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INVESTIGATIONS OF A ONE DIMENSIONAL SYSTEM OF "CHARGED" BOSONS UNDERGOING DELTA-FUNCTION INTERACTIONS

by

Terrence W. Craig

Submitted in partial fulfillment of the requirements

for the degree of Doctor of Philosophy

at

Dalhousie University

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Halifax, Nova Scotia

September, 1994

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ABSTRACT

A one-dimensional system consisting of equal numbers of two types of bosons undergoing interactions through delta function potentials is examined. All particles have the same mass but each boson carries a "charge" that distinguishes one boson type from the other. The interactions are such that like particles repel and unlike attract. The amount of attraction and/or repulsion is determined by two adjustable parameters so that the amount of repulsion is not necessarily equal to that of attraction.

Analysis of the behavior of the system is determined by using the Bogoliubov approximation method to reduce the original Hamiltonian to an approximate form that is solvable. Although the approximation method does restrict the parameter space that can be analyzed, it turns out this limitation fortuitously still allows the determination of some interesting thermodynamic properties of the system. Among these properties is the feature of having a system length which exhibits thermodynamic stab.lity provided the temperature is below some finite temperature. This stable length can be quite simply related to the number of particles in the system but this simple relationship is quite different for periodic boundary conditions as compared to Dirichlet boundary conditions.

V

LIST OF SYMBOLS

Below is given a list of symbols used. If the symbol can be defined easily with a few words than those words are given. Otherwise the equation number in which the symbol first appears is given. The meaning of the symbol is usually defined in the text immediately before or after the equation. Most of the symbols used in Chapter 1 are not included in this list since they are not used in other than the introductory material where work of other authors, and thus their symbols, is called upon frequently. The symbols are arranged in order of their first appearance.

Η	a Hamiltonian
c, g, e	(1)
N	number of particles in a particular system
p	momentum
Ξ	grand canonical partition function
a^{\dagger}, a	creation and annihilation operators for a type of particle
b [†] , b	creation and annihilation operators for a type of particle
ß	inverse of temperature (Units such that Boltzmann constant $= 1$)
Т	temperature
Ę	single particle kinetic energy
μ	chemical potential
ζ	Riemann zeta function

L	length
No	number of particles in the Bose-Einstein condensate
N _{ex}	number of particles not in Bose-Einstein condentate
Р	pressure
E	energy of a system of perticles
S	entropy
Eo	(41)
ρ	density of particles, N/L
γ	<i>;</i> / <i>ρ</i>
e((41) and (44)
e,e'	(62)
d_p	(63)
f_p	(63)
θ	(71)
φ	(72)
λ_p	(74)
<i>Ф</i> р	(75)
H _{grd}	(78)
EBKS	(82)
Lo	a particular length of a system, its stable length or minimum length
H _o	Hamiltonian when $g = 0$

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λ_n	(102)
H _{grd(o;}	ground state energy when $g = 0$
$G_c(x - y)$	single particle density function, type a particle, (107)
$G_b(x-y)$	single particle density function, type b particle
g _{aa} (x - y)	pair correlation function, two type a particles, (110)
866(x-y)	pair correlation function, two type b particles
$g_{ab}(x - y)$	pair correlation function, type a and type b particle, (112)
e _o ,e'	(113)
λ_{p}°	(113)
ω [°] _p	(113)
C_L	specific heat
<i>E</i> ₍₀₎	energy of $g = 0$ system
P ₍₀₎	pressure of $g = 0$ system
S ₍₀₎	entropy of $g = 0$ system
C _{L(0)}	specific heat of $g = 0$ system
$\langle N_{ex} \rangle_{(o)}$	number of particles not in condensate in $g = 0$ system
J(c hoeta,g/c)	(137)

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F Helmholtz potential

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ACKNOWLEDGMENTS

There are always a number of people who provide support and inspiration when one undertakes a project such as this but at this point the author wishes to single out a few of those who provided a very large and important share of that inspiration and support. First, there is my supervisor, Dr. David Kiang. Not only was he able to provide the aforementioned inspiration and support but he was also able to do it with a considerable amount of patience which was much appreciated on my part. The second person I wish to single out is Dr. Akira Niégawa who was able to provide so much insight into the mathematical approach to the project. Finally I wish to thank my wife for her ever so important support.

I. INTRODUCTION

The Primary Focus

The primary focus of what is to follow will be a one-dimensional assemblage of spinless bosons. All the particles present in the system have identical masses but there are two types of particles. The particles of a given type are *i*-lentical in all respects. Each boson carries what will be called a "charge" for lack of a better word and it is this "charge" that distinguishes one type of boson from the other. As with electrical charge the "charge" causes an interaction between likes that is different from the interaction between unlikes. In contrast with electrical charge that has an infinite range over which to interact, the "charge" on these bosons has a range of interaction that is at the other extreme of distance. Namely, if these bosons were considered as classical macroscopic particles, they would only interact with each other on contact. Unlike classical particles, these bosons may penetrate or pass through each other. An additional difference between this interaction and the Coulomb one is that the repulsion between like need not be of the same magnitude as the attraction between unlike.

Picture this system of bosons $rac{1}{2}$ a string of particles laid out along the only dimension available in its one-dimensional world. Calling this direction the x-axis, at some point in time each particle can be viewed as occupying some position x_i . In the most general approach to describing this system's properties there would be no reason to restrict the

range of x_i along the x-axis but it will be required by the approximation method to be used that the system be confined to some finite size. The Hamiltonian that will be used to fit the description of the system of bosons described above is

$$H(c,g,N) = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + 2\sum_{i < j=1}^{N} (g + ce_i e_j) \delta(x_i - x_j)$$
(1)

where $e_i = \begin{cases} +1 \text{ if } 1 \le i \le \frac{N}{2} \\ -1 \text{ if } \frac{N}{2} + 1 \le i \le N \end{cases}$

The units have been chosen so as to have $\hbar = 1$ and, where *m* is the mass of each boson, 2m = 1. The form of the delta function not only indicates the point like nature of the interactions but also that all interactions are between pairs only. The second summation symbol is a shortened form to convey that the sum is to include all possible pairs. Here the system is assumed to have equal numbers of the two types of bosons (1 to N/2 for one group and N/2 + 1 to N for the other). Thus the *e*, determine that the strength of the contact potential is g + c between like particles and g - c between unlike particles. In the new work that is to be presented here the values of the parameters *g* and *c* are restricted so that there is repulsion between like particles and attraction between unlikes, that is $0 \le g < c$.

A) Why only one-dimension

The first point about this system of bosons to be considered is its restriction to only onedimension. As the sensible world about oneself is apparently three-dimensional, then the advantage in analyzing a one-dimensional system should be addressed. The interest in onedimensional systems has been present for a long time. If one were to go back in time more than twenty-five or thirty years, then the rationale for studying such a system would have a different emphasis than now. However, the past twenty-five years have shown that there are systems that have fewer than three-dimensions. Various surfaces and layers have shown themselves to be two-dimensional in nature and the study of their properties has produced a large amount of interest. An effective one-dimensional system can be realized by restricting the width of a two-dimensional system to small values. An easily visualized example of this process would be the making of a one-dimensional gate in a semiconducting material by the appropriate deposition of various layers. It may also be that the physical properties of a two-dimensional system have a strongly directional nature which would make it effectively one-dimensional. For example, a conducting polymer might have a very low resistivity in one direction compared to another. As a final example, some materials such as Bechgaard salts have shown themselves to possess quasi onedimensional properties.

Another comment to be made concerning the merit of one-dimensional systems is the argument that one never can predict what useful consequences might follow. Consider the Ising model. It started out in 1925 as a one-dimensional model of a ferromagnet with seemingly only theoretical application but with the passage of time has certainly grown in a major way in its applications to research. The Hamiltonian in (1) may not be destined for the same level of interest and usefulness as the Ising model but, as has happened before,

one never knows at the beginning of research how many new areas will open up. In support of this idea it is interesting to point out that although one-dimensional systems with contact potentials 'nave been studied for many years, the interest in (1) has arisen recently from work in two-dimensional systems. Superficially these systems would seem to have no connection with a one-dimensional system of bosons. A more in depth look will now be taken to show how the connection can be made.

B) The Source of the Recent Interest in This Hamiltonian

The illustrative example of the recent interest in Hamiltonians derived from (1) finds its source in the study of disordered, or random, systems. To help in the explanation of how random system studies lead to one-dimensional systems of bosons, a digression will now be taken in order to give an overview of some of the results in this field. For the purposes of illustration the work of M. Kardar¹ will be used. Although the example chosen will use terms applied to the boundary between two domains in a two-dimensional random-bond Ising model, it could just as well be used on a model system for a polymer on a disordered substrate². Indeed the mathematical development of coherent wave propagation through randomly disordered media³ turns out to be very similar as well. Although the aforementioned models can be applied to other than two-dimensional systems, it is only the two-dimensional form that will be considered here. Also, as the intent of this digression is to show that there is a field of current interest where knowledge of the solutions of the Hamiltonian (1) would be useful, the full mathematical development will not be reproduced

here. Rather, the outline will hopefully illustrate by highlighting in a step to step fashion why and how the transition from such two-dimensional models to a one-dimension boson system can occur.

The basic approach used in these models is to follow a path through the system under study. The path may represent the boundary between domains in a magnetic material or along some polymer on a random substrate, for example. Since the system has randomness built into it, the direction of the path is influenced by the randomness within the material. For the domains and polymer models some form of impurity is added at random sites resulting in randomness in the strength of the bonds present. The path is not that of a random walk but rather a self-avoiding random walk. The self-avoiding random walk prevents self intersections in the path which is useful in the domain wall case, for example, if you want to limit consideration to the simpler interface between only two domains rather than three or more. Since the length of a true self-avoiding random walk is unpredictable, a weighted or preferred direction is assigned to the models to allow for paths of whatever length may be required. In the parlance of the field such paths are called "directed paths" or "directed polymers".

To be more specific, picture a two-dimensional square lattice as in Figure 1. Starting at point (0,0) the path goes one step in the preferred direction which in the figure is to the right. The step need not go to the point (1,0) but could also take a transverse step to one of this point's neighbors, that is either to (1,1) or (1,-1). Continuing this process would mean



that after n steps the end of the path is at one of 2n + 1 possible positions. (For the case of a polymer one could produce such a shape as the directed path by applying sufficient tension to the ends of the polymer to prevent self-crossings. The interactions of the random bonds between the substrate and the polymer would produce "sideways" deflections

that would have different statistical properties from the thermally produced ones of the pure material.) One of the things that is of interest in this field is how the amount of deflection, from the straight line direction, of the end of the path is dependent on the number of steps taken.

Kardar sets up his random-bond Ising model so that the spin sites are on a twodimensional lattice in the x-t plane with t being in the preferred direction mentioned above. The random-bond Ising model has a Hamiltonian of the form

$$H = -\sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \tag{2}$$

In the common Ising model the interaction energy or scrength of bonds between

neighboring spins is a constant J but here bonds can be chosen to have random values. The boundary or interface between two domains runs from (0,0) and roughly follows the *t*-axis seeking a path that tries to balance the demands of keeping the boundary length minimum and passing through sites of locally low energy. If no impurities were present and the temperature was zero the interface would go along the axis. The presence of impurities causes the interface to be distorted even at zero temperature because of the centers of relative attraction they create. For simplicity the bonds between nearest neighbor spin sites in the x-direction are assumed to be equal. Moreover these bonds are made strong enough to make the *t*-direction the preferred direction in the random path selection process. The random bonds of the model are in the *t*-direction and are assumed to be independent of each other. Although random, these bonds $\mu(x, t)$ are selected to have a gaussian distribution of mean $[\mu]$ and standard deviation of σ . Kardar uses the square brackets, [...] to indicate that an averaging over a sampling of random arrangements of impurities has been carried out.

Starting at (0,0), the beginning of the interface, Kardar generates the possible directed paths to (x, t) where t is predetermined and considered the independent variable. Each of the paths would represent a possible interface between domains and he assigns a probability or weight, W(x,t), to each path. The set of weights can then be used to generate a partition function. His method of determining W(x,t) is through the use of transfer matrices, $\Im(t')$, evaluated at each step along the path. He indicates that these transfer matrices become, in the continuous limit in the x direction,

$$\langle \mathbf{x}|\Im(t')|\mathbf{x}'\rangle \approx \exp\left(-\mu(\mathbf{x},t')+2\gamma+\gamma\frac{\partial^2}{\partial \mathbf{x}^2}\right)$$
 (3).

Here γ is determined by the bonds perpendicular to the interface and is a constant Boltzmann weighting factor. Then setting

$$W(x,t) = \langle 0|\Im(0)\Im(1)...\Im(t-1)|x\rangle$$
(4)

and going to the continuous limit in the t direction he arrives at

$$\frac{\partial W}{\partial t} = -\left(\mu(x,t) - 2\gamma - \gamma \frac{\partial^2}{\partial x^2}\right) W$$
(5).

If one views the t variable as an "imaginary time" then the operator in brackets determines the time evolution of W and thus could be considered a Hamiltonian. The equation could then be written with a time dependent Hamiltonian as in

$$\frac{\partial W}{\partial t} = -H(t)W \tag{6}$$

By examining the asymptotic behavior of the equation Kardar is able to determine that

$$W(x,t) \propto \exp\left\{-[f]t - g\left(\frac{x}{t^{\nu}}\right)\right\}$$
. The $[f]$ is the averaged interface free energy and ν , in

the function g(), determines how the deflection of the end of the path in the x-direction scales with the number of steps taken along the *t*-direction. After a large number of steps the average magnitude of the x position of the path end will be proportional to t^{v} . As will be pointed out in more detail below, there is disagreement among some authors as to the correct value of the scaling properties of some models, not this one of Kardar, when the $t \to \infty$ limit is applied. Some aspects of this scaling controversy will be considered later in the new work to be presented.

The difficulty with impurity averaged quantities like [f] being in the exponent is that it requires the determination of $[\ln W]$ rather than [W]. To overcome this problem Kardar utilizes what is known as the replica method. The replica method is based on the mathematical identity

$$\ln X = \lim_{n \to 0} \left(\frac{X^n - 1}{n} \right) \tag{7}.$$

Interpreting W^n as being the product of *n* versions, or replicas, of *W* then

$$\left[\ln W\right] = \lim_{n \to 0} \left(\frac{\left[W^n\right] - 1}{n}\right)$$
(8).

The replica method or, as some authors call it, replica trick is not novel or unique to the work of Kardar being discussed here. For example, it has also been used in spin glass studies⁴ and random lattice work⁵.

Referring to (3) one can see that if an interface (path) crosses the bond $\mu(x, t)$, a contribution of a factor of $\exp(-\mu)$ is made to W. Then in any collection of interfaces (paths), W^n , the same bond would be crossed by m interfaces (paths) with the restriction $0 \le m \le n$ and would contribute a factor of $\exp(-m\mu)$. On averaging over different selections of randomness Kardar gives the result as

$$\left[\exp(-m\mu)\right] = \exp\left\{-\left(\left[\mu\right] - \frac{1}{2}\sigma^{2}\right)m + \frac{1}{2}\sigma^{2}m(m-1)\right\}$$
(9).

The important feature of this result is the interpretation Kardar gives it. The *m* interfaces that cross a bond, if considered two at a time, could be viewed as making up $\frac{1}{2}m(m-1)$ different pairs. Since this same factor appears in the last term in the exponent $\ln (9)$, he ascribes this occurrence to the idea that there must be a connection between pairs of interfaces. In the context of (9) each member of one of these pairs is interacting with the other member via an attraction of strength σ^2 . In addition, as only the factor *m* is involved and not *n*, these interfaces only interact on contact with each other. So, in this case, application of the replica method replaces a single interface (path) problem with *n*-interfaces (paths) that are regarded as interacting with each other in a pair-wise fashion but only at the points of contact.

Where in the single interface model the transfer matrices of (4) could be used, here in the n-interface replica model the transfer matrices must be of an n-body type. The time dependent Hamiltonian found in (5) is now replaced by

$$H = \left(\left[\mu \right] - \frac{1}{2} \sigma^2 - 2\gamma \right) + \gamma \left\{ -\sum_{\alpha=1}^n \frac{\partial^2}{\partial x_{\alpha}^2} - \frac{\sigma^2}{\gamma} \sum_{\alpha < \beta} \delta \left(x_{\alpha} - x_{\beta} \right) \right\}$$
(10).

Thus by invoking the replica method Kardar is able to go from the two-dimensional operator (or the "time" dependent Hamiltonian) found in (5) to the one-dimensional (or "time" independent) (10). However, in a "conservation of difficulty" fashion, the one-dimensional Hamiltonian is an *n*-body one. As it turns out, this particular Hamiltonian has a known exact solution (whose form will be given later). Having an exact solution makes

easy the limiting process $n \rightarrow 0$ required by the replica method.

For our purposes here the analysis of this work of Kardar has now gone far enough. The whole rationale for the analysis is summarized by that part of (10) enclosed in the curty braces. A comparison of this part with (1) will show that it is of the same type of Hamiltonian but with c = 0 and $g = -\frac{\sigma^2}{2\gamma}$. As all the factors outside the curty braces are constants, knowing the eigenvalues of the Hamiltonian represented within the braces makes it straightforward to find the eigenvalues of (10).

In order to introduce another Hamiltonian of the form of (1), a variation or extension of Kardar's model discussed above will be used. As already mentioned the model used by Kardar belongs to a class referred to as directed paths, or directed polymers, in random media. Following a weighted but random path through the system results in the acquisition of random amplitudes at sites along the path. For the next model to be considered each step along the directed path results in the gaining of random phases rather than amplitudes. Some authors refer to this model as a complex directed path, or a complex directed polymer, in a random median where the "complex" arises from the need for complex numbers when dealing with phases. This model has proved useful in work on ma_netoconductance and conduction in insulators or semiconductors when the phenomenon of electron hopping is involved. As the name of the model suggests, it can be applied in low dimensional situations with random impurity distributions. Under these conditions the electron that will take part in conduction can be well localized at an impurity

location but at even small finite temperatures may tunnel or hop to another location. It can be shown⁶ that at low temperatures the temperature dependence of the conductivity is proportional to

$$\sigma \propto \exp\left(\left(-\frac{T_o}{T}\right)^{\frac{1}{d+1}}\right)$$
(11)

where T_o is a constant and d is the dimension of the system. Materials that have a conductivity of the form of (11) exhibit Mott variable range hopping conduction. The electron is not confined to hop to an adjacent impurity site. The average hopping distance may exceed the average distance between impurities. It is then assumed that the conduction could take place along a directed path.

With the above as background we will now turn to an overview of the work of Blum, Shapir and Koltun⁷ and Blum and Goldschmidt⁸. There is a close parallel between their work and the work of Kardar already described. One of their assumptions is that the electrons are so highly localized that only directed paths need be considered in the hopping conduction process. This feature combined with their use of Feynman path integrals rather than transfer matrices leads to the phrase "directed Feynman paths" as a description of their approach. Again using *t* as the distance along the directed axis and *x* as the distance perpendicular to the directed axis, a wavefunction or transmission amplitude for the electron along the path connecting (0,0) to (x,t) is given as

$$\Psi(x,t) = \int_{(0,0)}^{(x,t)} \mathcal{D}x \exp\left\{-\int_0^t \left(\frac{1}{4}\left(\frac{dx}{dt}\right)^2 + i\Theta(x(t),t)\right)\right\}$$
(12).

Here $\Theta(x(t), t)$ is the random variable giving the random phase acquired at each site. As in (5) the "time" development can be viewed as being determined by a "time" dependent Hamiltonian as in

$$\frac{\partial \Psi}{\partial t} = \left(i\Theta(x(t), t) + \frac{\partial^2}{\partial x^2} \right) \Psi$$
(13).

Although the conductance is proportional to $\Psi^*\Psi$, because they have to average over different realizations of the disorder in the system, it turns out they must average over $log(\Psi^*\Psi)$. To accomplish this averaging they turn as Kardar did to the replica method. In this case the *n* "replicas" cause Ψ to contribute *n* interacting paths and Ψ^* to contribute a further *n* paths. Each group of *n* paths has a repulsion between pairs as the interaction whereas there is an attraction between any pairing involving the two groups. Here again there appears a one-dimensional Hamiltonian as in (10) but, if the randomness is uncorrelated, with the form

$$H = -\sum_{i=1}^{2n} \frac{\partial^2}{\partial x^2} + 2c \sum_{i < j}^{2n} e_i e_j \delta(x_i - x_j)$$
(14).

If the Hamiltonian in (1) has g = 0 and N = 2n then it is the same as (14). Unfortunately this form does not have a known exact solution which makes the limiting process $n \rightarrow 0$ of the replica method problematic. As it turns out though, determining the large *n* behavior of the ground state energy of (14) offers a way around the difficulty.

As indicated by Blum and Goldschmidt⁸ when t is large the x positions of the ends of many paths, when averaged over realizations of the randomness, have a distribution such that $\overline{\langle x^2(t) \rangle} = At^{2\nu}$. However, the value of v in the exponent was cause for some disagreement. On carrying out numerical simulations on finite two-dimensional lattices, Medina, Kardar, Shapir and Wang⁹ obtained $v = 0.68 \pm 0.05$ and proposed that for large t the value should be v = 2/3. Zhang¹⁰ also did numerical simulations but arrived at $v = 0.74 \pm 0.01$ with a conjectured large t value of 3/4. Backing up for the moment to the directed polymer described already, if one assumes that continuum elastic theory can be used to calculate the polymer free energy, it can be shown that the free energy difference between two polymers scales as $\frac{d^2}{t}$. Here d is the distance between the ends of the two polymers after t steps. In addition d scales as t^{ν} and the free energy difference scales as t^{∞} . Tying these relationships together gives

$$2\nu - 1 = \omega \tag{15}.$$

This connection between exponents can be shown to hold in the exactly solvable directed polymer case. It is assumed to hold in the complex directed polymer case. Also, the ground state energy of the Hamiltonian (14) is postulated to be of the form⁸

$$E_o(n) = -\mathcal{E}_i n^\beta - \mathcal{E}_2 n \tag{16}$$

where *n* is the number of paths in the context of the replica method or, in terms of particles, the number of particles in a system of interacting bosons. The basis for assuming the ground state energy to have this form arises from the known exact solution of (1) when c = 0 and g < 0

$$E_o(n) = -\frac{g^2}{12}(n^3 - n)$$
(17).

The rationale for considering the ground state energy into the picture is based on two things. First, Kardar used the idea that in the large *n* regime it is only the largest eigenvalue of the transfer matrix that is important. The largest eigenvalue is the groundstate energy. Second, there is a relationship $\omega = \frac{1}{\beta}$ when *n* is large. This equality which was derived by

Zhang¹¹ means that (15) can now be written as

$$2\nu - 1 = \frac{1}{\beta} \tag{18}.$$

This relationship implies that knowing the large *n* behavior of (16) would enable the determination of β and then ν could be determined from (18). It was with this approach in mind that led Blum, Koltun and Shapir¹² to consider the ground *r* ate energy scaling of *n* not only for the Hamiltonian of (14) but for the more general form (1).

