrix equation (14) is applied M-times on (13).

This yields

$$Q_\phi^{-\left(\frac{\pi \Delta x}{\beta b}\right)^{\frac{M}{2}}} \sum_n e^{-\beta \Delta x M \epsilon_n} \int d\phi_{M+1} \Phi_n(\phi_{M+1} - cL) \Phi_n(\phi_{M+1}) . \quad (15)$$

Because the potential $V(\phi)$ is periodic the Bloch theorem applies, and we can write

$$\Phi_n(\phi) = e^{ik\phi} \psi_{\alpha,k}(\phi), \quad (16)$$

where $\psi_{\alpha,k}(\phi)$ has the periodicity of the potential. The index n is now replaced by a pair of indices: α denotes the band and k is in the first Brillouin zone.

$$k \in \left[-\frac{1}{2}, \frac{1}{2}\right] \quad (17)$$

Assuming the functions Φ_n to be normalized the spatial part of the partition function is given by

$$Q_\phi^{-\left(\frac{\pi \Delta x}{\beta b}\right)^{\frac{M}{2}}} \sum_\alpha \frac{1}{2\pi} \int_{-\frac{1}{2}}^{\frac{1}{2}} dk e^{-\beta L \epsilon_{\alpha,k}} e^{ikcL} . \quad (18)$$

The evaluation of the partition function using the transfer matrix equation formalism has shifted the mathematical problem from calculating the

integrals in (11) to solving the eigenvalue problem (14).

Writing out $K(\phi_i, \phi_{i+1})$ in the left side of (14) yields

$$\int d\phi_i e^{-\beta\Delta x \left(b \left(\frac{\phi_{i+1} - \phi_i}{\Delta x} + c \right)^2 + V(\phi_{i+1}) \right)} \Phi_n(\phi_i) \quad (19)$$

$$= e^{-\beta\Delta x \epsilon_n} \Phi_n(\phi_{i+1}) .$$

The function $\Phi_n(\phi_i)$ is now Taylor expanded around ϕ_{i+1} . The integration can now be performed to give

$$\sqrt{\frac{\pi \Delta x}{\beta b}} e^{-\beta\Delta x \left(-\frac{1}{4\beta^2 b} \frac{d^2}{d\phi_{i+1}^2} - \frac{c}{\beta} \frac{d}{d\phi_{i+1}} + V(\phi_{i+1}) \right)} \Phi_n(\phi_{i+1}) \quad (20)$$

$$= \sqrt{\frac{\pi \Delta x}{\beta b}} e^{-\beta\Delta x \epsilon_n} \Phi_n(\phi_{i+1}) .$$

Or

$$\left[-\frac{1}{4\beta^2 b} \frac{d^2}{d\phi^2} - \frac{c}{\beta} \frac{d}{d\phi} + V(\phi) \right] \Phi_n(\phi) = \epsilon_n \Phi_n(\phi) . \quad (21)$$

The transfer matrix equation in (21) is often referred to as a pseudo Schrödinger equation. Substituting (16) into (21) gives

$$\left[-\frac{1}{4\beta^2 b} \left(-k^2 + 2ik \frac{d}{d\phi} + \frac{d^2}{d\phi^2} \right) \right. \quad (22)$$

$$\left. - \frac{c}{\beta} \left(ik + \frac{d}{d\phi} \right) + V(\phi) \right] \Psi_{\alpha, k} = \epsilon_{\alpha, k} \Psi_{\alpha, k} .$$

This equation provides the eigenvalues $\epsilon_{\alpha, k}$ needed to evaluate the partition function Q .

$$Q = Q_\pi Q_\phi - \left(\frac{\pi}{\beta}\right)^M \left(\frac{1}{ab}\right)^{\frac{M}{2}} \sum_n \frac{1}{2\pi} \int_{-\frac{1}{2}}^{\frac{1}{2}} dk e^{-\beta L \epsilon_{\alpha,k}} e^{ikcL} \quad (23)$$

In the thermodynamic limit the major contribution is made by the first band $\alpha=0$, since $\exp(-\beta L \epsilon_{\alpha,0})$ is going to be much larger than $\exp(-\beta L \epsilon_{\alpha,k})$ ($\alpha \neq 0$) in the limit $L \rightarrow \infty$.