As indicated above, the foundation for the complex directed polymer model is based on some assumptions carried over from the directed polymer work. However, the work on the directed polymer model is not without its criticisms. Bouchaud and Orland¹³, for example, bring up a number of points but the most directly important one for here is their criticism of the use of the ground state energy eigenvalue. They point out that this use of the ground state would only be valid if there was a gap in the energy spectrum of the Hamiltonian. They feel, since the center of mass energy of the system of particles can be made arbitrarily small, that there is no gap. However, as the stated point of this overview was not to get heavily involved in the merits (or demerits) of this work on random media, this aside will be closed now that it has been shown knowledge of a one-dimensional Hamiltonian of the form of (1) is of current interest.

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II. SOME PARTICULAR SOLUTIONS

Initial comments

Now that motivation for considering a one-dimensional system has been established it is the intent in this section to review some of the work that has been done on systems whose Hamiltonian is some variation of the form presented in the previous section. Various interactions have been used other than the pair potential $V(x_1 - x_j) = \delta(x_1 - x_j)$ already mentioned. For example, B. Sutherland has solved the Hamiltonian for an N-body system of identical bosons where $V(x_1 - x_j) = \frac{g}{(x_1 - x_j)^2}$ not only for the ground state¹⁴ but also

for its thermodynamics¹⁵. F. Calogero¹⁶ has found solutions for the more complex form $V(x_i - x_j) = \frac{g}{(x_i - x_j)^2} + c(x_i - x_j)^2$. However, unless the interaction has some direct

bearing on the delta function version it will not be considered here.

What will be considered is the consequence of varying the parameters g and c that determine the strength of the delta function interactions. The goal is to determine something about the system behavior when $c \neq 0$ so the development will focus primarily on those features of the rest of the g, c parameter space that support this thrust. If an exact solution for the Hamiltonian were known it would not be necessary to seek such support. At this point there is no exact solution known so an approximation technique will be used and it is support for this approximation that is being sought. With these points in mind the first case to be considered is the free Bose gas.

The g = c = 0 case

Setting g = c = 0 turns off the interactions between particles and one is left with an ideal Bose gas. The three-dimensional ideal Bose gas is dealt with in many texts on statistical mechanics and so its properties have been broadly treated. Here, in contrast, the ideal Bose gas is not only one-dimensional but also consists of two types of particles. In consequence this gas has some properties that differ from the more familiar three-dimensional one. A number of these differences will be brought out in some detain three so that they are at hand and can be referred to when needed. The approximation method that is to be presented later will be applied to systems with interactions but where the interactions will be considered as being relatively weak. If the interactions are weak then it seems reasonable to expect the behavior of such systems to bear some form of resemblance to the ideal Bose gas. As a check on the possible validity of the method it is also useful to turn off the interactions, that is to set g = c = 0, in the resulting equations to see if the equations then fit the ideal Bose gas.

In addition to the requirement of weak interactions, the approximation method also requires that there be a "large" number of the system particles in the p = 0 state. The primary focus of the development of the one-dimensional Bose gas that will follow here will then be mostly on the parameter space where there is a Bose condensate present. In the threedimensional case when the Bose condensate is present the chemical potential is so small that it is usually set to zero for the purposes of simplicity. Although an excellent approximation in large three-dimensional systems, the setting of the chemical potential to zero in finite one-dimensional systems should not be done without some circumspection as will be brought out in the following.

When the one-dimensional system has g = c = 0 the grand canonical partition function from statistical mechanics is

$$\Xi = \operatorname{Tr}\left(e^{-\beta\left(\hat{R}-\mu_{a}\hat{N}_{a}-\mu_{b}\hat{N}_{b}\right)}\right)$$
(19).

Here, and throughout what is to follow, the units have been adjusted so that the Boltzmann constant has a magnitude of 1 ($k_B = 1$). Also to be used is the symbol $\beta = 1/T$. Although there are no interactions between the particles, the system is still made up of two types of bosons - here referred to as type a and type b. The Hamiltonian is

$$\hat{H} = \sum_{r=0}^{\infty} \varepsilon_r a_r^{\dagger} a_r + \sum_{s=0}^{\infty} \varepsilon_s b_s^{\dagger} b_s$$
(20)

and the number operators are

$$\hat{N}_a = \sum_{r=0}^{\infty} a_r^{\dagger} a_r \text{ and } \hat{N}_b = \sum_{s=0}^{\infty} b_s^{\dagger} b_s$$
(21).

The a_r^{\dagger} , a_r , b_s^{\dagger} , and b_s are the creation and annihilation operators for the two types of bosons and ε_r (or ε_s) is the kinetic energy of the n_r (or n_s) particles in a given state that occupy the $r^{\text{th}}(s^{\text{th}})$ energy level. As the system particles are bosons, the occupation numbers n_r (n_s) can be any value from 0 to N_a (or N_b) subject to the constraint,

$$\sum n_r = N_a \quad \left(\sum n_s = N_b\right).$$

Using these forms of the operators (19) becomes

$$\Xi = \operatorname{Tr}\left(\exp\left(-\beta\sum_{r=0}^{\infty} (\varepsilon_{r} - \mu_{a})a_{r}^{\dagger}a_{r} - \beta\sum_{s=0}^{\infty} (\varepsilon_{s} - \mu_{b})b_{z}^{\dagger}b_{s}\right)\right)$$
$$= \sum_{N_{a}=0}^{\infty} \sum_{all \, n_{r}} e^{-\beta\sum_{r} (\varepsilon_{r} - \mu_{a})n_{r}} \sum_{N_{b}=0}^{\infty} \sum_{all \, n_{s}} e^{-\beta\sum_{s} (\varepsilon_{s} - \mu_{b})n_{s}}$$
(22).

From here the calculation of the grand partition function is much the same as found in many texts on statistical mechanics where the single component free Bose gas is analyzed. (See Huang¹⁷, page 186, for example.). The difference is the appearance of the extra factor due to the presence of two types of particles. To trace through the effect of the extra factor the calculation goes as follows:

$$\Xi = \sum_{all n_{r}}^{\infty} \left(e^{-\beta(s_{0}-\mu_{a})} \right)^{n_{0}} \left(e^{-\beta(s_{1}-\mu_{a})} \right)^{n_{1}} \dots \sum_{all n_{s}}^{\infty} \left(e^{-\beta(s_{0}-\mu_{b})} \right)^{n_{0}} \left(e^{-\beta(s_{1}-\mu_{b})} \right)^{n_{1}} \dots$$

$$= \sum_{n_{0}=0}^{\infty} \left(e^{-\beta(s_{0}-\mu_{a})} \right)^{n_{0}} \dots \sum_{n_{s}=0}^{\infty} \left(e^{-\beta(s_{r}-\mu_{a})} \right)^{n_{s}} \dots \sum_{n_{0}=0}^{\infty} \left(e^{-\beta(s_{0}-\mu_{b})} \right)^{n_{0}} \dots \sum_{n_{s}=0}^{\infty} \left(\gamma^{-\beta_{1}(s_{s}-\mu_{b})} \right)^{n_{s}} \dots$$

$$= \prod_{r=0}^{\infty} \left(\sum_{n=0}^{\infty} \left(e^{-\beta(s_{r}-\mu_{a})} \right)^{n} \right) \prod_{s=0}^{\infty} \left(\sum_{n=0}^{\infty} \left(e^{-\beta(s_{s}-\mu_{b})} \right)^{n} \right)^{n} \right)$$

$$= \prod_{r=0}^{\infty} \left(1 - e^{-\beta(s_{r}-\mu_{a})} \right)^{-1} \prod_{s=0}^{\infty} \left(1 - e^{-\beta(s_{s}-\mu_{b})} \right)^{-1}$$
(23).

Now that the grand partition function is available one can readily use it to generate the expression

$$N = N_{a} + N_{b} = \frac{1}{\beta} \left(\frac{\partial (\ln \Xi)}{\partial \mu_{a}} \right)_{L,\beta} + \frac{1}{\beta} \left(\frac{\partial (\ln \Xi)}{\partial \mu_{b}} \right)_{L,\beta}$$
$$= \sum_{r=0}^{\infty} \frac{1}{e^{\beta(\epsilon_{r} - \mu_{a})} - 1} + \sum_{s=0}^{\infty} \frac{1}{e^{\beta(\epsilon_{s} - \mu_{b})} - 1}$$
$$= \sum_{s=0}^{\infty} \frac{2}{e^{\beta(\epsilon_{s} - \mu)} - 1}$$
(24).

The last step is taken because there are equal numbers of the two types of particles present. This fact, in combination with their identical dynamic properties, means the two types of particles must have the same chemical potential. In appearance this form is identical to that for a two component three-dimensional free Bose gas with equal numbers of particles for both components. For example, as in the three-dimensional case, μ cannot be greater than zero so as to avoid the non-physical negative occupation numbers for single particle kinetic energy states. In addition the magnitude of μ must decrease as the temperature decreases in order for N to be constant. In the three-dimensional system it is well known that there can be a large scale or macroscopic occupation number in the p = 0 state. However, when considering the feature of this so called Bose-Einstein condensation, there is an important difference between the one-and three-dimensional systems and what this difference is will now be developed.

Using periodic boundary conditions and a one-dimensional "box" of length L, then, in terms of momentum $p_s = \frac{2\pi s}{L}$,

 $\varepsilon_s = p_s^2 + p_{-s}^2 \tag{25}.$

Now (24) can be written as

$$N = \sum_{s=-\infty}^{\infty} \frac{2}{e^{\beta(p_s^2 - \mu)} - 1} = \frac{2}{e^{-\beta\mu} - 1} + \sum_{s=1}^{\infty} \frac{4}{e^{\beta(p_s^2 - \mu)} - 1}$$
(26).

The first term on the right yields the occupation number in the p = 0 state. In order to have the Bose-Einstein condensation, this term must yield a substantial proportion of N when the temperature is sufficiently low. This requirement also means the magnitude of the chemical potential must be small enough so that the product $-\beta\mu$ is small. Then, using the

approximation $e^{-\beta\mu} \approx 1 + \beta |\mu|$, one can say

$$\frac{2}{e^{-\beta\mu}-1} \approx \frac{2}{\beta|\mu|} \to N \quad \text{as} \quad T \to 0$$
(27)

or, for small T,

$$|\mu| \approx \frac{2T}{N}$$
(28).

Now going back to (26) and writing the summation in the continuous form by making the

substitution
$$\sum \rightarrow \frac{L}{2\pi} \int_{0}^{\omega} dp$$
 we have

$$N = \frac{2}{e^{-\beta\mu} - 1} + \frac{L}{2\pi} \int_{0}^{\omega} \frac{4dp}{e^{\beta(p^2 - \mu)} - 1}$$
(29).

The first term in (29) gives the number of particles in the p = 0 state and the second term the number of particles in excited states. This form is analogous to the three-dimensional form. In the three-dimensional case it is usually pointed out that replacing the summation with an integration can be justified if one goes to the thermodynamic limit. (See Scharf¹⁸ for a discussion of this point for the three-dimensional case.) Evaluating the integral in (29) in the *N/L* form necessary for going to the thermodynamic limit gives

$$\frac{1}{2\pi} \int_{0}^{\infty} \frac{4dp}{e^{\beta(p^{2}-\mu)}-1} = \frac{2}{\pi} \int_{0}^{\infty} \frac{e^{-\beta(p^{2}-\mu)}dp}{1-e^{-\beta(p^{2}-\mu)}}$$
$$= \frac{2}{\pi} \int_{0}^{\infty} e^{-\beta(p^{2}-\mu)} \sum_{m=0}^{\infty} e^{-\beta m (p^{2}-\mu)} dp$$
$$= \frac{2}{\pi} \sum_{m=0}^{\infty} e^{\beta \mu (m+1)} \int_{0}^{\infty} e^{-\beta (m+1)(p^{2}-\mu)} dp$$
$$= \frac{1}{\sqrt{\pi\beta}} \sum_{m=0}^{\infty} \frac{e^{\beta \mu (m+1)}}{\sqrt{m+1}}$$
(30).

As stated above the primary area of interest here is in the region of parameter space where there is a significant occupation number in the p = 0 state. In the three-dimensional case the chemical potential is so small at temperatures below the Bose condensation temperature that the integral corresponding to the one above is computed by setting $\mu = 0$ for mathematical convenience. However, in the one-dimensional case with this value of μ the integral in (30) evaluates to $\frac{1}{\sqrt{\pi\beta}} \varsigma(\frac{1}{2})$ and, as the Riemann zeta function ζ diverges, the integral diverges for all temperatures except T = 0. For (30) to converge the magnitude of μ must be larger than zero even in the process of going to the thermodynamic limit. The result of (28) suggests that in the thermodynamic limit, that is

$$N \rightarrow \infty$$
, $L \rightarrow \infty$, $\frac{N}{L} = \text{constant}$, the limit value of the chemical potential is $\mu = 0$. This

limit value of μ is not achievable in the allowed values of the chemical potential. This limitation does not preclude dealing with very large systems as the condition for convergence of the summation in (30) is only that $\mu < 0$. (This convergence condition can be determined by the application of the ratio test to the infinite series in (30)). Thus, as (28) indicates, this restriction does not put any practical limitation on the size of N but it certainly does provide a mathematical inconvenience.

To better see why one can set $\mu = 0$ in the three-dimensional system and not in the onedimensional system, one can go back to (29) and reexamine the process of going to the continuous limit. In a somewhat more rigorous form the equation could be written for the thermodynamic limit as

$$\frac{N}{L} = \lim_{L \to \infty} \frac{2}{L(e^{-\beta\mu} - 1)} + \frac{2}{\pi} \lim_{L \to \infty} \int_{\frac{2\pi}{L}}^{\infty} \frac{dp}{e^{\beta(p^2 - \mu)} - 1}$$
(31).

It is the lower limit of the integral in (31) that is the source of the "problem". To take a simpler form for the purposes of illustration, consider the three-dimensional integral $\lim_{R\to 0} \int_{R}^{1} \frac{dV}{r}$. It is finite but its one-dimensional analog $\lim_{a\to 0} \int_{a}^{1} \frac{dx}{x}$ is not. The one-dimensional system of bosons does not have the same phase space available to it as does the three-dimensional case.

Nothing in the one-dimensional development to this point suggests the presence of a Bose-Einstein condensation temperature so the next thing to be examined is the presence of a condensate in the thermodynamic limit. Again the requirement for what is to follow is that the p = 0 state must be occupied by a substantial fraction of the total particles in the system. Going to the thermodynamic limit is also very useful not only for enhancing the reliability of the thermodynamic results (Fluctuations are usually proportional to $1/\sqrt{N}$,

for example.) but it is only in this limit that a true phase transition will show up. (The reason for requiring the thermodynamic limit in order to see a phase transition was first put forward by Yang and Lee¹⁹.) For large N and L, with N/L constant one has, using (28), (29) and (30)

$$\frac{N_{o}}{N_{ex}} = \frac{\frac{2}{e^{-\beta\mu} - 1}}{\frac{L}{\sqrt{\pi\beta}} \sum \frac{e^{\beta\mu(m+1)}}{\sqrt{m+1}}} \rightarrow \frac{2\sqrt{\pi\beta}}{L(-\beta\mu)\sum \frac{e^{\beta\mu(m+1)}}{\sqrt{m+1}}} \approx \left(\frac{N}{L}\right) \left(\frac{\sqrt{\pi\beta}}{\sum \frac{e^{\beta\mu(m+1)}}{\sqrt{m+1}}}\right)$$
(32).

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As N is made larger the summation in the denominator becomes larger due to the corresponding decrease in the chemical potential. So the result in (32) can be made small showing that there is no Bose condensation in the thermodynamic limit. Obviously an approximation method that depends on the presence of a Bose condensate cannot be applied to "infinite" one-dimensional systems.

The next step of the development is then to show that there can be a Bose-Einstein condensate present in a finite one-dimensional system of free bosons. To do this we will go back to (26) and look at a numerical approach. Let us look at the summation in (26) and ignore the first term for the moment. This summation gives the number of particles that are not in the p = 0 state. Choosing the specific system values of $N = 10^{6}$, L = 10, and T = 100, the object is to now calculate numerically the value of this summation. The

difficulty in evaluating the summation lies in not knowing the value of the chemical potential. An easy way around this problem is to assume the chemical potential is zero. (Setting μ to zero may seem counter to the argument given above that μ could not be zero but it is the term that has been neglected that causes the problem of non convergence. The infinite series now under consideration does converge when μ is zero.) The actual value of μ is not zero and assuming it is will have the result of making the summation give a larger result than the correct one. When this summation is carried out the answer is 1.6x10³. Even though this number is not correct, it does tell us that more than 99.8% of the particles are in the p = 0 state for the values of the system parameters chosen. Evidently then there is some parameter space available in which the number of particles in the p = 0 state is a significant portion of the total number of particles. The approximation method referred to above will be used not in analyzing the free Bose gas but rather a gas in which there are interactions between particles. Knowing that the p = 0 state can have macroscopic occupation in the free case lends some credence to the assumption that this state can still have such significant occupation levels in an interacting gas providing the interactions are weak.

Showing that the p = 0 state has significantly large occupation number at a single poin. in parameter space does not make a strong case for the presence of a "condensate" in general so now a more extensive analysis will be made. Again going back to (26) but this time solving for N_0 , the number of particles in the p = 0 state, by using numerical methods one can determine that a condensate exists for various sets of parameters. The computer code
used to do this calculation can be found in the appendix.

The results of analyzing a system of L = 100 and $N = 10^6$ using numerical methods is given graphically in Figure 2. The correct value of μ has been determined in the numerical



process and used in generating the graph. The graph shows how the relative occupation level of the p = 0 state is related to the temperature. Unlike the three-dimensional case, there is no Bose-Einstein condensation temperature to mark a relatively sudden transition to large scale occupation of the p = 0 state. In the one-dimensional case the occupation number decreases smoothly with temperature. This effect is again the result of the greater density of energy states in three-dimensions compared to the situation in one-dimension. Mills²⁰ has shown that this same form of occupancy in the p = 0 state can be present in a three-dimensional system. He found that if the "box" containing the system had two of its dimensions reduced, keeping the third fixed, that a point would be reached where the ground-state occupancy would behave like the one-dimensional system described above. In addition to its dependence on temperature, N_0 is also dependent on the value of L chosen for the system as in shown in Figure 3. Two additional lengths of 70 and 85 have been added to the one of 100 already shown. The implication is clearly that system length and temperature are inversely related to the occupation number N_0 . These dependencies put limitations on the



approximation method but in principle all that has to be done is to check that N_0 is suitable large for the parameter space being examined. However, determining N_0 even approximately in the one dimensional system presents a difficulty not encountered in the three-dimensional case.

In three-dimensions at temperatures below the Bose-Einstein condensation temperature, the chemical potential for a free Bose gas is so small that it is usually assumed to be zero. This assumption for the large systems that are usually being considered is quite legitimate and simplifies calculations. In the one-dimensional free Bose gas of finite size one cannot assume that $\mu = 0$ without circumspection. In the three-dimensional large system version of (29) if the requirement is to determine the value of N_0 at temperatures below the condensation temperature then one uses the idea that the number of particles not in the ground state is adequately determined by the integral. One then ignores the first term on the right and evaluates the integral after setting $\mu = 0$ to get the number of excited particles E_x . Then the required result is easily arrived at be using $N_0 = N - E_x$. As already pointed out, this process does not work for the one-dimensional case as the integral in question diverges under these conditions.

As an illustration of the type of difficulty that can be encountered a few specific numerically derived examples will now be given. Instead of using integration to find the number of excited particles, the summation is carried out directly as the systems to be dealt with are to be finite. When setting $\mu = 0$, as pointed out above, it is the number of excited particles that must be determined as the term involving N_o diverges. Then N_o is found from $N_o = N - E_x$.

Figure 4 shows the results for the summation when carried out on a system of L = 100both with $\mu = 0$ and the system μ as determined numerically. Note that N_o can become negative which is a feature of the fact that each term in the E_x summation is larger than the correct value when setting $\mu = 0$. As can be seen in the graph this error is not very large for some L but as μ increases with L there is a point reached where the error can no longer be ignored. A three-dimensional system does not suffer from this problem because there is a finite "condensation temperature" which means the graph of N_o/N vs T does not approach





the temperature axis asymptotically with increasing T.

Figure 5 shows the results for a system with the same number of particles but whose length has been reduced to 50. Figure 6 shows the effect of changing the number of particles in the system. These Figures illustrate that the $\mu = 0$ calculation produces an accurate result as long as the ground state occupation level is 75% or more of the total system particles. Even at this point the error in the estimate is less than 2%.

The point that is to be brought forward here is, as already mentioned, the approximation method to be used later in analyzing an interacting Bose gas relies for its



validity on the presence of a large number of particles in the p = 0state. For the calculations that are done a check is made to ascertain that indeed the number of particles in the condensate is large.

However, the check on condensate occupation is carried out under the assumption that setting $\mu = 0$ is a reasonable approximation. One can

reasonably expect a large N_0 to be present if the interactions are weak and the calculations are carried out in the parameter space where the free Bose gas has a large N_0 .

A more flexible way to view the reliability can be taken from the looking at the Figures presented above from a somewhat different perspective. As pointed out above in the free Bose system, any calculation with $\mu = 0$ that yields an N_o that is larger than 75% of the total particles present is a quite accurate measure of the number of particles in the condensate. In the interacting system, since the interactions are assumed to be weak, it will be assumed that this same "rule of thumb" can be applied, namely, if the estimate produces an N_o of 90% or more than it is reasonably accurate reflection of the actual number. The 90% level is arbitrary but is chosen to be well on the conservative side. Other system properties that will receive attention when the interactions are present are the energy, pressure, and entropy. Each of these can be calculated from the partition function and for ease of reference the logarithm of the partition function in terms of momentum is given here from (23) and (25) as

$$\ln \Xi = -2 \left\{ \ln \left(1 - e^{\beta \mu} \right) + 2 \sum_{s=1}^{\infty} \ln \left(1 - e^{-\beta \left(p_s^2 - \mu \right)} \right) \right\}$$
(33).

The expression for pressure can now be written as

$$P = \frac{1}{\beta} \left(\frac{\partial (\ln \Xi)}{\partial L} \right)_{\beta,\mu} = \frac{8}{L} \sum_{s=1}^{\infty} \frac{p_s^2}{e^{\beta (p_s^2 - \mu)} - 1}$$
(34).

If this result is written in the continuous limit form

$$P = \frac{4}{\pi} \int_0^\infty \frac{p^2 dp}{e^{\beta(p^2 - \mu)} - 1} = \frac{1}{\sqrt{\pi}} \sum_{n=0}^\infty \frac{e^{\beta\mu(n+1)}}{\left(\beta(n+1)\right)^{\frac{3}{2}}}$$
(35)

it can be seen that convergence occurs for all $\mu \le 0$. In the thermodynamic limit when μ is effectively zero and zero can be inserted in (35) which then becomes

$$P = \frac{\zeta(\frac{3}{2})T^{\frac{3}{2}}}{\sqrt{\pi}}$$
(36).

This form could be viewed as the one-dimensional analogue of the three-dimensional equation of state for an ideal Bose gas below the Bose-Einstein condensation temperature. (See Huang¹⁷, page 290 for the three-dimensional form and background.) Under these conditions pressure is a function of temperature only but in the three-dimensional system this type of temperature dependence occurs below the finite Bose-Einstein condensation

temperature. Here, unlike the three-dimensional case, however, there is no finite condensation temperature and (36) would remain a valid approximation as long as the temperature is kept low enough to keep the chemical potential small.

Figure 7 illustrates the isothermal behavior for a system of $N = 10^6$ at a temperature of 10. As the length of the system is increased the pressure asymptotically approaches the value given by (36). However, in spite of what the graph indicates, the system is not behaving in the fashion indicated. The



minimum shown in the graph occurs at L = 1. According to (26) the number of particles in the first excited state, which would be the most populous of the excited states, is only about 0.08. Clearly what is happening is continuous equations are being applied to a situation where the discreteness of the system is not well approximated by continuous equations. Effectively only one or two particles are not in the p = 0 state. As the length of the system increases, more particles enter excited states making the use of statistical methods employing continuous values of density more reasonable. Under conditions of fairly numerous excited particles, the steep positive slope of the isotherm is not present. The slight positive slope present for larger values of L is still a remnant of the finiteness of the system. Lieb²¹ states that one can expect this sort of result in a finite system and the more physically acceptable slopes will be present in infinite systems. The caution to be taken from this is not to attempt to treat systems with very small numbers of excited particles in this fashion.

The energy, as determined from the partition function, is

$$E = -\left(\frac{\partial(\ln\Xi)}{\partial\beta}\right)_{L,\beta\mu} = 4\sum_{s=1}^{\infty} \frac{p_s^2 - \mu}{e^{\beta(p_s^2 - \mu)} - 1}$$
(37).

In similar fashion, the entropy is

$$S = -\left(\frac{\partial(T \ln \Xi)}{\partial T}\right)_{L,\mu}$$

= $-2\ln(1 - e^{\beta\mu}) - \frac{2\beta\mu e^{\beta\mu}}{1 - e^{\beta\mu}} + 4\sum_{s=1}^{\infty} \left\{ \ln\left(\frac{e^{\beta(p_s^2 - \mu)}}{e^{\beta(p_s^2 - \mu)} - 1}\right) + \frac{\beta(p_s^2 - \mu)}{e^{\beta(p_s^2 - \mu)} - 1}\right\}$ (38).

Neither energy or pressure depend directly on the number of particles in the p = 0 state and, when the chemical potential is small, calculating either one by setting $\mu = 0$ produces almost the same result as when using the correct value of μ . Entropy, like the calculation of N done above, does have connections with the p = 0 state and setting $\mu = 0$ causes problems with the first term in (38). However, for finite systems with small μ the



contribution to the entropy from the first two terms of (38) is relatively small. So the simple expedient of dropping the first two terms and setting $\mu = 0$ in the summation terms will be employed. The entropy value produced by this method is not largely different from the correct value.

To more clearly show the

difference in entropy values graphically the Gibbs free energy versus L is plotted in Figure 8 for T = 100. Since the Gibbs function contains a factor TS the entropy difference is magnified by 100. As is obvious from the figure, the two graphs indicate a distinct difference but compare the shapes of the two. For both Helmholtz and Gibbs functions the shape of the curves is similar whether one computes using the correct μ or $\mu = 0$. This feature of shapes will prove useful later on when curves portraying the Helmholtz free energy in particular will be used in an examination of the stability of the system under consideration. For the stability considerations it is more the shape than the magnitudes that is important.

The g < 0, c = 0 case

If just two particles were present in the system then the solution of the Schrödinger equation is relatively straightforward. One converts to the center of mass coordinates and arrives at a single particle with delta function potential Schrödinger equation. This equation can then be solved by integration. Interestingly, for our purposes here, there turns out to be only one bound state. (A more complete treatment of the handling of the delta function potential in the bound state scenario is given by Atkinson and Crater²².)

For three particles in a bound state (in one dimension of course) the same general theme of attack can be used. Namely, one changes coordinates to convert the problem from a three body one to an effective one body in two dimensions. Such a coordinate transformation is given by Amado and Coelho²³ in their work on K harmonics, for example. In contrast with the two body case which can be solved for whatever the masses of the two bodies happen to be, the three body story is more difficult because, in the general case, not only can the masses differ but interactions between different pairs may differ. Kiang and Niégawa²⁴ building on the work of McGuire²⁵ establish conditions under which some exact solutions can be found. However, if the particles all have equal mass and the delta interactions are all equal, the symmetries introduced make the problem solvable not only for three particles but for N particles. It was the work of McGuire cited above that fully exploited these symmetries and in so doing came up with an exact solution to the N body problem.

Some of the results of McGuire's work that apply directly to an N body system of bosons

will now be considered for their consequences on what is to follow. There is only one bound state. The energy of this bound state is

$$E = -\frac{1}{12}g^2N(N^2 - 1)$$
(39).

As a result of this N dependence the system cannot be considered in the thermodynamic limit, that is, E/N does not have a finite size in this limit. As a consequence of there being only one bound state, McGuire points out that regardless of temperature the system has to collapse to this state and so it would not make sense to apply statistical mechanics to this system. McGuire also pointed out that no two particles in the bound state can have zero relative velocity. Therefore, the approximation scheme to be used later cannot 'oe applied to this system as it depends on there being a large number of particles in the p = 0 state.

The g > 0, c = 0 case

It was Lieb and Liniger²⁶ that first solved this problem. Since they give explicit equations for determining the ground state energy in their work it is this aspect that will be considered briefly here. Material for the thermodynamics of the system will be drawn from another source later. The Lieb and Liniger approach was to assume that since the particles in the system only interact on "contact" the phase space available to the system could be divided into segments according to the ordering of the particles. Within each segment the particles are "free" and this suggests using planes waves in the makeup of the wavefunction of the system. Employing what has become known as the Bethe ansatz they set their N particle wave function to be

$$\Psi(x_1,\cdots,x_N) = \sum_{P} a(P) P \exp\left(i \sum_{j=1}^{N} k_j x_j\right)$$
(40)

where the summation over permutations is over all possible permutations of the "momenta" k_j and the a(P) are coefficients dependent on the permutation P. Then they matched Ψ at the boundary between segments with the appropriate boundary conditions - continuity for Ψ and the jump in the derivative of Ψ that is dependent on the strength of the delta interaction. (It should be pointed out here that Lieb and Liniger were considering the system to consist of N identical particles and not equal numbers of two types.) By matching all the boundary conditions and meeting all the symmetry conditions on permutations of the identical particles they are able to come up with all the eigenfunctions of the system. The k_j turn out to be real with no two equal but the set $\{k_j\}$ contains both k_j and $-k_j$. The largest k_j then provides the bounds, -K and K, for the set. The spacing of the k_j is not equal but is partly dependent on the value of g, the strength of the delta interactions.

In determining the ground state energy they start from general dimensional considerations to show that this energy must have the functional form

$$E_o = N\rho^2 e(\gamma)$$
 with $\rho = N/L$ and $\gamma = g/\rho$ (41).

They then choose the values of the internal quantum numbers they have determined in such a way as to minimize the k_j . Going to the thermodynamic limit so that they can pass to continuous forms of their discrete equations they derive three coupled integral equations that enable the numerical determination of the ground state energy. These equations are as follows:

$$1+2\lambda\int_{-1}^{1}\frac{h(x)dx}{\lambda^{2}+(x-y)^{2}}=2\pi h(y)$$
(42),

$$\gamma \int_{-1}^{1} h(x) dx = \lambda \tag{43}$$

and

$$e(\gamma) = \frac{\gamma^{3}}{\lambda^{3}} \int_{-1}^{1} h(x) x^{2} dx$$
 (44)

where $g = K\lambda$. The solution scheme is to pick a value of λ and then use (42) to compute h(y) for a particular y. Using this scheme the integral in (43) can be evaluated to solve for γ . Next (44) can be solved for $e(\gamma)$. With this solution the ground state energy can be computed from (41) bearing in mind, being in the thermodynamic limit, it is E_0/N that would be sought.

Lieb and Liniger also show that the above process will produce a $h(y, \gamma)$ and an $e(\gamma)$ that are analytic functions of γ except at the point $\gamma = 0$. They are unable to determine the exact nature, or cause, of this singularity. It does seem rather strange that this point, e(0), should cause problems because this is then the free particle system and so it must be that e(0) = 0. Nevertheless the numerical solution for $e(\gamma)$ proceeds quite well until the value of γ begins to approach zero closely. A graph of $e(\gamma)$ versus γ will be presented later when it will be used as a comparison with the results of the approximation method that will be introduced.

C. N. Yang and C. P. Yang²⁷ were able to extend the work of Lieb and Liniger to determine the thermodynamics of the system of bosons. They show that the Bethe ansatz

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produces all the states of the Hamiltonian and the k_j for all states are real with no two k_j for a given state being the same. For the ground state, as already pointed out above, Lieb and Liniger had shown that the k_j form a nonuniform distribution between a maximum K and a minimum -K. Excited states are characterized by having k_j outside the K limits and "holes" left behind. The Yangs are able to develop an expression for the entropy of the system in terms of the density of holes, ρ_n , and the density of k_j , ρ . Using the constraints on energy and particle density

$$\frac{E}{N} = \frac{L}{N} \int_{-\infty}^{\infty} \rho(k) k^2 dk$$
(45)

and

$$\frac{N}{L} = \int_{-\infty}^{\infty} \rho(k) dk \tag{46}$$

respectively, they maximize the contribution of a given state to the partition function to arrive at the integral equation

$$\varepsilon(k) = -\mu + k^2 - \frac{Tg}{\pi} \int_{-\infty}^{\infty} \frac{\ln\left\{1 + \exp\left[-\varepsilon(q)/T\right]\right\} dq}{g^2 + (k-q)^2}$$
(47).

Here μ is the chemical potential and the ratio of the density of holes to the density of the k_j is embodied in

$$\frac{\rho_h}{\rho} = \exp\left[\frac{\varepsilon(k)}{T}\right]$$
(48).

Now, by manipulating (47) and combining the result with their expression for entropy they

arrive at an equation giving the Helmholtz free energy. Then using $P = -\left(\frac{\partial F}{\partial L}\right)_{T,N}$ they

are ultimately able to reach the expression for pressure

$$P = \frac{T}{2\pi} \int_{-\infty}^{\infty} dk \ln \left(1 + \exp \left[-\frac{\varepsilon(k)}{T} \right] \right)$$
(49)

The solution scheme to arrive at the thermodynamic properties of the boson system is to solve (47) with a given μ and T and then to use these results of get the pressure from (49). Knowing the pressure as a function of μ and T enables one to determine other thermodynamic quantities from

$$dP = \frac{S}{L}dT + \frac{N}{L}d\mu$$
 (50).

Unfortunately the Yang results can not be used here to support the results of the approximation method to be introduced. The difficulty in solving (47) numerically is the stumbling block. The limits of integration are ∞ and numerically one replaces this value with some "large enough" number in the hope that the region .hus left out of the integration is small. Here one can get the limit K (and -K) for the ground state from the work of Lieb and Liniger. Presumably one should set the limit somewhat higher for finite temperatures. However, even using K proves to be too high. Yang and Yang show that (47) can be solved by iteration. They "seed" their iteration proof with $\varepsilon(k) = -\mu + k^2$ but when this value, as suiting the system parameters that will be used, is placed in that part of (47) containing $\exp(-\varepsilon(k)/T)$ it does not take all that large a value of k to give a value

smaller than the 10^{-300} available in a standard computing environment. This problem could be overcome if μ was much larger but this would require a strongly interacting system of bosons and the approximation technique would not be applicable.

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III. The Approximate Solution of the Hamiltonian

The Bogoliubov approximation

The approximation method to be employed here was first introduced by N. Bogoliubov²⁸ when he presented work to show how superfluity could be explained on the basis of degeneracy in a non-perfect Bose gas. The fundamental requirement in applying this approximation scheme is that there be a relatively large number of particles in the condensate state of the system. The term "condensate" here being used in the sense of the Bose-Einstein condensate. Since the explanation of the technique is most easily coached in terms of particle numbers, it will be convenient at this point to convert the previously introduced Hamiltonian

$$H(c, g, N) = -\sum_{i=1}^{N} \frac{\partial^{2}}{\partial x_{i}^{2}} + 2\sum_{i < j=1}^{N} (g + ce_{i}e_{j}) \delta(x_{i} - x_{j})$$

$$= -\sum_{i=1}^{N} \frac{\partial^{2}}{\partial x_{i}^{2}} - \sum_{i=\frac{N}{2}+1}^{N} \frac{\partial^{2}}{\partial x_{i}^{2}} + (g + c) \sum_{i,j=1, j \neq j}^{N} \delta(x_{i} - x_{j})$$

$$+ (g + c) \sum_{i,j=\frac{n}{2}+1, j \neq j}^{N} \delta(x_{i} - x_{j}) + 2(g - c) \sum_{i=1}^{N} \sum_{j=\frac{N}{2}+1}^{N} \delta(x_{i} - x_{j})$$
(51)

to a Fock space. For this purpose a "box" of length L will be assumed and the space will be

constructed using single particle wave functions, $\frac{\exp(ip_n x)}{\sqrt{L}}$, constrained by periodic

boundary conditions $\left(p_n = \frac{2\pi n}{L}, n = \dots - 2, -1, 0, 1, 2, \dots\right)$. The prescription for carrying

this procedure out is standard and can be found in many texts such as the one by L. E. Ballentine²⁹ (page 359). Using a^{\dagger} and a as the creation and annihilation operators for one type of boson and similarly b^{\dagger} and b for the other type of boson leads to the form

$$H = \sum_{p=-\infty}^{\infty} p^{2} \left(a_{p}^{\dagger} a_{p} + b_{p}^{\dagger} b_{p} \right) + \left(\frac{g+c}{L} \right) \sum_{p=-\infty}^{\infty} \left(a_{p_{1}}^{\dagger} a_{p_{2}}^{\dagger} a_{p_{3}} a_{p_{4}} + b_{p_{1}}^{\dagger} b_{p_{2}}^{\dagger} b_{p_{3}} b_{p_{4}} \right) \delta_{p_{1}+p_{2};p_{3}+p_{4}}$$

$$+ \frac{2(g-c)}{L} \sum_{p=-\infty}^{\infty} a_{p_{1}}^{\dagger} b_{p_{2}}^{\dagger} a_{p_{3}} b_{p_{4}} \delta_{p_{1}+p_{2};p_{3}+p_{4}}$$
(52).

If the temperature is low enough there is a condensate present in the free Bose gas. It is reasonable to assume that if interactions between the particles are introduced the condensate would still be present providing the interactions are weak. Of course, it would be expected that there would be fewer particles in the condensate with interactions present than with no interactions but the number could still be much larger than the occupation number of any other higher single particle energy state. This assumption of macroscopic occupation of the Bose-Einstein condensate when the interactions are weak (and temperatures low enough) forms the basis for the validity of the Bogoliubov approximation.

On the assumption, then, that the number of particles N_0 in the condensate is not only large but also much larger than the number of particles in any other single particle momentum state, the following approximations are reasonable for the numbers drawn out by the annihilation and creation operators:

$$a_{0} \rightarrow \sqrt{\frac{N_{o}}{2} - 1} \approx \sqrt{\frac{N_{0}}{2}}$$

$$a_{0}^{\dagger} \rightarrow \sqrt{\frac{N_{0}}{2} + 1} \approx \sqrt{\frac{N_{0}}{2}}$$
(53).

Of course this same approximation can be applied to the annihilation and creatior operators for the second type of boson present. In addition these approximations,

$$\frac{N_0}{2} = \frac{N}{2} - \sum_{p \neq 0} a_p^{\dagger} a_p \approx \frac{N}{2}$$

$$\left(\frac{N_0}{2}\right)^2 = \left(\frac{N}{2} - \sum_{p \neq 0} a_p^{\dagger} a_p\right)^2 \approx \frac{N^2}{4} - N \sum_{p \neq 0} a_p^{\dagger} a_p \qquad (54),$$

can be applied to both particle types. Effectively one substitutes the numbers of (53) for their corresponding operators in (52) subject to the additional approximations of (54).

Carrying out the above process for terms involving four p = 0 operators gives

$$a_0^{\dagger} a_0^{\dagger} a_0 a_0 \rightarrow \frac{N^2}{4} - N \sum_{p \neq 0} a_p^{\dagger} a_p$$
(55),

$$b_0^{\dagger} b_0^{\dagger} b_0 b_0 \to \frac{N^2}{4} - N \sum_{p \neq 0} b_p^{\dagger} b_p$$
 (56),

and

$$a_0^{\dagger} b_0^{\dagger} a_0 b_0 \rightarrow \frac{N^2}{4} - \frac{N}{2} \sum_{p \neq 0} a_p^{\dagger} a_p - \frac{N}{2} \sum_{p \neq 0} b_p^{\dagger} b_p$$
 (57).

Terms involving three p = 0 operators are excluded by the factor $\delta_{p_1+p_2;p_2+p_4}$ which imposes the conservation of momentum constraint on particles interactions. Picking out, from the interaction terms, those terms involving only two p = 0 operators gives

$$\sum_{p\neq0} a_{p_1}^{\dagger} a_{p_2}^{\dagger} a_{p_3} a_{p_4} \delta_{p_1 + p_2; p_3 + p_4} \rightarrow \frac{N}{2} \sum_{p\neq0} \left(a_p^{\dagger} a_{-p}^{\dagger} + a_p a_{-p} + 4 a_p^{\dagger} a_p \right)$$
(58),

$$\sum_{p\neq 0} b_{p_1}^{\dagger} b_{p_2}^{\dagger} b_{p_3} b_{p_3} \delta_{p_1 + p_2; p_3 + p_4} \rightarrow \frac{N}{2} \sum_{p\neq 0} \left(b_p^{\dagger} b_{-p}^{\dagger} + b_p b_{-p} + 4 b_p^{\dagger} b_p \right)$$
(59),

and

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$$\sum_{p\neq 0} a_{p_1}^{\dagger} b_{p_2}^{\dagger} a_{p_3} b_{p_4} \delta_{p_1 + p_2; p_3 + p_4} \rightarrow \frac{N}{2} \sum_{p\neq 0} \left(a_p^{\dagger} b_{-p}^{\dagger} + a_p b_{-p} + a_p^{\dagger} a_p + a_p^{\dagger} b_p + b_p^{\dagger} a_p + b_p^{\dagger} b_p \right) \quad (60).$$

Any terms within the interaction terms that involve one or no p = 0 operators are now dropped on the assumption that their contribution is small compared to those terms dealt with above.

If all of the above approximations are carried out in (52) the resulting approximate Hamiltonian can be written as

$$H \approx \frac{gN^{2}}{L} + \sum_{p \neq 0} \left(a_{p} \quad a_{-p}^{\dagger} \quad b_{p} \quad b_{\cdot p}^{\dagger} \right) \left(\begin{array}{cccc} e' + e & 0 & e' - e & e' - e \\ p^{2} + 2(e' + e) & e' + e & e' - e & e' - e \\ e' - e & e' - e & e' + e & 0 \\ e' - e & e' - e & p^{2} + 2(e' + e) & e' + e \end{array} \begin{pmatrix} a_{-p} \\ a_{p}^{\dagger} \\ b_{-p} \\ b_{p}^{\dagger} \\ b_{p}^{\dagger} \end{pmatrix}$$
(61)

where

$$e' = \frac{gN}{2L}$$

$$e = \frac{cN}{2L}$$
(62).

The square matrix in (61) is not symmetric but it is block symmetric. To take advantage of this feature the following canonical operators are introduced:

$$d_p = \frac{a_p + b_p}{\sqrt{2}} \tag{63}$$

and

$$f_p = \frac{a_p - b_p}{\sqrt{2}} \tag{64}.$$

In terms of these newly introduced operators (61) can now be written as

$$H = \frac{gN^{2}}{L} + \sum_{p \neq 0} \left(d_{p} \quad d_{-p}^{\dagger} \quad f_{p} \quad f_{-p}^{\dagger} \right) \left(\begin{array}{cccc} 2e' & e' - e & 0 & 0 \\ p^{2} + 3e' + e & 2e' & 0 & 0 \\ 0 & 0 & 2e & e - e' \\ 0 & 0 & p^{2} + e' + 3e & 2e \end{array} \right) \left(\begin{array}{c} d_{-p} \\ d_{p}^{\dagger} \\ f_{-p} \\ f_{p}^{\dagger} \end{array} \right)$$
(65)

or, in preparation for the next step,

$$H = \frac{gN^{2}}{L} + \sum_{p\neq 0} \begin{pmatrix} d_{p} & d_{-p}^{\dagger} \end{pmatrix} \begin{pmatrix} 2e' & e'-e \\ p^{2} + 3e' + e & 2e' \end{pmatrix} \begin{pmatrix} d_{-p} \\ d_{p}^{\dagger} \end{pmatrix} + \sum_{p\neq 0} \begin{pmatrix} f_{p} & f_{-p}^{\dagger} \end{pmatrix} \begin{pmatrix} 2e & e-e' \\ p^{2} + e' + 3e & 2e \end{pmatrix} \begin{pmatrix} f_{-p} \\ f_{p}^{\dagger} \end{pmatrix}$$
(66).

Each of the two square matrices in (66) is of the general form $\begin{pmatrix} a & b \\ c & a \end{pmatrix}$ so the next step is

to introduce the following transformation:

$$\begin{pmatrix} \cosh \theta & -\sinh \theta \\ -\sinh \theta & \cosh \theta \end{pmatrix} \begin{pmatrix} a & b \\ c & a \end{pmatrix} \begin{pmatrix} \cosh \theta & -\sinh \theta \\ -\sinh \theta & \cosh \theta \end{pmatrix} = \begin{pmatrix} 0 & k_{\theta} \\ l_{\theta} & 0 \end{pmatrix}$$
(67)

In order to satisfy the requirements of (67) the parameters must have the values

$$\exp(2\theta) = \sqrt{\frac{2a+b+c}{b+c-2a}}$$
(68),

$$k_{\theta} = -a \sinh 2\theta + \frac{b}{2} (\cosh 2\theta + 1) + \frac{c}{2} (\cosh 2\theta - 1)$$
(69),

and

$$l_{\theta} = -a \sinh 2\theta + \frac{b}{2} (\cosh 2\theta - 1) + \frac{c}{2} (\cosh 2\theta + 1)$$
(70).

With the above background in mind another set of cononical operators is now introduced through Bogoliubov transformations. These new operators are defined using the

parameters $\theta = \theta(|p|)$ and $\phi = \phi(|p|)$ as

$$\begin{pmatrix} d_p \\ d_{-p}^{\dagger} \end{pmatrix} = \begin{pmatrix} \cosh\theta & -\sinh\theta \\ -\sinh\theta & \cosh\theta \end{pmatrix} \begin{pmatrix} \beta_p \\ \beta_{-p}^{\dagger} \end{pmatrix}$$
(71)

and

$$\begin{pmatrix} f_p \\ f_{-p}^{\dagger} \end{pmatrix} = \begin{pmatrix} \cosh \phi & -\sinh \phi \\ -\sinh \phi & \cosh \phi \end{pmatrix} \begin{pmatrix} \alpha_p \\ \alpha_{-p}^{\dagger} \end{pmatrix}$$
(72).