Still the k integration is difficult to perform. One cannot see easily which term is dominant. Simply considering the magnitude is not enough because it is determined by a phase cancellation.

However, Gupta and Sutherland suggested to calculate instead of the canonical partition function the grand partition function.

$$Z = \sum_{N=-\infty}^{\infty} e^{N\mu\beta} Q_N \quad (24)$$

In our case N is given by the number of 2π steps in the phase difference defined by the imposed boundary condition. These 2π steps can be interpreted as solitons or additional electrons in long Josephson junctions for example.

Note that N can be negative as well because the boundary conditions allow negative values of phase differences $\phi(L) - \phi(0)$. It depends on the system under consideration how negative particle numbers are interpreted. For kinks one denotes a positive N with kinks and negative N with antikinks.

Recalling (6)

$$\phi(L) - \phi(0) - cL - 2\pi \frac{cL}{2\pi} = 2\pi N . \quad (25)$$

Therefore

$$Z = \left(\frac{\pi}{\beta}\right)^M \left(\frac{1}{ab}\right)^{\frac{M}{2}} \frac{1}{2\pi} \int_{-\frac{1}{2}}^{\frac{1}{2}} dk e^{-\beta L \epsilon_0 k} \int_{-\infty}^{\infty} dN e^{-N(\beta\mu + 2\pi k)} . \quad (26)$$

Gupta and Sutherland pointed out that (26) can be easily evaluated if one continues the chemical potential μ into the complex region.

$$\beta\mu = -2\pi i\lambda \quad (27)$$

Obviously, the last factor in (26) with (27) is the δ -function $\delta(k-\lambda)$.

Hence, the k -integration in (26) can be done to give

$$Z = \left(\frac{\pi}{\beta}\right)^M \left(\frac{1}{ab}\right)^{\frac{M}{2}} \frac{1}{2\pi} e^{-\beta L \epsilon_0 \lambda} . \quad (28)$$

Where k is defined by

$$k = \frac{\beta\mu}{2\pi} i . \quad (29)$$

The chemical potential is related to the particle number N by

$$N = z \frac{\partial}{\partial z} \ln Z . \quad (30)$$

where z is the fugacity defined by $z = \exp(\beta\mu)$. Equation (30) yields μ for a given N .

Guyer and Miller Formalism

The Hamiltonian used by Guyer and Miller is slightly different from equation (5) in the Gupta and Sutherland formulation. They add an extra term.

$$\bar{H} = H - \mu' \sum_{i=1}^M \Delta x \left(\frac{\phi_{i+1} - \phi_i}{\Delta x} \right) \quad (31)$$

Formally μ' is a Lagrangian multiplier that leaves the value $\phi(L) - \phi(0)$ open during the calculations. The phase difference $\phi(L) - \phi(0)$ is proportional to the number of solitons in the system therefore μ' is similar to the chemical potential used by Gupta and Sutherland in the grand partition function. One now has to change the boundary conditions according to the new Hamiltonian.

Because $\phi(L) - \phi(0)$ is a dynamical variable controlled by the Lagrangian multiplier μ' , the old boundary condition $\delta(\phi_{M+1} - \phi_1 - cL)$ is in contradiction with the freely changing dynamical variable $\phi(L) - \phi(0)$. But it is necessary to fix the system at one end to avoid a divergence arising from the global translational invariance in the ϕ space. Therefore the system is fixed at ϕ_1 expressed by $\delta(\phi_1 - a)$.