When θ and ϕ are set to satisfy the requirements of (68) then (66) becomes

$$H = \frac{gN^{2}}{L} + \sum_{p\neq0} \left(\beta_{p} \quad \beta_{-p}^{\dagger}\right) \begin{pmatrix} 0 & k_{\theta} \\ l_{\theta} & 0 \end{pmatrix} \begin{pmatrix} \beta_{-p} \\ \beta_{p}^{\dagger} \end{pmatrix} + \sum_{p\neq0} \left(\alpha_{p} \quad \alpha_{-p}^{\dagger}\right) \begin{pmatrix} 0 & k_{\phi} \\ l_{\phi} & 0 \end{pmatrix} \begin{pmatrix} \alpha_{-p} \\ \alpha_{p}^{\dagger} \end{pmatrix}$$
$$= \frac{gN^{2}}{L} + \sum_{p\neq0} \left\{k_{\theta} \left(\beta_{p}^{\dagger}\beta_{p} + 1\right) + l_{\theta}\beta_{p}^{\dagger}\beta_{p} + k_{\phi} \left(\alpha_{p}^{\dagger}\alpha_{p} + 1\right) + l_{\phi}\alpha_{p}^{\dagger}\alpha_{p}\right\}$$
$$= \frac{gN^{2}}{L} + 2\sum_{p\neq0}^{\infty} \left\{-p^{2} - 2e' - 2e + \frac{1}{2}\left(\lambda_{p} + \omega_{p}\right)\right\} + 2\sum_{p\neq0}^{\infty} \left(\lambda_{p}\alpha_{p}^{\dagger}\alpha_{p} + \omega_{p}\beta_{p}^{\dagger}\beta_{p}\right)$$
(73)

where

$$\lambda_p = |p|\sqrt{p^2 + 8e} \tag{74}$$

and

$$\boldsymbol{\omega}_{p} = |\boldsymbol{p}|\sqrt{\boldsymbol{p}^{2} + \boldsymbol{8}\boldsymbol{e}'} \tag{75}.$$

The results of satisfying the requirements of (66) are

$$\exp 2\theta = \frac{\sqrt{p^2 + 8e'}}{|p|} \tag{76}$$

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$$\exp 2\phi = \frac{\sqrt{p^2 + 8e}}{|p|} \tag{77}.$$

As a result of the approximations and transformations outlined above the Hamiltonian (73) that is the final product can be seen to describe a system made up of two types of bosons that do not interact with each other. This boson, or quasiparticle, system is like a system of photons rather than particles in that there is no fixed number of them. Unlike the photon system, if there are no quasiparticles present the system still has a finite energy providing c and g are not both zero. Interestingly, when considering the two interaction parameters g and c, the energy of the one type of quasiparticle depends on g only whereas the energy of the other type of quasiparticle is dependent on c only. Induct, except for the leading term, g and c play completely symmetric roles in (73).

The ground state

Using the approach that the ground state of a system is the state of minimum energy then for (73) that condition would be achieved by having no quasiparticles present. Thus the ground state energy of the system is, by this Bogoliubov approach,

$$H_{grd} = \frac{gN^2}{L} + 2\sum_{p>0}^{\infty} \left\{ -p^2 - 2e' - 2e + \frac{1}{2} \left(\lambda_p + \omega_p \right) \right\}$$
(78).

To get some sense of how reasonable this result for the ground state energy is let us first set c = 0 and then take the resulting form of (78) to its continuous limit form. This process gives

$$H_{grd}(c=0) = \frac{gN^{2}}{L} + 2\sum_{p>0}^{\infty} \left\{ -p^{2} - \frac{gN}{L} + \frac{1}{2} \left(p^{2} + p\sqrt{p^{2} + 4\frac{gN}{L}} \right) \right\}$$
$$= \frac{gN^{2}}{L} + \frac{L}{\pi} \int_{0}^{\infty} dp \left\{ -p^{2} - \frac{gN}{L} + \frac{1}{2} \left(p^{2} + p\sqrt{p^{2} + 4\frac{gN}{L}} \right) \right\}$$
$$= \frac{gN^{2}}{L} - \frac{4}{3\pi} g^{\frac{3}{2}} N \sqrt{\frac{N}{L}}$$
(79).

Using the symbols introduced with (41) the result of (79) can be written as

$$H_{grd}(c=0) = N\rho^{2}\left(\gamma - \frac{4}{3\pi}\gamma^{\frac{3}{2}}\right)$$
(80).

This is the result that Lieb and Liniger²⁶ arrived at when they used the Bogoliubov approximation method. For our purposes here this agreement shows that the method used does reproduce previously known results when c = 0 as one would hope it would. Lieb and Liniger used the Bogoliubov approach because they had the exact answer to the ground state energy and wanted to see how valid this approximation approach would be in



comparison. Again referring back to (41) one can see that such a comparison can be carried out using $e(\gamma)$, as computed using the coupled integral equations (42), (43), and '44), and the factor in brackets in (80). Figure 9 shows the results of the comparison when the calculations just described are carried out. The graphs shown in the figure are in agreement with those given by Lieb and Liniger. From this comparison Lieb and Liniger felt that the results of the Bogoliubov approximation were quite valid for $\gamma < 2$.

Indeed Lieb and Liniger were able to show that the first term in the Bogoliubov result is

exact and, from the good agreement shown in Figure 9 for small γ , felt that the second term was probably also exact. More weight to the correctness of the second term was given by M. Gaudin³⁰ who arrived at these same two terms by using another method. Having these two leading terms allowed Blum, Koltun and Shapir¹² to make an estimate of the ground state of the system when c > 0 by using the method of variation. Their trial wave function was of the Hartree type, $|a\rangle|b\rangle$, where $|a\rangle$ is the exact solution as found by Lieb and Liniger if only type *a* bosons were present and similarly for $|b\rangle$. In Fock space the Lieb-Liniger solution is

$$H_{LL}^{a}|a\rangle = \left\{\sum_{p=-\infty}^{\infty} p^{2}a_{p}^{\dagger}a_{p} + \frac{g}{L}\sum_{p=-\infty}^{\infty} a_{p_{1}}^{\dagger}a_{p_{2}}^{\dagger}a_{p_{3}}a_{p_{4}}\delta_{p_{1}+p_{2};p_{3}+p_{4}}\right\}|a\rangle$$

$$= E_{o}|a\rangle$$
(81)

where E_o is as given in (41). Utilizing this result and using the Hamiltonian of (52) gives the ground state energy, E_{BKS} , arrived at by Blum, Koltun and Shapir

$$E_{BKS} = \langle b | \langle a | H | a \rangle | b \rangle$$

= $\langle b | \langle a | H_{LL}^{a} | a \rangle | b \rangle + \langle b | \langle a | H_{LL}^{b} | a \rangle | b \rangle$
+ $\frac{2(g-c)}{L} \langle b | \langle a | \sum_{p=-\infty}^{\infty} a_{p_{1}}^{\dagger} b_{p_{2}}^{\dagger} a_{p_{3}} b_{p_{4}} \delta_{p_{1}+p_{2};p_{3}+p_{4}} | a \rangle | b \rangle$ (82).
= $2E_{o} + \frac{2(g-c)}{L} \left(\frac{N}{2}\right)^{2}$

Here the E_o of (41) is modified to reflect the fact that only half the system particles are of each type $(N \rightarrow N/2)$ and the parameter determining the amount of repulsion is $g \rightarrow g + c$. In terms of these parameters one has

$$\gamma = \frac{2(c+g)L}{N} \tag{83}$$

and corresponding to the E_o of (41)

$$E_{o} = \frac{N}{2} \left(\frac{N}{2L}\right)^{2} e(\gamma)$$
(84).

Using (83) and (84) E_{BRS} can be written as

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$$E_{BES} = N \left\{ \frac{\left(g+c\right)^2}{\gamma^2} e(\gamma) + \frac{g^2 - c^2}{\gamma} \right\}$$
(85)

which is in a form that will prove to be useful later. The drawback to this form is that it must be solve numerically so Blum, Koltun and Shapir chose to use the Bogoliubov form introduced in (80), namely

$$e(\gamma) \approx \gamma - \frac{4}{3\pi} \gamma^{\frac{3}{2}}$$
(86)

With the introduction of the Bogoliubov form the ground state energy estimate becomes

$$E_{BES} = \frac{gN^2}{L} - \frac{2\sqrt{2}}{3\pi} (g+c)^{\frac{3}{2}} \frac{N^{\frac{3}{2}}}{\sqrt{L}}$$
(87)

As has been stated above, the Bogoliubov form is an approximation whose validity is good for $\gamma < 2$. Therefore, E_{BKS} should be valid for (g + c)L < N.

Going back to (78) and writing that equation in its continuous limit form gives

$$H_{grd} = \frac{gN^{2}}{L} + \frac{L}{\pi} \int_{0}^{\infty} dp \left\{ -p^{2} - \frac{gN}{L} - \frac{cN}{L} + \frac{1}{2} \left(p\sqrt{p^{2} + \frac{4gN}{L}} + p\sqrt{p^{2} + \frac{4cN}{L}} \right) \right\}$$

$$= \frac{gN^{2}}{L} - \frac{4}{3\pi} \left(g^{\frac{3}{2}} + c^{\frac{3}{2}} \right) \frac{N^{\frac{3}{2}}}{\sqrt{L}}$$
(88).

From this it can be seen that H_{grd} is much the same result as E_{BKS} . Therefore it seems reasonable to assume that the results of the approximation technique being used are valid at least when describing the ground state. So far no restriction has been given on the range the parameters can vary over. A systematic way of determining numerically whether a given set of parameters can be used will be developed later.

Blum, Koltun and Shapir were interested in determining how the ground state energy scaled with N and viewing L as a variational parameter in (87) they minimized E_{BKS} with respect to L to get

$$L_{o}(c,g,N) = \frac{9\pi^{2}g^{2}}{2(c+g)^{3}}N$$
(89)

and thus

$$E_{BKS}(c,g,N,L=L_o) = -\frac{2}{9\pi^2} \frac{(c+g)^3 N}{g}$$
(90).

Since they were working with problems involving the replica approach, as described earlier, the N dependence of the ground state energy was of keen interest. In a similar manner, minimizing H_{grd} with respect to L will yield

$$L_{o}(c, g, N) = \frac{9\pi^{2}g^{2}}{4\left(c^{3/2} + g^{3/2}\right)^{2}}N$$
(91)

with

$$H_{grd}(c,g,N,L=L_{o})=-\frac{4}{9\pi^{2}}\frac{\left(c^{\frac{3}{2}}+g^{\frac{3}{2}}\right)^{2}}{g}N$$
(92).

It is easily seen from the above that both E_{BRS} and H_{grd} are directly proportional to N at $L = L_o$. It is also clear from both (90) and (92) that the case of g = 0 is not handled by the treatment above. Going back to (87) and (88) it is easy to see that on setting g = 0 the minimum energy is reached at a system length of L = 0 - that is, the system would collapse. It should also be noted that mathematically the minimum in the ground state energy given in (92) is achievable whether g is greater or less than c. Physically the requirement for the bound state is that g < c and this restriction will be applied here.

Initially one might question whether the system would in fact collapse if g = 0 or whether the collapse was only implied because both approximation methods have only two terms present with smaller ones being dropped. Perhaps these smaller terms could prevent the collapse. For the H_{grd} case this question remains unanswered. However one can look more closely at the E_{BKS} derivation by going back to (85) and taking the derivative of that expression with respect to L,

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$$\frac{\partial E_{BKS}}{\partial L} = \frac{2(g+c)^2}{\gamma^2} \left\{ \left(g+c\right) \left(\frac{\partial e(\gamma)}{\partial \gamma} - \frac{2e(\gamma)}{\gamma}\right) - \left(g-c\right) \right\}$$
(93).

The condition for an extremum here is

$$\frac{\partial e(\gamma)}{\partial \gamma} = \frac{2e(\gamma)}{\gamma} + \frac{g-c}{g+c}$$
(94).

This equation can be solved numerically but there is enough information about the behavior of $e(\gamma)$ from the Lieb-Liniger work to determine some general features of the solution. The Bogoliubov results can be used to deal with the region $\gamma < 2$ and they give an algebraic expression for $e(\gamma)$ that is valid for large γ . Indeed they claim their large γ results are good to within 1% for γ as small as 10. The range of $2 < \gamma < 10$ that is not covered in the form needed here by their work was dealt with numerically.

The left hand side of (94) has a value of 1 at $\gamma = 0$ and decreases monotonically and asymptotically to zero as γ approaches ∞ . The ratio of $e(\gamma)$ to γ appearing on the right side of the equation has a value of 1 at $\gamma = 0$ and decreases monotonically and asymptotically to zero as γ approaches ∞ . Thus the right side of (94) has a value of 2 + (g - c)/(g + c) at $\gamma = 0$ and diminishes monotonically to the asymptote (g - c)/(g + c) as γ approaches ∞ . It was also apparent when we carried out the numerical work mentioned above in the region $2 < \gamma < 10$ that $2e(\gamma)/\gamma$ is always larger than $\partial e(\gamma)/\partial \gamma$ for these intermediate values of γ . As already mentioned above, both of these terms are equal at $\gamma = 0$. Again, from the work



of Lieb and Liniger it is easy to show that this relative relationship remains true for both small and large values of γ .

Now to help in putting together the intent of giving all the description of the components of (94) Figure 10 shows an example of a numerical solution to the equation. For the example given in the figure both the left and right sides of the equation are plotted as functions of γ with (g-c)/(g+c) = -0.5. Had g been set equal to c then the two curves would not have intersected because, as pointed out above, the left side term of the equation is always less than the resulting right side. If g > c there can be no solution as the asymptote for the right side of the equation is then greater than zero. If g = c then the solution is the limit point

E,

 $\gamma = \infty$ and this implies a system particle density of zero as $\gamma = 2(g+c)/\rho$. For 0 < g < cthere is one and only one value of γ that will solve the equation and Figure 10 illustrates this feature. For such a solution (that is, $\gamma = \text{constant}$) it readily follows that $L_o \propto N$. As g is made to approach zero, then so does γ approach zero and the density of the system will also increase. At g = 0 the solution is $\gamma = 0$ and to achieve this the system would have to have infinite density. In summary, the only physically meaningful solutions for a bound system have 0 < g < c and a length $L_o \propto N$.

The g = 0 case

The implication from the above discussion is that setting g = 0 requires some special consideration. For Blum, Koltun and Shapir it was important to know the N dependence of E_o under this condition on g so they introduced the term $\pi^2 N/L^2$ into their expression for the ground state energy when g = 0. This term represents the zero point energy of N free particles in a "box" of length L when Dirichlet boundary conditions are used. The introduction of this term avoids the tendency of the system to collapse and it also gives a distinctly different L_o behavior than the previously derived one, namely $L_o \propto N^{-\frac{1}{3}}$ which in turn leads to $E_o \propto N^{\frac{5}{3}}$. This seemingly arbitrary tool to get around a problem lead Craig, Kiang and Niégawa³¹ to examine the effect of both periodic and Dirichlet boundary conditions using the Bogoliubov approximation technique for the apparently distinct cases

of g > 0 and g = 0. The case of periodic boundary conditions with g > 0 has already been developed above and more on it is to come. The Dirichlet boundary case (g > 0) lead to the necessity of introducing a boson transformation which could only be carried out at the expense of degrading the accuracy of the Bogoliubov technique. Since no basically new results came out of this treatment, it will not be pursued further here. As has already been noted in the development above, the g = 0 case with periodic boundary conditions implies system collapse. The fourth scenario, g = 0 with Dirichlet boundary conditions, will be considered now in a little more detail.

Rather than insert the zero point free particle kinetic energy term as Blum, Koltun and Shapir did, it seemed more reasonable to start with Dirichlet boundary conditions and see if this term did arise naturally in the treatment of an interacting system. On going to a Fock space, with g = 0, one arrives at

$$H = \sum_{n=1}^{\infty} p_n^2 \left(a_n^{\dagger} a_n + b_n^{\dagger} b_n \right)$$

$$= \frac{c}{2L} \sum_{m',n',m,n} f_{m',n',m,n} \left(a_{m'}^{\dagger} a_{n'}^{\dagger} a_m a_n + b_{m'}^{\dagger} b_{n'}^{\dagger} b_m b_n - 2a_{m'}^{\dagger} b_{n'}^{\dagger} a_m b_n \right)$$
(95).

The difficulty with this expression, compared to the corresponding one in the periodic boundary case, is the relative complexity of the Kronecker delta, namely

$$f_{m'n'mn} = \delta_{m'-n'+m-n} + \delta_{m'-n'-m+n} + \delta_{m'+n'-m-n} - \delta_{m'-n'+m+n} - \delta_{m'-n'+m+n} - \delta_{m'-n'-m+n} - \delta_{m'+n'-m+n}$$
(96).

In invoking the Bogoliubov approximation where one picks out terms involving four or two lowest single particle momentum modes, the Kronecker delta combination introduces coupling between single particle modes n and n + 2. In the Craig, Kiang, and Niégawa work mentioned above a trial wave function was introduced and a switch made to the variational method. The ground state energy found as a consequence showed no Cependence on the mode coupling and showed that the same result would have been achieved if, in following the Bogoliubov method, the Kronecker delta had been assumed to consist of the first three terms on the right side of (96) only. It will be assumed here that this ignoring of coupling is reasonable in developing the approximate Hamiltonian.

With the reduction in the complexity of the Kronecker delta form the carrying out of the Bogoliubov approximation scheme follows the same general development scheme as already described in the periodic boundary case. An examination of (95) shows that the sum of all terms containing four lowest mode, or p = 1, operators will produce a zero. Removing the p = 1 operators from the first summation in (95) will yield $\pi^2 N/L^2$ as $p_1 = \pi/L$. This term, was previously mentioned as being introduced by Blum, Koltun and Shapir in their treatment of the g = 0 case. Now it can be seen that this term can naturally arise, at least in a weakly interacting system, when Dirichlet boundary conditions are invoked. The approximate Hamiltonian is now

$$H_{o} = \frac{\pi^{2}N}{L^{2}} + \sum_{n=2}^{\infty} \left(a_{n} \quad a_{n}^{\dagger} \quad b_{n} \quad b_{n}^{\dagger}\right) \begin{pmatrix} e & 0 & -e & -e \\ p_{n}^{2} + 2e & e & -e & -e \\ -e & -e & e & 0 \\ -e & -e & p_{n}^{2} + 2e & e \end{pmatrix} \begin{pmatrix} a_{n} \\ a_{n}^{\dagger} \\ b_{n} \\ b_{n}^{\dagger} \end{pmatrix}$$
(97).

On using the operators introduced in (63) and (64) the Hamiltonian becomes

$$H_{o} = \frac{\pi^{2} N}{L^{2}} + \sum_{n=2}^{\infty} \left(d_{n} \quad d_{n}^{\dagger} \right) \begin{pmatrix} 0 & -e \\ p_{n}^{2} + e & 0 \end{pmatrix} \begin{pmatrix} d_{n} \\ d_{n}^{\dagger} \end{pmatrix} + \sum_{n=2}^{\infty} \left(f_{n} \quad f_{n}^{\dagger} \right) \begin{pmatrix} 2e & e \\ p_{n}^{2} + 3e & 2e \end{pmatrix} \begin{pmatrix} f_{n} \\ f_{n}^{\dagger} \end{pmatrix}$$
(98).

As can now be seen, the terms in the first summation are of the required form but those in the second summation have to undergo a transformation of the Bogoliubov type as given in (67) and meeting the conditions outlined in (68), (69), and (70). Then carrying out the transformation

$$\begin{pmatrix} f_n \\ f_n^{\dagger} \end{pmatrix} = \begin{pmatrix} \cosh \varphi & -\sinh \varphi \\ -\sinh \varphi & \cosh \varphi \end{pmatrix} \begin{pmatrix} \alpha_n \\ \alpha_n^{\dagger} \end{pmatrix}$$
(99)

yields, on meeting the conditions for φ ,

$$H_{o} = \frac{\pi^{2}N}{L^{2}} + \sum_{n=2}^{\infty} (d_{n} \quad d_{n}^{\dagger}) \begin{pmatrix} 0 & -e \\ p_{n}^{2} + e & 0 \end{pmatrix} \begin{pmatrix} d_{n} \\ d_{n}^{\dagger} \end{pmatrix} + \sum_{n=2}^{\infty} (\alpha_{n} \quad \alpha_{n}^{\dagger}) \begin{pmatrix} 0 & \frac{p\sqrt{p_{n}^{2} + 8e} - (p_{n}^{2} + 2e)}{2} \\ \frac{p\sqrt{p_{n}^{2} + 8e} + (p_{n}^{2} + 2e)}{2} & 0 \end{pmatrix} \begin{pmatrix} \alpha_{n} \\ \alpha_{n}^{\dagger} \end{pmatrix}$$
(100).

Simplifying this expression leads to

$$H_o = \frac{\pi^2 N}{L^2} + \frac{1}{2} \sum_{n=2}^{\infty} \left(-p_n^2 - 4e + \lambda_n \right) + \sum_{n=2}^{\infty} \left(p_n^2 d_n^{\dagger} d_n + \lambda_n \alpha_n^{\dagger} \alpha_n \right)$$
(101)

where

$$\lambda_n = p_n \sqrt{p_n^2 + 8e} \tag{102}.$$

Like the Hamiltonian in (73), the Hamiltonian in (100) describes a system consisting of two types of none interacting bosons. Again there is no fixed number of bosons, or

quasiparticles, specified. Note that one of the two types of quasiparticles has the same energy spectrum as one of the real bosons making up the system would have if it were a free particle. The ground state of this system

$$H_{grd(o)} = \frac{\pi^2 N}{L^2} + \frac{1}{2} \sum_{n=2}^{\infty} \left(-p_n^2 - 4e + \lambda_n \right)$$
(103)

has as its first term the free particle kinetic energy but it appears as a natural consequence of the method used rather than the more *ad hoc* insertion used by Blum, Koltun and Shapir. If this ground state energy is put in its continuous form

$$H_{grd(o)} = \frac{\pi^2 N}{L^2} - \frac{4}{3\pi} N \left(\frac{N}{L}\right)^{\frac{1}{2}} c^{\frac{3}{2}}$$
(104)

and then minimized with respect to L the result is similar to that given by Blum, Koltun and

Shapir, namely $L_o \propto N^{-\frac{1}{3}}$ and $H_{grd(o)}(L = L_o) \propto N^{\frac{5}{3}}$. However the actual value of this minimum ground state energy

$$H_{grd(o)}(L = L_o) = -\frac{c^2 N^{\frac{3}{3}}}{3^{\frac{1}{3}} \pi^2}$$
(105)

is lower than that of Blum, Koltun and Shapir.

The one particle density matrix and pair correlation function

In the next chapter the approximate Hamiltonian will be used to examine its predictions on the thermodynamics of the system. Before launching into the macroscopic behavior of the
system we will have a brief look at what the approximate Hamiltonian has to say about the microscopic behavior of the ground state. To carry this out we will use the one-particle density matrix and the pair correlation function.

The single particle density matrix, (See G. Baym³², for example.) can be written as $G_a(x-y) = \langle \chi | \Psi_a \setminus \tau \rangle \Psi_a(y) | \chi \rangle$ (106)

where $\Psi_a(x)$ is the field operator that removes a type "a" particle from position x and $\Psi_a^{\dagger}(x)$ adds a type "a" at position x. Of course, the same formulation could be made up for type "b" particles. $|\chi\rangle$ is the ground state vector.

In momentum terminology, using the previously defined operators a^{\dagger} and a, we have

$$G_{a}(x-y) = \langle \chi | \sum_{p_{1}=-\infty}^{\infty} \frac{e^{-ip_{1}x}}{\sqrt{L}} a_{p_{1}}^{\dagger} \sum_{p_{2}=-\infty}^{\infty} \frac{e^{ip_{2}y}}{\sqrt{L}} a_{p_{2}} | \chi \rangle$$

$$= \frac{1}{L} \sum_{p=-\infty}^{\infty} e^{ip(y-x)} \langle \chi | a_{p}^{\dagger} a_{p} | \chi \rangle$$

$$= \frac{1}{L} a_{0}^{\dagger} a_{o} + \frac{1}{L} \sum_{p\neq 0} e^{ip(y-x)} \langle \chi | a_{p}^{\dagger} a_{p} | \chi \rangle$$
(107).

(Note the long range order in the condensate implied by the first term.) The first term is now replaced by its exact value rather than using the approximation from the first equation of (54). On so doing, the single particle density matrix becomes

$$G_{a}(\boldsymbol{x}-\boldsymbol{y}) = \frac{N}{2L} + \frac{1}{L} \sum_{p\neq 0} \left(e^{ip(\boldsymbol{y}-\boldsymbol{x})} - \mathbf{1} \right) \langle \boldsymbol{\chi} | \boldsymbol{a}_{p}^{\dagger} \boldsymbol{a}_{p} | \boldsymbol{\chi} \rangle$$
(108).

Next converting to the quasiparticle operators of (71) and (72) the result is

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$$G_{a}(x-y) \approx \frac{N}{2L} + \frac{1}{2L} \sum_{p \neq 0} \left(e^{\varphi(y-x)} - 1 \right) \left(\chi \left| \cosh^{2} \phi \, \alpha_{p}^{\dagger} \alpha_{p} + \sinh^{2} \phi \, \alpha_{p} \alpha_{p}^{\dagger} + \cosh^{2} \theta \, \beta_{p}^{\dagger} \beta_{p} + \sinh^{2} \theta \, \beta_{p} \beta_{p}^{\dagger} \right| \chi \right)$$

$$= \frac{N}{2L} + \frac{1}{4L} \sum_{p \geq 0} \left(\cos p(y-x) - 1 \right) \left(\frac{\lambda_{p}}{p^{2}} + \frac{p^{2}}{\lambda_{p}} + \frac{\omega_{p}}{p^{2}} + \frac{p^{2}}{\omega_{p}} - 4 \right)$$
(109).

Not surprisingly, for the other type of particle present, $G_b(x - y) = G_a(x - y)$.

The next graph, Figure 11, shows the numerical results when only the |x - y| dependent part of (109) is plotted for the values of the parameters given in the figure caption. For this particular length of the system over 95% of the particles are in the condensate. (How the



Figure 11 -Single particle density matrix for ground state. Parameters are L = 10, $g = 2 \times 10^{-5}$, c = 0.1, and $N = 10^{6}$. Condensate occupancy exceeds 95%. Note that it is only the |x - y| dependent part that is plotted.

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percentage of particles in the condensate is calculated will be given in Chapter 4.) It should be noted that the relatively large, but constant, part of (109) that is not included in the plot is the contribution from the particles in the condensate. This contribution has a magnitude of $N_o/(2L)$ where N_o is the number of particles in the condensate. The symmetry of the graph about a vertical line drawn through the point |x - y| = 5 is attributable to the periodic boundary conditions. If the interactions between particles were "turned off" then the graph would be a straight line along the horizontal axis which would indicate a homogeneous distribution of particles. With the interactions present there is a large homogeneous "background" due to most particles being in the condensate but the moving particles are apparently not uniformly distributed.

Taking the interpretation of the single particle density matrix as the amplitude of being able to remove a particle from one position and put it back in another, then the graph shows that this amplitude is greatest if the particle is replaced in the same position it is removed from. This amplitude diminishes with increased distance between point of removal and point of replacement until a minimum is reached at L/2. Since the removed particle must have the same momentum as the inserted particle then the implication is that particles which are not in the condensate but with the same momentum have a tendency to be near each other or move as a group.



Figure 12 shows the effect of changing the length of the system. Note the horizontal axis gives the *percentage* of |x - y| so that the two graphs can be compared for shape. Increasing the length diminishes the tendency of particles of the same momentum to be near each

other.

Figure 13 shows the dependence of the |x - y| part of the single particle density matrix on N. Here again the general shape of the curve is much the same as in the other plots of this function. Increasing the parameters g and/or c will also produce effects like increasing N



values of N. Other parameters are L = 10, $g = 2 \times 10^{-5}$, c = 0.1.

but again there is no basic change in the over all shape.

The pair correlation function (See Baym³³, for example.) can be written as

$$g_{aa}(x-y) = \left(\frac{2}{N}\right)^{2} \langle \chi | \Psi_{a}^{\dagger}(x) \Psi_{a}^{\dagger}(y) \Psi_{a}(y) \Psi_{a}(x) | \chi \rangle$$
(110).

A similar definition would apply to the "b" type particles and $g_{bb}(x-y) = g_{aa}(x-y)$.

Now carrying out the same basic process as for the single particle density matrix where the goal was to transform to the quasiparticle operators to get

$$\left(\frac{N}{2}\right)^{2} g_{aa}(x-y) = \frac{1}{L^{2}} \langle \chi | \sum_{all \ p} e^{i(p_{4}-p_{1})x+i(p_{3}-p_{2})y} a_{p_{1}}^{\dagger} a_{p_{2}}^{\dagger} a_{p_{3}} a_{p_{4}} | \chi \rangle$$

$$= \frac{N^{2}}{4L^{2}} + \frac{N}{L^{2}} \sum_{p=-\infty}^{\infty} \cos p(x-y) \langle \chi | a_{p}^{\dagger} a_{p} | \chi \rangle$$

$$= \frac{N^{2}}{4L^{2}} + \frac{N}{L^{2}} \sum_{p>0} \cos p(x-y) \{ \sinh^{2} \theta + \sinh^{2} \phi \}$$

$$= \frac{N^{2}}{4L^{2}} + \frac{N}{4L^{2}} \sum_{p>0} \cos p(x-y) \{ \frac{\lambda_{p}}{p^{2}} + \frac{p^{2}}{\lambda_{p}} + \frac{p^{2}}{\omega_{p}} - 4 \}$$
(111).

Here use of the approximations in (54) was made and, in keeping with the Bogoliubov approximation method, terms containing one or no p = 0 indexed operators were dropped as being small. Note that the functional form of the |x - y| dependent part is identical to that of the single particle density matrix in (109).

One can also define two pair correlation functions involving both types of particles as

$$g_{ab}(x-y) = \left(\frac{2}{N}\right)^{2} \langle \chi | \Psi_{a}^{\dagger}(x) \Psi_{b}^{\dagger}(y) \Psi_{b}(y) \Psi_{a}(x) | \chi \rangle$$

$$g_{ab}(x-y) = \left(\frac{2}{N}\right)^{2} \langle \chi | \Psi_{a}^{\dagger}(y) \Psi_{b}^{\dagger}(x) \Psi_{b}(y) \Psi_{a}(x) | \chi \rangle$$
(112).

The first of these two forms, which can be interpreted as removing an "a" and a "b" type particle and then replacing them in the same locations as their removal, produces a constant for the result. More interesting is the second form which can be interpreted as removing one each of the two types of particles and then replacing them in exchanged positions. This second form becomes

$$\left(\frac{N}{2}\right)^{2} g_{ab}(x-y) = \frac{1}{L^{2}} \langle \chi | \sum_{p=-\infty}^{\infty} e^{i(p_{1}-p_{2})(x-y)} a_{p_{1}}^{\dagger} a_{p_{1}} b_{p_{2}}^{\dagger} b_{p_{2}} | \chi \rangle$$

$$= \frac{N^{2}}{4L^{2}} + \frac{N}{4L^{2}} \sum_{p>0} (\cos p(x-y) - 1) \left(\frac{\lambda_{p}}{p^{2}} + \frac{p^{2}}{\lambda_{p}} + \frac{\omega_{p}}{p^{2}} + \frac{p^{2}}{\omega_{p}} - 4\right)$$
(113).

Note that once again the functional form of the |x - y| dependent part of this expression is the same as that of the single particle density matrix (109).

Going back to (111) and writing out the expansion is a different way will give

$$\left(\frac{N}{2}\right)^{2} g_{aa}(x-y) \approx \frac{N_{o}^{2}}{4L^{2}} + \frac{1}{L^{2}} \sum_{p\neq 0} \left\{ 2a_{o}^{\dagger}a_{o}a_{p}^{\dagger}a_{p} + 2(\cos p(x-y))a_{o}^{\dagger}a_{o}a_{p}^{\dagger}a_{p} \right\}$$
(114).

Here, as has been the usual practice, the rest of the terms have been dropped as being small. The reason for writing the form in this way is that it is somewhat more useful to see what is going on to produce the final form. The first term in the expression comes from pair exchanges involving particles in the condensate only. This term is by far the largest contributor to the magnitude of the result because of the large number of particles in the condensate and it is also constant which indicates a uniform distribution of these particles. The next term, the sum of the $a_o^{\dagger}a_o a_p^{\dagger}a_p$, is also a constant and it involves pair exchanges in which only one of the pair is in the condensate. In these exchanges the particles are returned to their original positions. The final part again involves pair exchanges in which only one of the pair is from the condensate but the position of the particles also gets interchanged. However, because the particles in the condensate are so numerous and uniformly distributed, this type of exchange amounts to essentially the same type of exchange as the single particle density matrix calculation. Thus no basically new information is brought forward by the pair correlation function.

One other feature of the results of the single particle density matrix (and pair correlation function) that deserves some mention is the symmetry in the occurrence of the interaction parameters g and c. This symmetry also will come up in some of the thermodynamic functions to be derived in the next chapter and it is surprising considering that this symmetry is not present in the original Hamiltonian. If one goes back to (114) and does not use the approximations of (54), the resulting form can be diagonalized using operator transformations exactly of the forms as were used in arriving at the approximate Hamiltonian (73). The resulting approximate Hamiltonian under these conditions has the form

$$H^{\circ} = \frac{gN_{o}^{2}}{L} + 2\sum_{p>0} \left\{ -p^{2} - 6e_{o}' - 2e_{o} + \frac{1}{2} \left(\lambda_{p}^{\circ} + \omega_{p}^{\circ}\right) \right\} + 2\sum_{p>0} \left(\lambda_{p}^{\circ} \alpha_{p}^{\dagger} \alpha_{p} + \omega_{p}^{\circ} \beta_{p}^{\dagger} \beta_{p}\right) \quad (115)$$

where

$$e_{o} = \frac{cN_{o}}{2L}, e_{o}' = \frac{gN_{o}}{2L}, \lambda_{p}^{o} = \sqrt{(p^{2} + 4e_{o}')(p^{2} + 8e_{o} + 4e_{o}')},$$

and $\omega_{p}^{o} = \sqrt{(p^{2} + 4e_{o}')(p^{2} + 12e_{o}')}$ (116).

The difficulty with this form is in the occurrence of N_o which is an unknown. However, it can be determined by using $N_o = N - \langle N_{ex} \rangle$. As has already been mentioned parenthetically an expression for N_{ex} will be derived in the next chapter. This expression for N_{ex} contains N and not N_o so it is convenient. An equivalent expression for N_{ex} can also be derived in terms based on the elements in (116) but in this form N_o can be solved for by using $N_o = N - \langle N_{ex} \rangle$ in a self consistent manner. Both methods give approximately the same result.

Now in terms of this second formulation of an approximate Hamiltonian we have

$$\left(\frac{N}{2}\right)^{2} g_{aa}(x-y) = \frac{N_{o}^{2}}{4L^{2}} + \frac{N_{o}}{4L^{2}} \sum_{p \geq 0} (1 + \cos p(x-y)) \left\{ \frac{\lambda_{p}^{o}}{p^{2} + 4e'_{o}} + \frac{p^{2} + 4e'_{o}}{\lambda_{p}^{o}} + \frac{\omega_{p}^{o}}{p^{2} + 4e'_{o}} + \frac{p^{2} + 4e'_{o}}{\omega_{p}^{o}} - 4 \right\}$$
(117).

This form produces the same results as the previous one to a good approximation so, in that respect, it is not particularly interesting. However, what is of some interest is that it produces the same results without being symmetric in the occurrence of the interaction parameters g and c as can be seen by referring back to the definitions in (116) when looking at the structure of (117). However, the symmetry still must be there and the source of this symmetry must be N_o . N_o is dependent on g and c but this feature is buried out of sight in the original formulation of the approximate Hamiltonian. It is through the second of the approximations in (54) that this connection is made. Thus the symmetry between cand g exists through this interconnection at least in the parameter range where this Bogoliubov approximation method is valid.

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IV. The Thermodynamics of the System

The partition function

In developing the examination of the thermodynamic properties of the boson system when both g and c are greater than zero the first step in the process will be the calculation of the partition function from

$$\Xi = Tr \left\{ \exp(-\beta H) \right\}$$
(118)

One feature of the partition function that should be dealt with first is the lack of mention of a chemical potential. The Hamiltonian that will be used in developing the partition function is not the original Hamiltonian but rather the approximate Hamiltonian (73) derived from it. This approximate Hamiltonian, as already mentioned, describes a system consisting of two types of bosons (the quasiparticles) whose number is not fixed. The number of real particles in any state of the original system is, of course, fixed at the constant value N. A quasiparticle requires the presence of excitations which do not exist in the ground state of the system. As Callen³³, page 412, points out the chemical potential of a nonconserved Bose system is zero. So here, as the number of quasiparticles is not fixed, the grand canonical formalism will be used after first setting the chemical potential to zero.

As a check on the reasonableness of using the partition function of (118) with the approximate Hamiltonian one can rotate back to real particle space by setting g and c to zero. On so doing, the partition function has the appearance of a system of free real particles with a chemical potential of zero. (See (19) and (20)). Such a system of free real bosons does not in fact have a chemical potential of zero but as has been pointed out here, in the development following (19), the setting of the chemical potential to zero does produce quite reasonable approximations when the number of particles in the condensate is macroscopic. The dropping of terms, as being small, in the derivation of the approximate Hamiltonian has reproduced this argument in a more indirect way.

Inserting the approximate Hamiltonian in (118) gives

$$\Xi(\beta, L, N) = Tr \left\{ \exp\left(-\beta H_{grd} - \beta \sum_{p \neq 0} \left(\lambda_{p} \alpha_{p}^{\dagger} \alpha_{p} + \omega_{p} \beta_{p}^{\dagger} \beta_{p}\right)\right) \right\}$$

$$= \exp\left(-\beta H_{grd}\right) Tr \left\{ \exp\left(-\beta \sum_{p \neq 0} \left(\lambda_{p} \alpha_{p}^{\dagger} \alpha_{p} + \omega_{p} \beta_{p}^{\dagger} \beta_{p}\right)\right) \right\}$$

$$= \exp\left(-\beta H_{grd}\right) \prod_{p \neq 0} \left(\frac{1}{1 - \exp\left(-\beta \lambda_{p}\right)} \frac{1}{1 - \exp\left(-\beta \omega_{p}\right)}\right)$$
(119).

Here the H_{grd} is as given in (78).

Some of the thermodynamic functions

With form (119) of the partition function it is now reasonably straightforward to calculate the thermodynamic measures of the system. A number of those measures will now be

determined, the first of which being the energy. Using $E = -\left(\frac{\partial}{\partial\beta}\ln\Xi\right)_L$ gives

$$E = H_{grd} + 2\sum_{p>0}^{\infty} \left(\frac{\lambda_p}{\exp(\beta\lambda_p) - 1} + \frac{\omega_p}{\exp(\beta\omega_p) - 1} \right)$$
(120).

For the pressure, using $P = \frac{1}{\beta} \left(\frac{\partial}{\partial L} \ln \Xi \right)_{\beta}$, one arrives at

$$P = -\frac{\partial H_{grd}}{\partial L} + \frac{4}{L} \sum_{p>0}^{\infty} \left(\frac{\lambda_p - 2e \frac{p^2}{\lambda_p}}{\exp(\beta \lambda_p) - 1} + \frac{\omega_p - 2e' \frac{p^2}{\omega_p}}{\exp(\beta \omega_p) - 1} \right)$$
(121)

where

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$$-\frac{\partial H_{grd}}{\partial L} = \frac{H_{grd}}{L} - \frac{2}{L} \sum_{p>0}^{\infty} p^2 \left\{ 1 - \frac{1}{4} \left(\frac{p^2}{\lambda_p} + \frac{\lambda_p}{p^2} + \frac{p^2}{\omega_p} + \frac{\omega_p}{p^2} \right) \right\}$$
(122).

The entropy is also derivable from the partition function using $S = -\left(\frac{\partial(T \ln \Xi)}{\partial T}\right)_L$ to give

$$S = 2\sum_{p>0}^{\infty} \left\{ \ln \left(\frac{\exp(\beta \lambda_p)}{\exp(\beta \lambda_p) - 1} \right) + \ln \left(\frac{\exp(\beta \omega_p)}{\exp(\beta \omega_p) - 1} \right) \right\} + 2\sum_{p>0}^{\infty} \left(\frac{\beta \lambda_p}{\exp(\beta \lambda_p) - 1} + \frac{\beta \lambda_p}{\exp(\beta \lambda_p) - 1} \right)$$
(123).

Another thermodynamic property of the system that will be considered is its specific heat which can be evaluated using

$$C_{L} = \left(\frac{\partial E}{\partial T}\right)_{L} = 2\beta^{2}\sum_{p>0}^{\infty} \left(\frac{\lambda_{p}^{2}\exp(\beta\lambda_{p})}{\left[\exp(\beta\lambda_{p})-1\right]^{2}} + \frac{\omega_{p}^{2}\exp(\beta\omega_{p})}{\left[\exp(\beta\omega_{p})-1\right]^{2}}\right)$$
(124).

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A validity check

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Until now no concrete way has been specified that would test whether a specific calculation met the requirements of the approximation method. At this point it would seem appropriate to develop such a strategy. Since the very foundation of the Bogoliubov method as is being used here is the assumption that there is a large number of the system's constituent particles in the p = 0 mode, then a method of estimating the occupation level of the condensate will now be developed.

The average number of particles in excited modes, $\langle N_{\alpha} \rangle$, can be found from

$$\langle N_{\alpha} \rangle = \frac{Tr \left[e^{-\beta H} \sum_{p \neq 0} \left(a_p^{\dagger} a_p + b_p^{\dagger} b_p \right) \right]}{Tr \left[e^{-\beta H} \right]}$$
(125).

It will be assumed here that the approximate Hamiltonian will be adequate to make an estimate of this result. That being the case, then using the relationships between operators given in (63), (64), (71) and (72) one can write

$$\sum_{p\neq0} \left(a_p^{\dagger} a_p + b_p^{\dagger} b_p \right) = \sum_{p>0}^{\infty} \left\{ -2 + \left(\frac{p^2}{\lambda_p} + \frac{\lambda_p}{p^2} \right) \left(\frac{1}{2} + \alpha_p^{\dagger} \alpha_p \right) + \left(\frac{p^2}{\omega_p} + \frac{\omega_p}{p^2} \right) \left(\frac{1}{2} + \beta_p^{\dagger} \beta_p \right) \right\} \quad (126)$$

Now using

$$\frac{Tr(e^{-\beta H}\beta_{p}^{\dagger}\beta_{p})}{Tr(e^{-\beta H})} = \frac{1}{e^{\beta \omega_{p}} - 1} \frac{Tr(e^{-\beta H})}{Tr(e^{-\beta H})}$$
(127)

and similar results for the other type of quasiparticle operator leads to the expression

$$\langle N_{\alpha} \rangle = \sum_{p>0}^{\infty} \left\{ -2 + \left(\frac{p^2}{\lambda_p} + \frac{\lambda_p}{p^2} \right) \left(\frac{1}{2} + \frac{1}{e^{\beta \lambda_p} - 1} \right) + \left(\frac{p^2}{\omega_p} + \frac{\omega_p}{p^2} \right) \left(\frac{1}{2} + \frac{1}{e^{\beta \omega_p} - 1} \right) \right\}$$
(128).

The thermodynamic functions for the g = 0 case

The thermodynamic functions derived above can also be determined for the g = 0 case. The development of these expressions is so similar to that already done above that only the final results will be listed here. These results are:

$$\Xi_{(o)}(\boldsymbol{\beta}, L, N) = \exp\left(-\boldsymbol{\beta}H_{grd(o)}\right) \prod_{n=2}^{\infty} \left(\frac{1}{1 - \exp\left(-\boldsymbol{\beta}p_n^2\right)} \frac{1}{1 - \exp\left(-\boldsymbol{\beta}\lambda_n\right)}\right)$$
(129),

$$E_{(o)} = H_{grd(o)} + \sum_{n=2}^{\infty} \left(\frac{p_n^2}{\exp(\beta p_n^2) - 1} + \frac{\lambda_n}{\exp(\beta \lambda_n) - 1} \right)$$
(130),

$$P_{(o)} = -\frac{\partial H_{gnd(o)}}{\partial L} + \frac{2}{L} \sum_{n=2}^{\infty} \left(\frac{p_n^2}{\exp(\beta p_n^2) - 1} + \frac{\lambda_n - 2e \frac{p_n^2}{\lambda_n}}{\exp(\beta \lambda_n) - 1} \right)$$
(131),

$$-\frac{\partial H_{grd(o)}}{\partial L} = \frac{1}{L}H_{grd(o)} + \frac{\pi^2 N}{L^3} - \frac{1}{4L}\sum_{n=2}^{\infty}p_n^2 \left\{2 - \left(\frac{p_n^2}{\lambda_n} + \frac{\lambda_n}{p_n^2}\right)\right\}$$
(132),

$$S_{(o)} = \sum_{n=2}^{\infty} \left\{ \ln\left(\frac{\exp(\beta p_n^2)}{\exp(\beta p_n^2) - 1}\right) + \ln\left(\frac{\exp(\beta \lambda_n)}{\exp(\beta \lambda_n) - 1}\right) + \frac{\beta p_n^2}{\exp(\beta p_n^2) - 1} + \frac{\beta \lambda_n}{\exp(\beta \lambda_n) - 1} \right\}$$
(133),

$$C_{L(o)} = \beta^2 \sum_{n=2}^{\infty} \left\{ \frac{p_n^4 \exp(\beta p_n^2)}{\left[\exp(\beta p_n^2) - 1\right]^2} + \frac{\lambda_n^2 \exp(\beta \lambda_n)}{\left[\exp(\beta \lambda_n) - 1\right]^2} \right\}$$
(134).