The partition function can be evaluated in essentially the same way as in the Gupta and Sutherland case. The spatial part of the partition function is now

$$Q_\phi = \sum_n \int d\phi_{M+1} \dots \int d\phi_1 \Phi_n^*(a') \quad (32)$$

$$\cdot \prod_{i=1}^M e^{-\beta \Delta x \left(b \left(\frac{\phi_{i+1} - \phi_i}{\Delta x} + c \right)^2 + V(\phi_{i+1}) - \mu' \frac{\phi_{i+1} - \phi_i}{\Delta x} \right)} \Phi_n(\phi_1) .$$

The transfer matrix equation takes the same form as (14) but with a modified operator

$$K(\phi_i, \phi_{i+1}) = e^{-\beta \Delta x \left(b \left(\frac{\phi_{i+1} - \phi_i}{\Delta x} + c \right)^2 + V(\phi_{i+1}) - \mu' \frac{\phi_{i+1} - \phi_i}{\Delta x} \right)} . \quad (33)$$

Accordingly the transfer matrix equation (21) is changed to

$$\left[-\frac{1}{4\beta^2 b} \frac{d^2}{d\phi^2} + \left(\frac{\mu'}{2\beta b} - \frac{c}{\beta} \right) \frac{d}{d\phi} - \frac{\mu'^2}{4b} \right. \quad (34)$$

$$\left. + c\mu' + V(\phi) \right] \Phi_n(\phi) = \varepsilon'_n \Phi_n(\phi) .$$

Applying M times (14) and using (16) gives

$$Q_\phi = \left(\frac{\pi \Delta x}{\beta b} \right)^{\frac{M}{2}} \sum_\alpha \int_0^{2\pi} d\phi \frac{1}{2\pi} \int_{-\frac{1}{2}}^{\frac{1}{2}} dk \psi_{\alpha, k}^*(a') \quad (35)$$

$$\cdot e^{-ia'k} e^{-\beta L \varepsilon'_{\alpha, k}} \psi_{\alpha, k}(\phi) e^{ik\phi} .$$

Where the prime is added to the eigenvalue to distinguish it from the corresponding quantity in the Gupta and Sutherland formalism.

In the limit $L \rightarrow \infty$ only the lowest band $\alpha = 0$ is important. Moreover, since $\psi(\phi)$ is 2π periodic, the ϕ integration is different from zero only for $k=0$. Also set $a'=0$ for convenience.

We thus have

$$Q = \left(\frac{\pi}{\beta}\right)^M \left(\frac{1}{ab}\right)^{\frac{M}{2}} \frac{e^{-\beta L \epsilon'_{0,0}}}{2\pi} . \quad (36)$$

Of course μ' should satisfy the condition

$$\langle \phi_M - \phi_1 \rangle = 2\pi N = -\frac{\partial}{\partial(\beta\mu')} \epsilon'_{0,0}(\mu') . \quad (37)$$

This has the same form as the grand partition function of Gupta and Sutherland, i.e., equation (28). Therefore the Guyer and Miller and the Gupta and Sutherland formalisms are equivalent if $\epsilon_{0,k}$ in (22) is equal to $\epsilon'_{0,0}$ in (34).

Note that it does not matter that this work compares a canonical partition function and a grand partition function because if they are equal the statistical mechanical properties are equal too.

Equivalence of the two Formulations

We now compare the two quantities $\epsilon_{0,k}$ and $\epsilon'_{0,0}$. $\epsilon_{0,k}$ is the lowest eigenvalue of the pseudo Schrödinger eigenvalue equation (22) with

$$k = \frac{\beta\mu}{2\pi} i , \quad (38)$$

that is,

$$\left[-\frac{1}{4\beta^2 b} \frac{d^2}{d\phi^2} - \left(\frac{c}{\beta} - \frac{1}{2b\beta} \frac{\mu}{2\pi} \right) \frac{d}{d\phi} - \frac{1}{4b} \left(\frac{\mu}{2\pi} \right)^2 \right. \\ \left. - c \frac{\mu}{2\pi} + V(\phi) \right] \psi_{0,k} = \epsilon_{0,k} \psi_{0,k} . \quad (39)$$

The condition (30) for μ is rewritten as

$$2\pi N = -L \frac{\partial}{\partial \left(\frac{\mu}{2\pi} \right)} \epsilon_{0,k} . \quad (40)$$

On the other hand, $\epsilon'_{0,0}$ is the lowest eigenvalue of the pseudo Schrödinger equation (34) with the condition (37) for μ' .

One can easily see that (39) and (40) are identical to (34) and (37) with the identification

$$\mu' = \frac{\mu}{2\pi} , \quad (41)$$

thus proving the equivalence of the two formalisms.