To complete the parallel development with the $g \neq 0$ case, the expression for the number of

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particles in excited modes is

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$$\langle N_{\alpha} \rangle_{(o)} = \sum_{n=2}^{\infty} \left\{ -\frac{1}{2} + \frac{1}{\exp(\beta p_n^2) - 1} + \frac{1}{2} \left(\frac{\lambda_n}{p_n^2} + \frac{p_n^2}{\lambda_n} \right) \left(\frac{1}{2} + \frac{1}{\exp(\beta \lambda_n) - 1} \right) \right\}$$
(135).

A graphical description of the thermodynamics

The thermodynamic relationships given above were first presented by Craig, Kiang, and Niégawa³⁴. As was done there, a description of the thermodynamic behavior of the system will now be given. The given equations for energy, entropy, pressure and specific heat are rather complicated as they now stand, so the purpose now is to see some of the features that might be buried under this layer of complexity.

As a first step the continuous form of these equations will be examined. The continuous fimit form of the logarithm of the partition function (119) is

$$\ln \Xi = -\beta H_{grd} - \frac{L}{\pi} \int_0^\infty dp \left\{ \ln \left(1 - \exp(-\beta \lambda) \right) + \ln \left(1 - \exp(-\beta \omega) \right) \right\}$$
(136).

With the goal of seeking functional forms, let us first extract part of (136) for further consideration, namely

$$\frac{L}{\pi} \int_0^\infty dp \left\{ \ln\left(1 - \exp\left(-\beta p \sqrt{p^2 + 4cN/L}\right)\right) + \ln\left(1 - \exp\left(-\beta p \sqrt{p^2 + 4gN/L}\right)\right) \right\}$$
$$= \frac{L}{\pi} \int_0^\infty dp \left\{ \ln\left(1 - \exp\left(-\beta \sqrt{\frac{cN}{L}} p \sqrt{\frac{Lp^2}{cN} + 4}\right)\right) + \ln\left(1 - \exp\left(-\beta \sqrt{\frac{cN}{L}} p \sqrt{\frac{Lp^2}{cN} + 4\frac{g}{c}}\right)\right) \right\}$$
$$= \frac{\sqrt{cNL}}{\pi} \int_0^\infty dx \left\{ \ln\left(1 - \exp\left(-c\rho\beta x \sqrt{x^2 + 4}\right)\right) + \ln\left(1 - \exp\left(-c\rho\beta x \sqrt{x^2 + 4\frac{g}{c}}\right)\right) \right\}$$

$$= \sqrt{cNL} J\left(c\rho\beta, \frac{g}{c}\right)$$
(137).

As the chemical potential of the quasiparticles is zero then the Helmholtz free energy, F, can be determined from the logarithm of the partition function and (88) which gives

$$F = -\frac{1}{\beta}\ln\Xi = Nc\left(\frac{g}{c}\rho + \sqrt{c\rho}\left\{-\frac{4}{3\pi}\left[1 + \sqrt[3]{\frac{g}{c}}\right] + \frac{1}{c\rho\beta}J\left(c\rho\beta,\frac{g}{c}\right)\right\}\right)$$
(138).

From this functional form of the logarithm of the partition function the continuous form of (120) becomes

$$E = -\frac{\partial}{\partial\beta}\ln\Xi = Nc\left(\frac{g}{c}\rho + \sqrt{c\rho}\left\{-\frac{4}{3\pi}\left[1 + \sqrt[3]{\frac{g}{c}}\right] + \frac{\partial}{\partial(c\rho\beta)}J(c\rho\beta,\frac{g}{c})\right\}\right)$$
(139).

The continuous limit version of (121) is

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$$P = -\left(\frac{\partial F}{\partial L}\right)_{\beta} = g\rho^{2} + \sqrt[3]{c\rho} \left\{-\frac{2}{3\pi} \left[1 + \sqrt[3]{g}\right] + \sqrt{c\rho\beta} \frac{\partial}{\partial(c\rho\beta)} \left[\frac{1}{\sqrt{c\rho\beta}} J(c\rho\beta, \frac{g}{c})\right]\right\}$$
(140).

For the entropy the continuous version of (123) is

$$S = \beta(E - F) = \frac{Nc}{\sqrt{c\rho}} (c\rho\beta)^2 \frac{\partial}{\partial(c\rho\beta)} \left[\frac{1}{c\rho\beta} J \left(c\rho\beta, \frac{g}{c} \right) \right]$$
(141).

Finally, the continuous form of the specific heat (124) is

$$C_{L} = \left(\frac{\partial E}{\partial T}\right)_{L} = \frac{Nc}{\sqrt{c\rho}} (c\rho\beta)^{2} \frac{\partial^{2}}{\partial (c\rho\beta)^{2}} J\left(c\rho\beta, \frac{g}{c}\right)$$
(142).

Examining the above continuous forms will show that the energy, entropy and specific heat

are all proportional to N as extensive functions should be. Pressure, being intensive, is not proportional to N. All of the functions, E/N, S/N, C_L/N , and P have the general functional form of $f(\rho, c, g, c\rho\beta)$. One other interesting feature that can be picked out is that the temperature dependence appears through $c\rho\beta$. Before moving on it should be pointed out is that the above method of going to the continuous limit form can be applied to the thermodynamic functions derived for the g = 0 case. Doing so produces the same results as given above if g is set equal to zero in the results.

Next an examination of the characteristics of the thermodynamic functions will be made using numerical techniques. To do this specific values of the parameters have to be chosen. After each calculation a check will be made to ensure that the occupation level of the condensate is large for the particular selection of parameters. As the numerical results will be presented graphically, each graph will be marked at the points where calculations show 95% of the system's particles are still in the condensate. If not marked, then all points on the graph have condensate occupation levels exceeding 95%. The parameters g and c that determine the strength of the interactions enter the calculation (128) of the number of particles not in the p = 0 mode in a symmetrical fashion. However, the original Hamiltonian (1) does not show this same symmetry as g + c is the strength of the interactions between like particles and g - c is the strength of the interactions between unlike. Referring back to the condition for the validity of E_{BKS} after (87) which was derived from the work of Lieb and Liniger, namely (g + c)L < N, and inserting L_o from (91) leads to the relationship between g and c of

$$9\pi^2 \left(\frac{g}{c}+1\right) \left(\frac{g}{c}\right)^2 < 4 \left(1+\left(\frac{g}{c}\right)^3+\left(\frac{g}{c}\right)^{\frac{3}{2}}\right)$$
(143).

This condition will be met if g/c < 0.2. Now it could be argued that choosing a smaller value of L than that of L_o would ease this restriction on the magnitude of g. Indeed L could be so chosen as to make g many times larger than c.

There are two reasons for not taking this approach here. First, unless $g \ll c$, the leading term in the expression for L *th E* and *P* which is gN^2/L dominates the calculated values to such an extent that the effects of temperature variations are suppressed. In order to get the effects of increased temperatures to show up the condensate must be depleted beyond the point at which the approximation method is considered valid. Not being able to see the effects of temperature makes for uninteresting thermodynamics. The second reason hinges on the fact that if g > c then there are no attractions between particles, only repulsions as determined by g + c and g - c. Nevertheless the mathematical form of H_{grd} is such that a minimum can be achieved even if g > c. So the physics requires g < c if H_{grd} is to be applicable and the desire to see interesting thermodynamic effects requires g < c.

The first function to be dealt with numerically will be pressure. Mathematically for large L the expression for pressure given in (121) becomes, in the limit,

$$P = \frac{8}{L} \sum_{p>0}^{\infty} \frac{p^2}{\exp(\beta p^2) - 1} \to \frac{4}{\pi} \int_0^{\infty} \frac{p^2 dp}{\exp(\beta p^2) - 1} = \frac{\zeta(\frac{3}{2})T^{\frac{3}{2}}}{\sqrt{\pi}}$$
(144).

The pressure in the g = 0 case also becomes this value in the limit of large L. For small enough L the pressure for both $g \neq 0$ and g = 0 is positive. For the ground state F = E

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where F is the Helmholtz potential and, as $P = -\left(\frac{\partial F}{\partial L}\right)_r$, then the zero for pressure will be

at the point where there is a minimum in the ground state energy. This point, L_o , has already been shown to exist. With these features a plot of an isotherm for the ground state would be expected to have positive pressure values for small L which would diminish with increasing L to zero pressure at L_o . Since for large L the pressure curve approaches the value zero (for the ground state as T = 0), then the pressure curve must approach this zero from negative values - there being only one extremum in the ground state energy. With an increase in temperature the asymptotic approach to the positive value of the pressure for large L as given in (144) would require the pressure curve to cut the P = 0 axis at two points at least for temperatures low enough and hence close to the ground state.



In Figure 14 the results of plotting the ground state isotherm show the features of the pressure graph as described above. The pressure curve is asymptotically approaching the horizontal axis from below at the larger values of L in the plot. Larger values of L would have to be used before the occupation level of the condensate dropped below the 95% level. At the temperature chosen, T = 0, the Helmholtz potential is the ground state energy



so the plot could just as well be considered to be of the ground state energy.

The next plot, Figure 15, is again one of pressure and the Helmholtz potential but this time at a temperature of T = 100. The graphs do not look very different from those in the previous plot but note that the condensate occupation level is now less than 95% for lengths larger than about L = 75. For a given g and c the occupation level of the

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condensate is inversely related to L and T.

The higher temperature of Figure 16 shows in a more readily apparent fashion the effect of temperature. To the eye it is as if the pressure curve has been moved higher up the vertical axis with its shape basically the same as for lower temperatures. The feature of the pressure curve crossing the horizontal axis in two places is also shown. Note that the Helmholtz

potential has two extrema, one at each of the points where P = 0. Of course, since $(\partial F/\partial L)_T = -P$, the extrema should occur at these points. However, the fact that the numerical results show the correct general behavior implies that the approximation has produced the correct shape for the function F = E - TS in spite of the insensitivity to the entropy of the condensate.



If the temperature is increased even further then the situation shown in Figure 17 will be reached. Here there is only one point of contact between the pressure curve and the



horizontal axis. Note that the Helmholtz potential correctly reflects this situation by having

an inflection point at the length where $(\partial F/\partial L)_{\tau} = 0$.

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Increasing the temperature even further does continue to move the pressure curve upward so that eventually, as shown if Figure 18, the pressure curve does not cut the horizontal axis at all. As is also shown in the figure the Helmholtz potential continues to behave as it should in showing no point with a horizontal slope. In those plots of pressure versus temperature where the Helmholtz potential shows a minimum, this minimum indicates a point of stability for the system. The length at which this minimum occurs would be the size the system could "support" itself at without the need of constraints. For the ground state this length was referred to as L_o but now the meaning of L_o will be extended to cover the stable length at other temperatures. The maximum in the Helmholtz potential indicates that the other length at which P = 0 is not thermodynamically stable. Of course, the section of the pressure curves where $(\partial P/\partial L)_{\tau} > 0$ indicates thermodynamic instability and more will be said about this region later.

So far no plot has given the behavior of C_L . Figure 19 is such a plot. Three different values of L are used and, for the range of temperatures chosen, no point has a condensate occupation level of less than 95%. Nothing in the shape of the graphs suggests any unusual features in the system. The graph for L = 20 is of the same basic form as those for the other two lengths in spite of the fact that L = 20 is in the thermodynamic unstable region of the isotherm. The requirement that $C_L > 0$ for stability is met by all points on the graphs.



Figure 19 - Plot of C_L versus T for three values of L. Other parameters are c = 0.1, $g = 2 \times 10^{-5}$, and $N = 10^{6}$. No points are below the 95% condensate occupation level.

All the plots to this point have had the number of particles set to $N = 10^6$. This parameter value was chosen, as were the values for g and c, because it allows the showing of the features of the isotherms while staying within the restrictions required by the approximation method. In addition to this aspect is that the choice of parameter values also kept the computing time down to convenient levels. An examination of (128) will show that if the value of N was increased by some factor and at the same time the values of g and c were

decreased by the same factor then N_{ex} would not be affected. However, the percentage of particles in excited states would diminish because of the increase in N. Such new values of g, c, and N would also not change the values of entropy and specific heat. However, both pressure and entropy have leading terms of gN^2/L and would thus not remain at the same values with the new parameters. On the other hand, since the chosen value of g in the plots is so much smaller than c, the effect of g in the summations is dominated by the c terms. Thus if g was reduced not by the factor that N was increased by but by that factor squared then the leading term in both energy and pressure calculations would be unchanged. Carrying out such a process would enable the increasing of N to larger values and produce plots that are visually identically to the ones so tar presented. The decrease in the percentage of excited particles at a given length would enable the plots to meet the "cutoff" at greater values of L but there is little value in this as the plots already presented have the 95% cutoff well into the thermodynamically unstable region.

Figure 20 shows the general effect on the shape of the isotherms of varying the parameter g. The 95% cutoff is at about the same value of L for all three graphs. The value of L_o decreases with a decrease in g but this behavior is quite consistent with the L_o already determined for the ground state in the continuous limit. For the periodic boundary value case the decrease in L_o continues as g is decreased until the system goes into collapse at g = 0. As already mentioned this collapse at g = 0 can be prevented with the introduction of Dirichlet boundary conditions and some plots illustrating this feature will be given



shortly.

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Finally, the effect on the general shape of the isotherm when the parameter c is varied is given in Figure 21. Again from the knowledge of L_o for the ground state, it is now surprising to see that there is an inverse relationship between L_o and c. As in Figure 20, the decrease in L_o is accompanied by a deeper minimum in the isotherm and a steeper slope to the



isotherm in the region $L < L_o$.

The behavior of the g = 0 system with Dirichlet boundary conditions is very similar to that of the $g \neq 0$ (periodic boundary conditions) already portrayed in the graphs given to this point. Figure 22 gives the isotherm for two different values of T for the g = 0 system. The main difference for the parameters chosen is the greater "insensitivity" to temperature



compared to the previous plots.

One other comparison of interest can be done between the two systems, g = 0 and $g \neq 0$, and that is how L_o is affected by N. In the ground state discussion the L_o dependence was determined by going to the continuous limit forms of the ground state energy. In Figure 23 it is shown that the same behavior persists when using the summation forms, solved numerically, and at finite temperatures. It is to be restated that the different behaviors

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between the two systems is boundary condition dependent.

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CONCLUDING REMARKS

The focus of interest here has been an effort to gain some insight into the physical behavior of the one dimensional system of bosons governed by the Hamiltonian

$$H(c,g,N) = -\sum_{i=1}^{N} \frac{\partial^{2}}{\partial x_{i}^{2}} + 2\sum_{i < j=1}^{N} (g + ce_{i}e_{j})\delta(x_{i} - x_{j})$$
(145).

This Hamiltonian and its parameters are described in Chapter 1. That chapter is also used to put forward the motivation for examining this particular Hamiltonian. After having established some rationale for pursuing the topic then the second chapter was used to review some of the previous work of others on various forms of this Hamiltonian. The third and fourth chapter then presented the material that is new and provides the rationale for this thesis. At this point it is worthwhile to present a brief summary of the new material.

Working in the parameter space $0 \le g \ll c$ an approximate Hamiltonian was developed based on the Bogoliubov perturbation method. Using this new approximate Hamiltonian it was then straightforward to develop a new expression for the ground state energy. This ground state energy approximation was shown to be consistent with the approximation, based on the variational method, of Blum, Koltun and Shapir.

One of the features of the ground state was the prediction of system collapse when g = 0. To show that this prediction was probably not a result of a limitation in the approximation method the same variational method setting of Blum, Koltun and Shapir was used. Whereas Blum, Koltun and Shapir had built their result on an approximation of the work of Lieb and Liniger, we used the exact results of the Lieb and Liniger work.

To prevent the collapse of their g = 0 system Blum, Koltun and Shapir had introduced in an *ad hoc* manner the term $\pi^2 N/L^2$. By modifying the boundary conditions under which the approximate Hamiltonian was derived from periodic to Dirichlet boundary conditions we were able to show that this term, $\pi^2 N/L^2$, was a natural consequence of the Dirichlet boundary conditions. Then having two forms of the approximate Hamiltonian, one from using periodic boundary conditions and the other from Dirichlet boundary conditions, we developed the thermodynamics of the two systems - the one to apply to the g > 0 situation and the other to the g = 0.

Since the method of solution presented has been an approximation method it seemed important to establish some legitimacy to the results. Chapter 2 contains some important material from which the argument for the reasonableness of the solution can be built. With this intent in mind let us return for the moment to the free boson system. The Hamiltonian reduces to the free particle system if the strength of interaction parameters are reduced to zero. It would be expected that any solution to the Hamiltonian would contain a description of the free particle system simply by setting g = c = 0. The expressions for energy, pressure, etc., derived using the approximation will produce agreement with the free case at a temperature of zero but not at finite temperatures. The source of the disagreement is the chemical potential. In the thermodynamic development of the approximation in Chapter 4 the point of view used was since the approximate Hamiltonian (73) is in terms of quasiparticles, whose chemical potential is zero, then the derivation of the grand partition function could be based on this point. This quasiparticle point of view may provide some rationale for setting μ to zero but, in the end, it still does not provide the correct answer. Working from the point of view of the real particles the $H - \mu N$ factor in the partition function proved more than nettlesome unless one assumed that μ was small enough to be ignored. Of course, even so, one is still forced to use the approximate Hamiltonian. Whichever of the two points of view is taken leads to the same requirement for getting a solution - the classical potential is small enough to be ignored. Some of the material of Chapter 2 was directed toward substantiating the idea that, at least for the non interacting boson gas, ignoring μ produced a good approximation under suitable conditions.

Another important foundation stone for the approximation method was the required presence of a Bose-Einstein condersate. Again material in Chapter 2 was presented to show that, here again for a non-interacting gas, there is such a condensate but again under suitable conditions. Thus the argument is that if a free Bose gas can have a condensate and be well approximated as having $\mu = 0$, then turning on weak interactions should not change these features. The restrictions that arise out of this are that the temperature must be low and the system size must be finite. It is pointed out in Chapter 4 that finite size does not necessarily mean small size for a way of arranging parametere to give large systems while remaining within the scope of reliability of the approximation is given there.

By switching boundary conditions a very different behavior in the dependence of ground state size L_o on N is established as given in Figure 23. Since Blum, Koltun and Shapir were doing work involving the directed Feynman paths as described in Chapter 1, they were interested in the large N behavior of the system when g = 0. However, the $\pi^2 N/L^2$ term is not immune to collapse in the thermodynamic limit.

Another feature of interest involving the g and c parameters is their symmetric role in the expressions for entropy (123), specific heat (124), $\langle N_{ex} \rangle$ (128), and $G_a(x-y)$ in (109). Such symmetry is not present in the Hamiltonian but an explanation for it can be found in the alternate derivation of an approximate Hamiltonian that led to (112). It can be noted from (113) that, unlike the λ_p of (74), the λ_p^o of (113) is dependent on both g and c. The factors in λ_p^o appear in the expressions for entropy, specific heat, etc., derived in this alternate formulation, in such a way that the symmetry between g and c is no longer apparent from a visual examination of the equations. For example the specific heat expression is

$$C_{L}^{o} = 2\beta^{2} \sum_{p \geq 0}^{m} \left(\frac{\left(\lambda_{p}^{o}\right)^{2} \exp\left(\beta\lambda_{p}^{o}\right)}{\left[\exp\left(\beta\lambda_{p}^{o}\right) - 1\right]^{2}} + \frac{\left(\omega_{p}^{o}\right)^{2} \exp\left(\beta\omega_{p}^{o}\right)}{\left[\exp\left(\beta\omega_{p}^{o}\right) - 1\right]^{2}} \right)$$
(146)

which, although it has the same general form as the specific heat expression of (124), is not symmetric in g and c. However, both λ_p^o and ω_p^o are dependent on N_o which in turn is

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dependent on g and c. The end result of these relationships is that the numerical calculation of specific heat, and for that matter the other functions as well, produces essentially the same numerical results especially in the region where the condensate occupancy exceeds 90%. This agreement shows that the source of the apparent symmetry between g and c lies in the interconnection between N_c and the parameters g and c. In the parameter range where the approximations of (54) are valid this symmetry would be present. However, as the requirement here is $g \ll c$, this symmetry is mathematical and not physical.

The isotherms plotted in several of the Figures in Chapter 4 indicated some interesting aspects of the system behavior. It was shown, at least for the parameter space $g \ll c$, that the system has a stable size L_o if the temperature is low enough. However, a perplexing aspect of the isotherm is the region where $(\partial P/\partial L)_{\tau} > 0$. Perhaps the first thing that springs to mind is a phase change and the Maxwell construction but the shape of the curve is not correct for this approach. Nor can this region be attributable to the assumption of $\mu = 0$ in the partition function because the ground state also has this region.

Attributing the shape of the curve in the unstable region to the dropping of terms in the approximation also seems unlikely. Going to the expression for the ground state energy derived by Blum, Koltun and Shapir (85) with the Bogoliubov approximation form (86) one can show that their ground state isotherm also has a similar region where $(\partial P/\partial L)_T > 0$ for

$$L > \frac{8\pi^2 g^2}{(c+g)^3} N$$
 (147).

Here g and c can be chosen in such a way as to put the Bogoliubov form (86) into the region of Figure 9 where the approximation is very accurate. Thus it would seem that this region of instability is characteristic of the system.

As to what the nature of this instability is remains unknown. The equilibrium thermodynamics used offers no answers. This instability does not show up in the specific heat as (134), the expression for specific heat, contains only positive terms and thus C_L can never be negative. The single particle density function and the pair correlation function of Chapter 3 also did not show any change that would point to entering a region of instability when the parameter L was increased to take the system from a region of stability to one of instability. The contribution of the peculiarities of one-dimensional systems in general and the finite system size used here are felt to be at the root of this interesting behavior. However, the method used here does not seem to be able to substantiate this speculation and it will need a different approach in the future to sort it out.

APPENDIX

Comments on the numerical work

The computer program used to generate the numerical results was written using the Borland® C⁺⁺, Version 2, programming platform. As the computer used for executing the program was of the IBM® clone variety, then some of the library functions used in the program are only suitable for this computing environment. Almost all of the program uses features that are of the C programming language with very little taken from C⁺⁺.

The listing of the computer program that is to follow is divided into five sections but only for reasons of economy of time in recompiling as the program grew and for cutting down paper consumption as new listings were sent to hard copy. As the program is the end product of a project that not only grew with time but also had many edits as various avenues were explored, the listing will show some vestigial and some "left over" areas. These areas could have been revised and polished but since it was a single user program and time was precious the attitude of "If it ain't broken, don't fix it." was taken to avoid the strong possibility of introducing bugs that occurs whenever software is altered.