CHAPTER III

NONHERMITIAN PSEUDO HAMILTONIAN

In the last chapter, the path integrals in the partition function were evaluated by the transfer matrix method. The problem is reduced to the eigenvalue problem

$$\left[-\frac{1}{4\beta^2 b} \frac{d^2}{d\phi^2} - \frac{c}{\beta} \frac{d}{d\phi} + V(\phi) \right] \Phi_n(\phi) = \epsilon_n \Phi_n(\phi). \quad (42)$$

The pseudo Hamiltonian

$$H = -\frac{1}{4\beta^2 b} \frac{d^2}{d\phi^2} - \frac{c}{\beta} \frac{d}{d\phi} + V(\phi) \quad (43)$$

is not hermitian because the adjoint operator is given by

$$H^\dagger = -\frac{1}{4\beta^2 b} \frac{d^2}{d\phi^2} + \frac{c}{\beta} \frac{d}{d\phi} + V(\phi) \neq H. \quad (44)$$

As a result, the eigenfunctions Φ_n are not orthogonal. This can be seen as follows.

First

$$\langle \Phi_m | H^\dagger - H | \Phi_n \rangle = (\epsilon_m^* - \epsilon_n) \langle \Phi_m | \Phi_n \rangle. \quad (45)$$

From (43) and (44) we have

$$H^\dagger - H = 2 \frac{c}{\beta} \frac{d}{d\phi} . \quad (46)$$

But the commutator is not zero

$$\left[H, \frac{d}{d\phi} \right] = - \frac{d}{d\phi} V(\phi) , \quad (47)$$

and therefore ϕ_n cannot be a simultaneous eigenfunction of H and $H^\dagger - H$. Thus equation (45) shows that the eigenfunctions are not orthogonal to each other.

The analysis in Chapter II implicitly assumed orthogonal eigenfunctions of the transfer matrix equation when the δ -function is expanded as equation (12).

Indeed the same implicit assumption was made in the previous transfer matrix analyses, and the previous results are under serious question. We now develop below a new procedure concerning the nonorthogonal wavefunctions, and show that the results of the previous transfer matrix analyses for the nonhermitian pseudo Hamiltonian still hold.

A set of eigenfunctions can always be orthogonalized by using the Schmidt orthogonalization method.

Assume a set of eigenfunctions is given by $\{|\phi_{0,k}\rangle, |\phi_{1,k}\rangle, \dots\}$. The first eigenfunction of the orthonormalized set is simply proportional to the first one of the old eigenfunctions.

$$c_0 |\Phi'_{0,k}\rangle = |\Phi_{0,k}\rangle, \quad c_0 = \langle \Phi_{0,k} | \Phi_{0,k} \rangle, \quad (48)$$

where c_0 denotes the normalization. The next step is to write $|\Phi'_{1,k}\rangle$ as a superposition of $|\Phi_{1,k}\rangle$ and $|\Phi'_{0,k}\rangle$ that satisfies $\langle \Phi'_{0,k} | \Phi'_{1,k} \rangle = 0$.

$$c_1 |\Phi'_{1,k}\rangle = |\Phi_{1,k}\rangle + f |\Phi'_{0,k}\rangle \quad (49)$$

Applying the orthogonality condition specifies

$$f = -\langle \Phi'_{0,k} | \Phi_{1,k} \rangle. \quad (50)$$

In general $|\Phi'_n\rangle$ can be expressed as

$$c_n |\Phi'_{n,k}\rangle = |\Phi_{n,k}\rangle + \sum_{j=0}^{n-1} f_{nj} |\Phi'_{j,k}\rangle \quad (51)$$

with

$$f_{nj} = -\langle \Phi'_{j,k} | \Phi_{n,k} \rangle, \quad (52)$$

$$c_n = \langle \Phi_{n,k} | \Phi_{n,k} \rangle + \sum_{j=0}^{n-1} f_{nj} \langle \Phi'_{j,k} | \Phi_{n,k} \rangle. \quad (53)$$

Now the δ -function is expanded in the orthonormal function set $\{|\Phi'_{0,k}\rangle, |\Phi'_{1,k}\rangle, \dots\}$.

$$\delta(\phi_{M-1} - \phi_1 - cL) = \sum_n \Phi_n^*(\phi_{M-1} - cL) \Phi'_n(\phi_1) \quad (54)$$

The task is now to show that this new expansion does not affect the result of the partition function derived in Chapter II.

The partition function is written as a sum.

$$Q_\phi = \sum_n Q_n \quad (55)$$

Where

$$\begin{aligned} Q_n = & \sum_k \int d\phi_1 \dots \int d\phi_{M+1} \Phi'_{n,k}^*(\phi_{M+1} - c L) \\ & \cdot \prod_{i=1}^M K(\phi_i, \phi_{i+1}) \Phi'_{n,k}(\phi_1) \\ = & \sum_k | \langle \Phi_{n,k} | \sum_{j=0}^{n-1} f_{nj} | \Phi'_{j,k} \rangle |^{-2} \int d\phi_1 \dots \int d\phi_{M+1} (\Phi_{n,k} \\ & - \sum_{j=0}^{n-1} \langle \Phi'_{j,k} | \Phi_{n,k} \rangle \Phi'_{j,k})^*(\phi_{M+1} - c L) \prod_{i=1}^M K(\phi_i, \phi_{i+1}) \\ & \cdot (\Phi_{n,k} - \sum_{j=0}^{n-1} \langle \Phi'_{j,k} | \Phi_{n,k} \rangle \Phi'_{j,k})(\phi_1) . \end{aligned} \quad (56)$$

This rather long equation is divided into three terms:

$$\begin{aligned} term_1 = & \int d\phi_1 \dots \int d\phi_{M+1} \Phi'_{n,k}^*(\phi_{M+1} - c L) \\ & \cdot \prod_{i=1}^M K(\phi_i, \phi_{i+1}) \Phi'_{n,k}(\phi_1) \end{aligned} \quad (57)$$

$$\begin{aligned}
\text{term}_2 = & - \int d\phi_1 \dots \int d\phi_{M+1} \Phi'_{n,k}{}^*(\phi_{M+1} - cL) \prod_{i=1}^M K(\phi_i, \phi_{i+1}) \\
& \sum_{j=0}^{n-1} \langle \Phi'_{j,k} | \Phi_{n,k} \rangle \Phi_{j,k}(\phi_1)
\end{aligned} \tag{58}$$

$$\begin{aligned}
\text{term}_3 = & - \int d\phi_1 \dots \int d\phi_{M+1} \sum_{j=0}^{n-1} \langle \Phi'_{j,k} | \Phi_{n,k} \rangle^* \Phi'_{j,k}{}^*(\phi_{M+1} - cL) \\
& \cdot \prod_{i=1}^M K(\phi_i, \phi_{i+1}) \Phi_{n,k}(\phi_1)
\end{aligned} \tag{59}$$

Term_1 and term_3 are immediately evaluated as before

$$\text{term}_1 = \left(\frac{\pi \Delta x}{\beta b} \right)^{\frac{M}{2}} e^{-\beta L \epsilon_{n,k}} e^{ikcL} \tag{60}$$

$$\begin{aligned}
\text{term}_3 = & - \sum_{j=0}^{n-1} \langle \Phi'_{j,k} | \Phi_{n,k} \rangle^* \int d\phi_{M+1} \Phi'_{j,k}{}^*(\phi_{M+1}) \\
& \cdot \Phi_{n,k}(\phi_{M+1}) e^{-\beta L \epsilon_{n,k}} e^{ikcL} \\
= & - \sum_{j=0}^{n-1} |\langle \Phi'_{j,k} | \Phi_{n,k} \rangle|^2 e^{-\beta L \epsilon_{n,k}} e^{ikcL} .
\end{aligned} \tag{61}$$