Some additional results

In Chapter 3 an alternative way of developing the Bogoliubov approximation was presented in developing the results for the pair correlation functions. The resulting Hamiltonian was given in (115) and (116) and the form of the specific heat was given in (146). Since routines will be presented that compute other functions in this alternate version then, to be complete, the remainder of these forms will now be given.

$$E^{\circ} = H_{grd}^{\circ} + 2\sum_{p>0} \left(\frac{\lambda_{p}^{\circ}}{\exp(\beta \lambda_{p}^{\circ}) - 1} + \frac{\omega_{p}^{\circ}}{\exp(\beta \omega_{p}^{\circ}) - 1} \right)$$
(148)

,

$$P^{\circ} = -\frac{\partial H_{gnd}^{\circ}}{\partial L} + \frac{4}{L} \sum_{p>0} \left(\frac{\lambda_{p}^{\circ} - \frac{e_{o}' \lambda_{p}^{\circ}}{p^{2} + 4e_{o}'} - \frac{(2e_{o} + e_{o}')(p^{2} + 4e')}{\lambda_{p}^{\circ}}}{\exp(\beta \lambda_{p}^{\circ}) - 1} \right) + \frac{4}{L} \sum_{p>0} \left(\frac{\omega_{p}^{\circ} - \frac{e_{o}' \omega_{p}^{\circ}}{p^{2} + 4e_{o}'} - \frac{(3e_{o}')(p^{2} + 4e')}{\omega_{p}^{\circ}}}{\exp(\beta \omega_{p}^{\circ}) - 1} \right)$$
(149)

$$S^{\circ} = 2\sum_{p \ge 0} \left\{ \ln \left(\frac{\exp(\beta \lambda_{p}^{\circ})}{\exp(\beta \lambda_{p}^{\circ}) - 1} \right) + \ln \left(\frac{\exp(\beta \omega_{p}^{\circ})}{\exp(\beta \omega_{p}^{\circ}) - 1} \right) \right\}$$

$$+ 2\sum_{p \ge 0} \left(\frac{\exp(\beta \lambda_{p}^{\circ})}{\exp(\beta \lambda_{p}^{\circ}) - 1} + \frac{\exp(\beta \omega_{p}^{\circ})}{\exp(\beta \omega_{p}^{\circ}) - 1} \right)$$
(150)

$$\langle N_{ex}^{\circ} \rangle = \sum_{p \ge 0} \left\{ -2 + \left(\frac{p^2 + 4e'_o}{\omega_p^{\circ}} + \frac{\omega_p^{\circ}}{p^2 + 4e'} \right) \left(\frac{1}{2} + \frac{1}{\exp(\beta \omega_p^{\circ}) - 1} \right) \right\}$$

$$+ \sum_{p \ge 0} \left(\frac{p^2 + 4e'_o}{\lambda_p^{\circ}} + \frac{\lambda_p^{\circ}}{p^2 + 4e'} \right) \left(\frac{1}{2} + \frac{1}{\exp(\beta \lambda_p^{\circ}) - 1} \right)$$

$$(151)$$

$$H_{grd}^{o} = \frac{gN_{o}^{2}}{L} + 2\sum_{p>0} \left\{ -p^{2} - 2e_{o} - 6e_{o}' + \frac{1}{2} \left(\lambda_{p}^{o} + \omega_{p}^{o}\right) \right\}$$
(152)

A list of the functions in the program

Function name	Applicable equation
ener	120 and 130
press	121 and 131
entropy	123 and 133
spht	124 and 134
hgrd	78 and 103
ratio	128 and 135
spdf	109
nzero	151
hgrdno	152
energyno	148
pressureno	149
entropyno	150
nzero	151
lieb	42, 43, and 44
nex, chem	26
freepress	34

freeenergy	37
freecntropy	38

First section of program

This section controls the input and output from the program. For most options the output is sent to a file from where it is picked up by the commercial software Microsoft® Excel for plotting purposes.

#include <conio.h>
#include <stdio.h>
#include <math.h>

double c,g,temp,bign; double pi,pi2,rt2; int gflag,errcodes=8,error_no[8]={0,0,0,0,0,0,0,0,0};

double ener(double ell); double press (double ell); double entropy (double ell); double ratio (double ell); double spht (double ell); double hgrd (double ell); int spdf (double ell, double step); void probcheck(int flag); void setwindow(int ulc,int ulr,int lrc,int lrr); void restorescrn(int flag); double nzero(double ell,double trial); double hgrdno(double ell,double num); double pressureno(double ell,double num); double energyno(double ell,double num); double entropyno(double ell,double num); void lieb(double lamda,int n,double *gamma,double *egamma); double nex(double tp,double mu,double ell); double chem(double tp,double mu,double ell); double freepress(double tp,double ell,double mu); double freeenergy(double tp,double ell,double mu); double freeentropy(double tp,double ell,double mu);

```
int error_check(int signal)
  {int flag,n;
```

```
flag = 0;
```

The second

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for(n=0;n<errcodes;n++)
{if(error_no[n]!=0)
        {flag++;
        if(!signal)
        {cprintf("\r\nError code %d",n);
        error_no[n] = 0;}
    }
    if((flag) && (!signal))
    {cprintf("\r\nPress any key to continue.");
        getch();}
return flag;
}</pre>
```

main()

{double x,y,z,xx,xxx,ell,ell_1,ell_2,pp,ti,tf,tp,tinc,num,gib,gibo;

```
int again,again_1,j,k,m,n,ni,nf,tni,tnf,f_flag,flag,c_flag;
char choice;
FILE *f ptr;
```

pi=3.141592653589793; pi2=pi*pi; rt2=sqrt(2.0); again=1; c=0.1; g=0.00002; gflag=1; temp=100.0; bign=1.0e6; textmode(C80); textbackground(BLUE); textcolor(YELLOW); while (again) {clrscr(); $cprintf("\r 1 g = \%10.5e, c = \%10.5e", g, c);$ cprintf("rn 2 T = %7.4f, N = %10.2e", temp, bign);cprintf("\r\n 3 Pressure"); cprintf("\r\n 4 Specific heat and entropy"); cprintf("\r\n 5 General (N)"); cprintf("\r\n 6 General (No)"); cprintf("\r\n 7 No"); cprintf("\r\n 8 Single particle density"); cprintf("\r\n 9 Lieb energy"); cprintf("\r\n 0 Free Bose gas - No"); cprintf("\r\n A Free Bose gas - Po"); cprintf("\r\n B Exit\r\n"); choice=getch();

```
switch (choice)
 \{case '1': again 1=1;
            while (again_1)
              {clrscr();
              cprintf("1 Change g from %10.5e\r\r\n",g);
              cprintf("2 Change c from %10.5e\r\r\n",c);
              cprintf("3 Exit\r\r\n");
              cl.oice=getch();
              switch(choice)
               {case '1':cprintf("Enter new value for g. ");
                           scanf ("%le",&g);
                           break;
                case '2':cprintf("Enter new value for c. ");
                           scanf ("%le",&c);
                           break:
                case '3':if (g==0.0) gflag=0;
                           else gflag = 1;
                           again 1=0;
                           break;
                }
              }
            break;
   case '2': again 1=1;
            while (again_1)
             {clrscr();
              cprintf("1 Change T from %7.4f\r\r\n", temp);
              cprintf("2 Change N from %10.2e\r\r\n", bign);
              cprintf("3 Exit\r\r\n");
              choice=getch();
              switch(choice)
               {case'1':cprintf("Enter new value for T. ");
```

K

```
scanf ("%le", &temp);
                   break:
            case'2':cprintf("Enter new value for N. ");
                   scanf ("%le",&bign);
                   break;
            case'3':again 1=0;
                   break;
            }
          }
        break:
case '3':cprintf(" Pressure starting at L = ");
        scanf("%le",&ell);
        cprintf(" Ending at L = ");
        scanf("%le",&ell_1);
   cprintf(" Increment = ");
   scanf("%le",&ell 2);
        if(NULL==(f ptr=fopen("c:\\dad\\pressure.dat", "w+t")) error no[0]=1;
        if(error check(0)) break;
        setwindow(45,1,79,25);
        f flag = 0;
        num = bign;
        while (ell<=ell 1)
         {xxx = press(chi);
          num = nzero(e^{t}, num);
          if(error check(0)) break;
          xx = pressureno(ell,num);
          fprintf(f_ptr,"%12.5f
                                                     %12.5e\n",ell,xxx,xx);
                                      %12.5e
          cprintf("\r\n%12.5f
                                   %12.5e",ell,xx);
          cll += ell 2;
          if(kbhit())
           \{f f f lag = 1;
```

```
getch();
            break;
             }
          }
        fclose(f_ptr);
        restorescrn(f_flag);
        break;
case '4':cprintf("Enter start value for L. ");
        scanf("%le",&ell);
        xx=temp;
        cprintf("Enter initial value for T. ");
        scanf("%le",&temp);
        cprintf("Enter increment for T. ");
        scanf("%le",&ell 1);
        cprintf("Enter final value for T. ");
        scanf("%le",&ell 2);
        if((f_ptr=fopen("C:\\dad\\tuxermal4.dat", "w+t"))==NULL) error no[0]=1;
        if(error check(0)) break;
        while (temp \le 2)
         {fprintf(f_ptr,"%10.2f
                                      %12.5f",temp,entropy(ell));
          fprintf(f ptr,"%12.5f\n",spht(ell));
          cprintf("%10.2f\r\n",temp);
          temp+=ell 1;
          }
        fclose(f ptr);
        temp=xx;
        cprintf("Finished\r\n");
        choice=getch();
        break;
case '5':cprintf(" General (N) - starting at L = ");
        scanf("%le",&ell);
```

```
cprintf(" Increment = ");
        scanf("%le",&ell 1);
        cprintf(" Ending at L = ");
        scanf("%le",&eil_2);
        if(NULL==(f_ptr=fopen("c:\\dad\\general.dat","w+t"))) error_no[0]=1;
        if(error check(0)) break;
        setwindow(45,1,79,25);
        f flag = 0;
        while (ell<=ell 2)
         {x = ener(ell);}
          y = press(ell);
          z = entropy(ell);
          xx = ratio(ell)*100;
          fprintf(f_ptr,"%12.2f
                                      %15.6e
                                                     %15.6e",ell,x,y);
          fprintf(f ptr,"
                              %15.6e
                                              %8.2f\n",z,xx);
          cprintf("\r\n%12.2f",ell);
          ell += ell 1;
          if(kbhit())
           {f_flag = 1;
            getch();
            break;
            }
          }
        fclose(f_ptr);
        restorescrn(f flag);
        break;
case '6':cprintf(" General (No) - starting at L = ");
        scanf("%le",&ell);
        cprintf(" Increment = ");
        scanf("%le",&ell_1);
        cprintf(" Ending at L = ");
```

```
scanf("%le",&ell_2);
        if(NULL==(f ptr=fopen("c:\\dad\\genern0.dat", "w+t"))) error no[0]=1;
        if(error check(0)) break;
        setwindow(45,1,79,25);
        f flag = 0;
        num = bign;
        while (ell<=ell 2)
          {num = nzero(ell,num);
          if(error check(0)) break;
          x = energyno(ell,num);
          y = pressureno(ell,num);
          z = entropyno(ell,num);
          fprintf(f_ptr,"%12.2f
                                                     %15.6e",ell,x,y);
                                      %15.6e
          fprintf(f ptr,"
                              %15.6e
                                             %12.1fe\n",z,num);
          cprintf("\r\n%12.2f",ell);
          ell += ell 1;
          if(kbhit())
           {f flag = 1;}
            getch();
            break;
            }
          }
        fclose(f ptr);
        restorescrn(f flag);
                                                  ٠.,
        break;
case '7':cprintf(" No for L = ");
        scanf("%le",&ell);
        cprintf(" Starting at T = ");
        scanf("%le",&ti);
        cprintf(" Ending at T = ");
        scanf("%le",&tf);
```

```
cprintf(" Increment = ");
        scanf("%le",&tinc);
       if(NULL==(f ptr=fopen("c:\\dad\\nzero.dat","w+t"))) error_no[0]=1;
        if(error check(0)) break;
        setwindow(45,1,79,25);
       f_flag = 0;
        xx = temp;
        temp = ti;
        num = bign;
        while (temp<=tf)
         {xxx = nzero(ell,num);
         if(error check(0)) break;
         fprintf(f_ptr,"%12.2f
                                     %10.1f\n",temp,xxx);
          cprintf("\r\n%12.2f %10.1f",temp,xxx);
          temp += tinc;
          num = xxx;
          if(kbhit())
           {f flag =1;
            getch();
            break;
            }
          }
        fclose(f ptr);
        temp = xx;
        restorescrn(f flag);
        break;
case '8':cprintf(" Single particle density function.\r\n");
        cprintf(" Enter value for L. ");
        scanf("%le",&ell);
        cprintf(" Enter number of intervals in L. ");
        scanf("%d",&m);
```

```
ell 1 = ell/m;
       probcheck(spdf(eil,eil 1));
        break:
case '0':cprintf("(Lieb) Enter value of lamda. ");
        scanf("%le",&x);
        cprintf("Enter number of intervals. ");
        scanf("%d",&j);
        lieb(x,j,\&y,\&z);
        cprintf("\r\ngamma = %15.6fe(gam) = %15.6f",y,z);
        getch();
        break;
case 'A':
case 'a':cprintf("Free Bose gas - enter L. ");
        scanf("%le",&ell);
        cprintf(" Starting at T = ");
        scanf("%le",&ti);
        cprintf(" Ending at T = ");
        scanf("%le",&tf);
        cprintf(" Increment = ");
        scanf("%le",&tinc);
        if(NULL==(f ptr=fopen("c:\\dad\\freebose.dat", "w+t"))) error no[0]=1;
        if(error check(0)) break;
        fprintf(f_ptr,"L
                              N\n%10.1f
                                             10.0f(n), ell, bign);
        fprintf(f ptr,"T
                              No
                                     No(mu=0)
                                                     No+Nex
                                                                    mu\n");
        setwindow(45, 1, 79, 25);
        f flag = 0;
        while ((ti<=tf)&&(!f flag))
         \{xxx = chem(ti,ell);
         if(error check(0)) break;
         xx = bign-nex(ti, 0.0, ell);
         x = 2.0/(exp(-xxx/ti)-1.0);
```

```
y = x + nex(ti, xxx, ell);
          fprintf(f_ptr,"%12.2f
                                                     ",ti,x);
                                      %10.1f
          fprintf(f ptr,"%10.1f
                                      %10.1f
                                                      %12.6e\n",xx,y,xxx);
          cprintf("\r\n%12.2f %10.1f",ti,x);
          ti += tinc;
          if(kbhit())
            {f flag =1;
            getch();
            break;
            }
          }
        fclose(f_ptr);
        restorescrn(f_flag);
        break;
                                                                     •
case 'B':
case 'b':cprintf("Free Bose gas - isotherm 0, isochore 1 ");
        scanf("%d",&c flag);
        if(!c flag)
         {cprintf("Enter value of T ");
          scanf("%le",&tp);
          cprintf("Starting at L = ");
          scanf("%le",&ell);
          pp = ell;
          cprintf("Ending at L = ");
          scanf("%le",&x);
          cprintf("Increment in L = ");
          scanf("%le",&y);
          }
        else
         {cprintf("Enter value of L ");
          scanf("%le",&ell);
```

```
cprintf("Starting at T = ");
  scanf("%le",&tp);
  pp = tp;
  cprintf("Ending at T = ");
  scanf("%le",&x);
  cprintf("Increment in T = ");
 scanf("%le",&y);
  }
if(NULL==(f ptr=fopen("C:\\dad\\freepres.dat", "w+t"))) error no[0]=1;
if(error check(0)) break;
setwindow(45,1,79,25);
f flag = 0^{\circ}
fprintf(f ptr,"N\n%10.0f\n\n",bign);
fprintf(f ptr,"L
                      T
                                     Pmu
                                             Po
                                                     ");
                              in U
fprintf(f ptr,"Emu
                      Eo
                              Smu
                                      So
                                             No
                                                     ");
fprintf(f ptr,"G
                                      mugo\n");
                      Go
                              mug
while((pp<=x)&&(!f flag))
 {xx = chem(tp,ell);}
 if(error check(0)) break;
 fprintf(f_ptr,"%12.2f
                              %12.2f%12.7f",ell,tp,xx);
  xxx = freepress(tp,ell,xx);
  z = freepress(tp,ell,0.0);
 fprintf(f ptr,"%12.2f
                              %12.2f",xxx,z);
  xxx = free energy(tp,ell,xx);
  z = freeenergy(tp,ell,0.0);
 fprintf(f_ptr,"%12.2f
                              %12.2f",xxx,z);
 xxx = freeentropy(tp,ell,xx);
 z = freeentropy(tp,ell,0.0);
 fprintf(f_ptr,"%12.2f
                              %12.2f<sup>"</sup>,xxx,z);
 xxx = 2.0/(exp(-xx/tp)-1.0);
  gib = freegibbs(tp,ell,xx);
```

```
gibo = freegibbs(tp,ell,0.0);
                 fprintf(f_ptr,"%12.0f
                                              %12.2f%12.2f",xxx,gib,gibo);
                 fprintf(f ptr, "%12.6f
                                              %12.6f\n",gib/bign,gibo/bign);
                 cprinti("\r\n%12.2f %12.2f",ell,tp);
                 if(!c_flag)
                   \{ell += y;
                    pp = ell;
                    }
                  else
                   {tp += y;
                    pp = tp;
                    }
                  if(kbhit())
                   \{f f a = 1;
                    getch();
                    break;
                    }
                  }
                fclose(f_ptr);
                restorescrn(f_flag);
                break;
       case 'C':
       case 'c':again=0;
                break;
       }
   }
void probcheck(int flag)
 {switch(flag)
  {case 1:cprintf(" Could not open file.");
```

}

break;

```
case 2:cprintf(" Convergence too slow.");
    break;
case 3:cp.rintf(" Could not get memory asked for.");
    break;
case 4:cprintf("\r\nNo has become invalid.");
}
if(flag) getch();
return;
}
```

Second section of program

```
#include <math.h>
```

extern double c,g,bign,pi,pi2,temp,rt2; extern int gflag;

double hgrd (double ell)
{double a,a1,ab,nf,n2,sum,sum2,xx;
double alpha,rtalpha,ee,eep,p,p2;
long int n,lim;

```
if (gflag==0)
    {alpha=2.0*pi2/c/bign/ell;
    rtalpha=sqrt(alpha);
    lim=sqrt(8000.0/alpha);
    sum=0.0;
    sum2=pi2/6.0-1.0;
    for (n=lim;n>1;n--)
      {nf=n;
```

```
n2=nf*nf;
   a1=alpha*n2;
   xx=a1+4.0-rtalpha*nf*sqrt(a1+8.0);
   sum + = xx;
   sum2-=1.0/n2;
   }
 sum+=8.0/alpha*sum2;
 a1=bign/ell*(pi2/ell-c*sum/4.0);
 retuin (a1);
 }
else
 {alpha=2.0*pi/ell;
 lim=sqrt(1000.0*c*bign*ell/pi2);
 sum=0.0;
 sum2=pi2/6.0;
 ee=4.0*c*bign/ell;
 eep=4.0*g*bign/ell;
 ab=(ee+eep)/4.0;
 for(n=1;n<=lim;n++) sum2-=(1.0/n)/n;
 for(n=lim;n>0;n--)
   {p=alpha*n;
   p2=p*p;
   sum + = -p2-ab+0.5*p*(sqrt(p2+ee)+sqrt(p2+ee));
   }
 sum-=bign*bign*(c*c+g*g)/4.0/pi2*sum2;
 a1=bign*bign*g/ell+2.0*sum;
 return (a1);
 }
```

}

```
double spht (double ellv)
{double alpha,sum,ce,cep,p,p2,a,b,pa,pb,betapa,betapb,a1,a2;
long int nmin,lim,n;
```

```
if (temp==0.0) return (0.0);
alpha=2.0*pi/ellv;
nmin=1.0;
if(gflag==0)
 {alpha/=2.0;
 nmin=2;
  }
sum=0.0;
ee=4.0*c*bign/ellv;
eep=4.0*g*bign/ellv;
a=0.5*(sqrt(eep*eep+5184.0*temp*temp)-eep);
lim=sqrt(a)/alpha;
for(n=lim;n>=nmin;n--)
 {p=alpha*n;
 p2=p*p;
 a=sqrt(p2+ee);
 b=sqrt(p2+eep);
 betapa=p*a/temp;
  betapb=p*b/temp;
 if(betapb>21.0) sum+=betapb*betapb*exp(-betapb);
 clse
   {a1=exp(betapb);
   a2=a1-1.0;
   sum+=betapb*betapb*a1/a2/a2;
    }
 if(betapa<36.0)
   {if(betapa>21.0) sum+=betapa*betapa*exp(-betapa);
```

```
else
{a1=exp(betapa);
a2=a1-1.0;
sum+=betapa*betapa*a1/a2/a2;
}
}
if(gflag==0) return (sum);
return (2.0*sum);
}
```

```
double press (double ell)
{double alpha,a1,a,b,ee,eep,e,ep,p,p2,pa,pb;
double sum,sum2,summ,betapa,betapb;
long int n,lim;
```

```
sum=0.0;
ee=4.0*c*bign/ell;
e=ee/4.0;
eep=4.0*g*bign/ell;
ep=eep/4.0;
alpha=2.0*pi/ell;
if(gflag==0) alpha/=2.0;
if(temp!=0.0)
{if (eep<ee) b=eep;
else b=ee;
a=0.5*(sqrt(b*b+5184.0*temp*temp)-b);
lim=sqrt(a)/alpha;
if(gflag==0)
{for(n=lim;n>1;n-)
```

```
{p=alpha*n;
p2=p*p;
a=sqrt(p2+ee);
pa=p*a;
betapa=pa/temp;
sum.+=p2/(exp(p2/temp)-1.0);
if(betapa<36.0) sum+=(pa-e*p/a)/(exp(betapa)-1.0);
}
sum*=2.0/ell;
}
```

```
else
```

```
{for(n=lim;n>0;n--)
       {p=:lpha*n;
        p2=p*p;
        a=sqrt(p2+ee);
        b=sqrt(p2+eep);
        pa=p*a;
        pb=p*b;
        betapa=pa/temp;
        betapb=pb/temp;
        if(betapb<36.0) sum+=(pb-ep*p/b)/(exp(betapb)-1.0);
        if(betapa < 36.0) sum + = (pa-e*p/a)/(exp(betapa)-1.0);
        }
      sum*=4.0/ell;
      }
  }
summ=0.0;
if (c>g) lim=10.0*sqrt(c*bign*ell);
else lim=10.0*sqrt(g*bign*ell);
if(gflag==0)
 {sum2=pi2/6.0-1.0;
```

```
for(n=2;n<=lim;n++) sum2-=(1.0/n)/n;
 for(n=lim;n>1;n--)
     {p=alpha*n;
     p2=p*p;
     a=sqrt(p2+ee);
     summ + = p2*(2.0-(a/p+p/a));
      }
  summ-=4.0/pi2*c*c*bign*bign*sum2;
  summ/=4.0*ell;
 }
else
 {sum2=pi2/6.0;
  for(n=1;n<=lim;n++) sum2-=(1.0/n)/n;
 for(n=lim;n>0;n--)
     {p=alpha*n;
     p2=p*p;
     a=sqrt(p2+ee);
     b=sqrt(p2+eep);
     summ+=p2*(1.0-0.25*(p/a+a/p+p/b+b/p));
      }
 summ-=bign*bign/4.0/pi2*(c*c+g*g)*sum2;
 summ*=2.0/ell;
  }
sum-=summ;
sum+=hgrd(ell)/ell;
if(gflag==0) sum+=pi2*bign/ell/ell;
return (sum);
}
```

double ener (double ell)

{double alpha, a, b, ee, eep, sum, p, p2, pa, pb, betapa, betapb; long int lim, n, nmin;