Now to perform the transfer integral in term_2, the new eigenfunctions $\Phi'_{j,k}$ are expressed in terms of the old eigenfunctions $\Phi_{h,k}$ as

$$\Phi'_{j,k}(\phi) = \sum_{h=0}^j g_h \Phi_{h,k}(\phi) . \quad (62)$$

Therefore

$$\begin{aligned} \text{term}_2 = & \sum_{j=0}^{n-1} \sum_{h=0}^j g_h \langle \Phi'_{j,k} | \Phi_{n,k} \rangle \int d\phi_{M+1} \Phi'_{n,k}{}^*(\phi_{M+1}) \\ & \cdot e^{-\beta L e_{n,k}} e^{ikcL} \Phi_{h,k}(\phi_{M+1}) . \end{aligned} \quad (63)$$

It is now clear that term₂ is zero, because $\Phi_{h,k}$ is a linear combination of $\Phi'_{m,k}$ with $m \leq h \leq j \leq n-1$ all of which are orthogonal to $\Phi'_{n,k}$. Summing up all three terms results in

$$\begin{aligned} Q_n = & \left(\frac{\pi \Delta x}{\beta b} \right)^{\frac{M}{2}} \sum_k \left| \langle \Phi_{n,k} | - \sum_{j=0}^{n-1} f_{nj} | \Phi'_{j,k} \rangle \right|^{-2} \\ & \cdot \left(1 - \sum_{j=0}^{n-1} |\langle \Phi'_{j,k} | \Phi_{n,k} \rangle|^2 \right) e^{-\beta L e_{n,k}} e^{ikcL} . \end{aligned} \quad (64)$$

This can be reduced further to

$$Q_n = \left(\frac{\pi \Delta x}{\beta b} \right)^{\frac{M}{2}} \sum_k e^{-\beta L e_{n,k}} e^{ikcL} , \quad (65)$$

which is identical with the previous result (15) in Chapter II where the δ -function was not expanded properly.

We have thus shown that the transfer matrix method works formally the same way for the nonhermitian pseudo Hamiltonians as for the hermitian pseudo Hamiltonians.

CHAPTER IV

CONCLUSION

Two formulations for evaluating the partition function using the transfer matrix technique, the first one by Gupta and Sutherland and the second one by Guyer and Miller, have been discussed in Chapter II of this thesis. The partition functions and the pseudo Schrödinger equations have been derived in both formulations and were compared. It was shown that these formulations are equivalent to each other. We have thus given a firm basis to the reasonable idea of continuation into the complex space of the chemical potential in the evaluation of the grand partition function.

Chapter III focuses on the pseudo Schrödinger equation with nonhermitian pseudo Hamiltonian. Nonhermitian means that the eigenfunctions are not orthogonal to each other and the previous analyses assuming the orthogonality are questionable. A new correct analysis based on the Schmidt orthonormalization method, however, has shown that the previous results are not changed. We have thus extended the transfer integral technique to nonhermitian pseudo Hamiltonian systems.

BIBLIOGRAPHY

- Gupta, N., & Sutherland, B. (1976). Investigation of a class of one-dimensional nonlinear fields. Physical Review B, 5, 1790.
- Guyer, R. A., & Miller, M. D. (1979). Commensurability in one dimension at $T=0$. Physical Review Letters, 11, 718.
- Krumhansl, M. J., & Schrieffer, J. A. (1975). Dynamics and statistical mechanics of a one-dimensional model Hamiltonian for structural phase transitions. Physical Review B, 11, 5317.
- McMillan, W. L. (1976). Theory of discommensurations and the commensurate-incommensurate charge-density-wave phase transition. Physical Review B, 4, 1496.
- Scalapino, D. J., Sears, M., & Ferrell R. A. (1972). Statistical mechanics of one-dimensional Ginzburg-Landau fields. Physical Review B, 9, 3409.
- Schneider, T., & Stoll, E. (1980). Long-time behavior and dynamic scaling properties of displacement fluctuations in the sine-Gordon chain. Physical Review B, 1, 395.
- Suits, B. H., Couturie, S., & Slichter, C.P. (1980). Confirmation of McMillan's concept of "Discommensurations". Physical Review Letters, 3, 194.
- Turkevich, L. A., & Doniach, S. (1982). Critical behavior of the one-dimensional commensurate-incommensurate transition. Annals of Physics, 139, 343.