```
sum=0.0;
if(temp!=0.0)
 {alpha=2.0*pi/ell;
  if(gflag==0) alpha /=2.0;
  ee=4.0*c*bign/ell;
  eep=4.0*g*bign/ell;
  if(gflag==0) nmin=2;
  else nmin=1;
  a=0.5*(sqrt(eep*eep+5184.0*temp*temp)-eep);
  lim=sqrt(a)/alpha;
  for(n=lim;n>=nmin;n--)
   {p=alpha*n;
   p2=p*p;
   a=sqrt(p2+ee);
   b=sqrt(p2+eep);
   pa=p*a;
   pb=p*b;
   betapa=pa/temp;
   betapb=pb/temp;
   if(betapa>36.0) sum+=pb/(exp(betapb)-1.0);
   clse sum+=pa/(exp(betapa)-1.0)+pb/(exp(betapb)-1.0);
   }
  }
if(gflag!=0) sum*=2.0;
return (sum+hgrd(ell));
}
```

double ratio (double ell) {double alpha,sum,sum2,ee,eep,p,p2,a,b,xx,yy,betapa,betapb; double b1,b2,b3,b4,bg,s1,s2,s3,s4,sm,t,term,x; long int lim1,lim2,n,nmin;

```
if(gflag==0)
 {alpha=pi/ell;
 nmin=2;
 }
else
 {alpha=2.0*pi/-li:
 nmin=1;
  }
if (g<c)
 {bg=c;
  sm=g;
  }
else
 {bg=g;
  sm=c;
  }
x=bg*bign/ell;
b1=2.0*x;
b2=b1*x;
b3=2.0*b2;
b4=4.0*x;
x=sm*bign/ell;
s1=2.0*x;
s2=s1*x;
s3=2.0*s2;
s4=4.0*x;
```

```
lim1=10.0*sqrt(sm*bign*ell/pi2);
lim2=10.0*sqrt(bg*bign*ell/pi2);
if (temp==0.0) t=1.0e-40;
else t=temp;
sum=0.0;
cc=4.0*bg*bign/ell;
eep=4.0*sm*bign/ell;
x=lim2+1;
do
 \{\text{term} = -2.0;
  p=alpha*x;
  p2=p*p;
 xx=2.0+b3/p2/p2*(1.0-b4/p2);
  yy=2.0+s3/p2/p2*(1.0-s4/p2);
  betapa=(p2+b1-b2/p2)/t;
  betapb=(p2+s1-s2/p2)/t;
  if (betapa>25.0) term += 0.5^{*}xx;
  else term += (0.5+1.0/(\exp(betapa)-1.0))*xx;
 if (betapb>25.9) term += 0.5*yy;
  else term += (0.5+1.0/(exp(betapb)-1.0))*yy;
  sum += term;
  x += 1.0;
  }
while (term > 1.0e-4);
sum2=0.0;
for(n=lim2;n>lim1;n--)
 {p=alpha*n;
  p2=p*p;
  a=sqrt(p2+cc);
 xx=a/p+p/a;
 yy=2.0+s3/p2/p2*(1.0-s4/p2);
```

```
betapa=p*a/t;
 betapb=(p2+s1-s2/p2)/t;
 if (betapa>25.0) sum 2 = 0.5 * xx;
 else sum2 += (0.5+1.0/(\exp(betapa)-1.0))*xx;
 if(betapb>25.0) sum2 += 0.5*yy;
 else sum2 += (0.5+1.0/(\exp(betapb)-1.0))*yy;
  }
sum += sum 2 - 2.0*(lim 2 - lim 1);
sum2=0.0;
for(n=lim1;n>=nmin;n--)
 {p=alpha*n;
 p2=p*p;
 a=sqrt(p2+ee);
 b=sqrt(p2+eep);
 xx=a/p+p/a;
 yy=b/p+p/b;
  betapa=p*a/t;
  betapb=p*b/t;
 if(betapa>25.0) sum2 += 0.5*xx;
  else sum2 += (0.5+1.0/(\exp(betapa)-1.0))*xx;
  if (betapb>25.0) sum2 += 0.5*yy;
  clse sum2 += (0.5+1.0/(exp(betapb)-1.0))*yy;
  ł
sum2 -= 2.0*(lim1-nmin+1);
sum += sum2;
if(gflag==0) return (sum/2.0/bign);
return (sum/bign);
}
```

double entropy (double ell) {double alpha,sum,p,p2,a,b,pa,pb,betapa,betapb,ee,eep;

```
long int nmin,lim,n;
```

_

```
if (temp==0.0) return (0.0);
alpha=2.0*pi/ell;
nmin=1.0;
sum=0.0;
ee=4.0*c*bign/ell;
eep=4.0*g*bign/ell;
if(gfla ==0)
 alpha/=2.0;
 nmin=2;
 }
a=0.5*(sqrt(eep*eep+5184.0*temp*temp)-eep);
lim=sqrt(a)/alpha;
for(n=lim;n>=nmin;n--)
 {p=alpha*n;
 p2=p*p;
 a=sqrt(p2+ee);
 b=sqrt(p2+eep);
 betapa=p*a/temp;
 betapb=p*b/temp;
 if(betapb>21.0) sum+=betapb*exp(-betapb);
 else
   {a=exp(betapb);
   b=a-1.0;
   sum+=log(a/b)+betapb/b;
   }
 if(betapa<36.0)
   {if{betapa>21.0} sum+=betapa*exp(-betapa);
   else
       {a=exp(betapa);
```

```
b=a-1.0;
sum+=log(a/b)+betapa/b;
}
}
if(gflag==0) return (sum);
return (2.0*sum);
}
```

Third section of program

#include <math.h>
#include <alloc.h>
#include <conio.h>
#include <stdio.h>

extern double c,g,temp,bign,pi;

void setwindow (int ulc,int ulr,int brc,int brr); double nzero(double ell, double trial); void restorescrn(int flag);

int spdf(double ell,double step)
{double alpha,sum,ec,eg,p,p2,a,b,beta,term,sa,sb,pt,pow,diff;
int r,n,flag;
double huge *ptr_1;
double huge *ptr_p;
FILE *f_ptr;

alpha = 2.0*pi/ell; ec = 4.0*c*bign/ell;

```
eg = 4.0*g*bign/ell;
if(temp==0.0) beta = 1.0e200;
else beta = 0.5/temp;
for (r=0;r<2;r++)
 {n = 0;}
  do
  {n++;
     p = alpha*n;
     if(r) ptr_p[n] = p;
     p2 = p*p;
     sa = sqrt(p2+ec);
     sb = sqrt(p2+eg);
     a = sa/p+p/sa;
     \mathbf{b} = \mathbf{sb/p+p/sb};
     pt = p*beta;
     pow = pt*sa;
     if(pow>36.0) term = a;
     else term = a/tanh(pow);
     pow = pt*sb;
     if(pow>36.0) term += b-4.0;
     else term += b/tanh(pow)-4.0;
     if(r) ptr_1[n] = term;
     }
 while ((\text{term} > 1.0\text{e-5})\&\&(n < 10000));
 if(n==10000) return 2;
 if(r==0)
  {if(NULL==(ptr_1=(double huge *)farcalloc(n+1,sizeof(double)))) return 3;
     if(NULL==(ptr p=(double huge *)farcalloc(n+1,sizeof(double))))
       {farfree(ptr 1);
       return 3;
       }
```

```
if(NULL==(f_ptr=fopen("c:\\dad\\spdf.dat", "w+t")))
       {farfree(ptr_1);
       farfree(ptr_p);
       return 1;
       }
     }
 }
setwindow(45,1,79,25);
flag = 0;
diff = 0.0;
do
 {sum = 0.0;
  for(r=n;r>0;r--) sum += cos(ptr_p[r]*diff)*ptr_1[r];
  sum /= 4.0*ell;
  fprintf(f_ptr,"%10.2f
                            %11.4f\n",diff,sum);
  cprintf("\r\n%10.2f
                            %11.4f",diff,sum);
  if(kbhit()) flag = 1;
  diff += step;
  }
while((diff<=ell)&&(!flag));
farfree(ptr_1);
farfree(ptr_p);
fclose(f ptr);
restorescrn(flag);
return 0;
}
```

Fourth section of program

#include <math.h>
#include <alloc.h>

#include <conio.h>
#include <stdio.h>

```
extern double c,g,temp,bign,pi;
extern int error_no[];
```

void setwindow (int ulc,int ulr,int brc,int brr)
{window(ulc,ulr,brc,brr);
textbackground(LIGHTGRAY);
textcolor(BLACK);
clrscr();
return;
}

```
void restorescrn(int flag)
{cprintf("\r\n");
  clreol();
  if(flag) cprintf("User break. Press key to continue. ");
  else cprintf("Finished. Press key to continue. ");
  getch();
  clrscr();
  window(1,1,80,25);
  textbackground(BLUE);
  textcolor(YELLOW);
  return;
}
```

}

double nzero(double ell,double trial) {double alpha,e1,e2,e3,beta,sum,p,p2,a,b,pow,term,part,bgr; int flag; long int lim,lwrlim,n;

÷

```
flag = 0;
if(temp==0.0) beta = 1.0e200;
else beta = 1.0/temp;
alpha = 2.0*pi/ell;
if(c>g) bgr = c;
else bgr = g;
lwrlim = 3.0*ell*sqrt(temp)/pi;
do
 \{e1 = 2.0*g*trial/ell;
 e2 = 3.0*e1;
  e3 = e1 + 4.0 + c + trial/ell;
  lim = sqrt(1500.0*bgr*trial*eil)/pi;
  if(lim<lwrlim) lim = lwrlim;
  sum = 0.0;
  for(n=lim;n>0;n--)
     {p = alpha*n;}
      p2 = p*p;
      a = sqrt(p2+e2);
      b = sqrt(p2+e1);
      part = beta*b;
      pow = part*a;
      if(pow>36.0) term = 0.5*(a/b+b/a);
      else term = (0.5+1.0/(\exp(pow)-1.0))*(a/b+b/a);
      a = sqrt(p2+e3);
      pow = part*a;
      if(pow>36.0) term += 0.5*(a/b+b/a)-2.0;
      else term += (0.5+1.0/(\exp(pow)-1.0))*(a/b+b/a)-2.0;
      sum += term;
```

```
}
if((fabs((bign-sum)/trial-1.0))<1.0e-5) flag = 1;
trial = bign-sum;
}
while((!flag)&&(trial>0.0));
if(trial<0.0) error_no[3] = 0;
return (trial);
}</pre>
```

```
double hgrdno(double ell,double num)
{double alpha,e1,e2,e3,e4,bgr,sum,sum2,p,p2,a;
long int lim,n;
```

```
alpha = 2.0*pi/ell;
e1 = c*num/ell+3.0*g*num/ell; /* 2e+6e' */
e2 = 2.0*g*num/ell; /* 4e' */
e3 = 4.0*c*num/ell+e2; /* 8e+4e' */
                /* 12e' */
e4 = 3.0 e2;
if(c>g) bgr = c;
else bgr = 3;
lim = sqrt(1500.0*bgr*num*ell)/pi;
sum = 0.0;
sum2 = 0.0;
for(n=lim;n>0;n--)
 {p = alpha*n;}
 p2 = p*p;
 a = sqrt(p2+e2);
 sum += 0.5*a*(sqrt(p2+e3)+sqrt(p2+e4))-p2-e1;
 sum2 = 1.0/p2;
 }
```

sum2 /= ell*ell; sum2 += 1.0/24.0; sum -= (g*g+c*c)*num*num*sum2; a = num*num*g/ell+2.0*sum; return (a); }

double pressureno(double ell,double num)
{double alpha,e1,e2,e3,c1,c2,c3,beta,beta1;
 double bgr,sum1,sum2,p,p2,d1,d2,d3,f1,f2,f3,f4,f5,f6;
 long int lim,n;

```
alpha = 2.0*pi/ell;
e1 = 2.0*g*num/ell; /* 4e' */
e2 = 3.0*e1; /* 12e' */
e3 = 4.0*c*num/ell+e1; /* 8e+4e' */
                   /* e' */
c1 = e1/4.0;
c2 = 3.0*c1; /* 3e' */
c3 = c*num/ell+c1; /* 2e+e' */
if(temp==0.0) beta = 1.0e200;
else beta = 1.0/\text{temp};
if(c>g) bgr = c;
else bgr = g;
lim = sqrt(1500.0*bgr*num*ell)/pi;
sum1 = 0.0;
sum2 = 0.0;
for(n=lim;n>0;n-)
 {p = alpha*n;}
 p2 = p*p;
```
```
d1 = sort(p2+e1);
  d2 = sqrt(p2+e2);
  d3 = sqrt(p2+e3);
  f1 = d1/d2;
  f2 = 1.0/f1;
  f3 = d1/d3;
  f4 = 1.0/f3;
  sum1 += p2*(4.0-f1-f2-f3-f4);
  f5 = d1*d2;
                                  /* w */
                                   /* mu */
  f6 = d1*d3;
  beta1 = beta*f5;
  if(beta1\leq36.0) sum2 += (f5-c1*f2-c2*f1)/(exp(beta1)-1.0);
  beta1 = beta*f6;
  if(beta1<36.0) sum2 += (f6-c^{1}f4-c^{3}f3)/(exp(beta1)-1.0);
  }
beta1 = (hgrdno(ell,num)-0.5*sum1+4.0*sum2)/ell;
return (beta1);
}
```

```
double energyno(double ell,double num)
{double alpha,e1,e2,e3,sum,p,p2,c1,c2,c3;
  double omega,mu,pow;
  long int lim,n;
```

```
if(temp==0.0) return (hgrdno(ell,num));
alpha = 2.0*pi/ell;
e1 = 2.0*g*num/ell; /* 4e' */
e2 = 3.0*e1; /* 12e' */
e3 = 4.0*c*num/ell+e1; /* 8e+4e' */
lim = (9.0*temp<sup>c</sup>ell-0.5*g*num)*ell;
```

```
if(lim<=0) return (hgrdno(ell,num));
lim = sqrt(lim)/pi;
sum = 0.0;
for(n=lim;n>0;n--)
 {p = alpha*n;}
 p2 = p*p;
 c1 = sqrt(p2+e1);
 c2 = sqrt(p2+e2);
 c3 = sqrt(p2+e3);
  omega = c1*c2;
 mu = c1*c3;
  sum += omega/(exp(omega/temp)-1.0);
  pow = mu/temp;
  if(pow < 36.0) sum += mu/(exp(pow)-1.0);
  }
return (hgrdno(ell,num)+2.0*sum);
}
```

```
double entropyno(double ell,double num)
{double alpha,e1,e2,e3,sum,p,p2,c1,c2,c3;
double pow,x;
long int lim,n;
```

```
if(temp==0.0) return (0.0);

alpha = 2.0*pi/ell;

e1 = 2.0*g*num/ell; /* 4e' */

e2 = 3.0*e1; /* 12e' */

e3 = 4.0*c*num/ell+e1; /* 8e+4e' */

lim = (9.0*temp*ell-0.5*g*num)*ell;

if(lim<=0) return (0.0);
```

```
lim = sqrt(lim)/pi;
sum = 0.0;
for(n=lim;n>0;n--)
 {p = alpha*n;}
  p2 = p*p;
  c1 = sqrt(p2+e1);
  c2 = sqrt(p2+e2);
  c3 = sqrt(p2+e3);
  pow = c1*c2/temp;
  x = exp(pow);
  sum += pow/(x-1.0);
  if(pow<20.0) sum += \log(x/(x-1));
  pow = c1*c3/temp;
  if(pow<36.0)
     {x = exp(pow);}
      sum += pow/(x-1.0);
     if(pow<20.0) sum += \log(x/(x-1.0));
      }
  }
return (2.0*sum);
}
```

```
double nex(double tp,double mu,double ell)
 {long int lim,n;
 double alpha,sum,p,x;
```

```
sum = 0.0;
lim = ell/2.0/pi*sqrt(36.0*tp+mu);
alpha = 2.0*pi/ell;
for(n=lim;n>0;n--)
```

```
{p = alpha*n;}
 x = (p*p-mu)/tp;
  sum += 1.0/(exp(x)-1.0);
  }
return 4.0*sum;
}
```

```
double chem(double tp, double ell)
 {double mu,mu1,mumid,fmid,dmu;
 int j,n;
 mu1 = -tp*log(1.0+2.0/bign);
 mu = mu1;
 do
   {mu *= 1.1;
   fmid = 2.0/(exp(-mu/tp)-1.0)+nex(tp,mu,ell)-bign;
```

```
}
```

```
while (fmid>0.0);
dmu = mu1-mu;
for(j=1;j<=40;j++)
 \{mumid = mu + (dmu *= 0.5);
 fmid = 2.0/(exp(-mumid/tp)-1.0)+nex(tp,mumid,ell)-bign;
 if(fmid<0.0) mu = mumid;
 if(fabs(fmid)<1.0e-7*bign) return mu;
  }
error_no[4] = 1;
return mu;
}
```

double freepress(double tp,double ell,double mu)

```
{double alpha,p,p2,term,sum;
long int lim,n;
```

```
alpha = 2.0*pi/ell;
lim = ell/2.0/pi*sqrt(40.0*tp+mu);
sum = 0.0;
for (n=lim;n>0;n--)
{p = alpha*n;
p2 = p*p;
term = p2/(exp((p2-mu)/tp)-1.0);
sum += term;
}
return 8.0/ell*sum;
}
```

```
double freeentropy(double tp,double ell,double mu)
{long int lim,n;
   double alpha,sum,p,x,y,term;
```

```
alpha = 2.0*pi/ell;
lim = ell/2.0/pi*sqrt(40.0*tp+mu);
sum = 0.0;
for(n=lim;n>0;n--)
{p = alpha*n;
x = (p*p-mu)/tp;
y = exp(x);
term = x/(y-1.0)+log(y/(y-1.0));
sum += term;
}
sum *= 4.0;
```

```
if(mu!=0.0)
{x = mu/tp;
y = exp(x);
sum -= 2.0*(log(1-y)+x*y/(1-y));
}
return sum;
}
```

double freeenergy(double tp,double ell,double mu)
{long int lim,n;
 double alpha,sum,p,x;

```
alpha = 2.0*pi/ell;
lim = ell/2.0/pi*sqrt(40.0*tp+mu);
sum = 0.0;
for(n=lim;n>0;n--)
  {p = alpha*n;
  x = p*p-mu;
  sum += x/(exp(x/tp)-1.0);
  }
return (4.0*sum);
}
```

double freegibbs(double tp,double ell, double mu)
{double alpha,p,p2,x,y,sum1,sum2;
long int lim,n;

alpha = 2.0*pi/ell; lim = ell/2.0/pi*sqrt(36.0*tp+mu);

```
sum1 = 0.0;
sum2 = 0.0;
for(n=lim;n>0;n--)
 {p = alpha*n;}
 p2 = p*p;
 x = \exp((p2-mu)/tp);
  sum1 += log(x/(x-1));
  sum2 += p2/(x-1.0);
  }
sum1 = 4.0*tp;
sum2 *= 8.0;
sum2 \rightarrow sum1;
if(mu != 0.0)
 {x = mu/tp;}
 y = exp(x);
 sum2 += 2.0*(tp*log(1-y)+mu*y/(1-y));
  }
return sum2;
}
```

Fifth part of program

This is the section of the program that solves the coupled integral equations taken from Lieb and Liniger²⁶, namely equations 42,43, and 44. The method is taken from Press, Teukolsky, Vetterling and Flannery³⁵ with modifications made to suit the requirements here.

#include <math.h>
#include <alloc.h>

#include <stdlib.h>
#include <conio.h>

#define TINY 1.0e-20 #define EPS 3.0e-11

extern double c,g,bign,pi,pi2,temp,rt2;

```
void fatal(int n)
 {switch (n)
   {case '1':
    case '2':
    case '3': cprintf("Could not allocate memory.\r\n");
               break;
    case '4': cprintf("Singular matrix in ludcmp.\r\n");
               break;
    case '5': cprintf("Error in polint.\r\n");
               break;
    case '6': cprintf("Too many steps in gromb.\r\n");
               break;
        }
    cprintf("Press key to terminate. ");
    getch();
    exit(EXIT_FAILURE);
    }
```

double far *vector(int n)
{double far *ptr;

if(NULL==(ptr=(double far *)farcalloc(n+1,sizeof(double)))) fatal(3);

```
return ptr;
  ł
double * far *matrix(int m,int n)
 {double * far *ptr;
  int i;
  /*Assumes m by n matrix with first element (1,1) */
  if(NULL==(ptr=(double * far *)calloc(m+1,sizeof(double * far*)))) fatal(3);
  if(NULL==(ptr[0]=(double tar *)farmalloc(m*n*sizeof(double)))) fatal(3);
  ptr[1] = ptr[0]-1;
  for(i=2;i<=m;i++) ptr[i] = ptr[i-1]+n;
  return ptr;
  }
void freematrix(double * far *ptr)
 {farfree(ptr[0]);
  free(ptr);
  }
int far *ivector(int n)
 {int far *ptr;
  if(NULL==(ptr=(int far *)farcalloc(n+1,sizeof(int)))) fatal(3);
  return ptr;
  }
```

void ludcmp(double far **a,int n,int *indx)

```
{int i,imax,j,k;
double big, dum, sum, temp;
double far *vv;
vv = vector(n);
for(i=1;i<=n;i++)
  {big = 0.0;}
  for(j=1;j<=n;j++) if((temp=fabs(a[i][j]))>big) big = temp;
  if (big == 0.0) fatal(4);
  vv[i] = 1.0/big;
  }
for(j=1;j<=n;j++)
  {for(i=1;i<j;i++)
      \{sum = a[i][j];
      for(k=1;k<i;k++) sum -= a[i][k]*a[k][j];
      a[i][j] = sum;
       }
  big = 0.0;
  for(i=j;i<=n;i++)
      \{sum = a[i][j];
      for(k=1;k<j;k++) sum -= a[i][k]*a[k][j];
       a[i][j] = sum;
       if((dum=vv[i]*fabs(sum)) >= big)
        {big = dum;
         imax = i;
         }
       }
  if(j != imax)
      {for(k=1;k<=n;k++)
         \{dum = a[imax][k];
         a[imax][k] = a[j][k];
```

```
a[j][k] = dum;
}
vv[imax] = vv[j];
}
indx[j] = imax;
if(a[j][j] == 0.0) a[j][j] = TINY;
if(j != n)
{dum = 1.0/a[j][j];
for(i=j+1;i<=n;i++) a[i][j] *= dum;
}
farfree(vv);
return;
}</pre>
```

```
void lubksb(double far **a,int n,int *indx,double b[])
{int i,ii=0,ip,j;
double sum;
```

```
for(i=1;i<=n;i++)
{ip = indx[i];
sum = b[ip];
b[ip] = b[i];
if (ii) for (j=ii;j<=i-1;j++) sum -= a[i][j]*b[j];
else if(sum) ii = i;
b[i] = sum;
}
for(i=n;i>=1;i--)
{sum = b[i];
for(j=i+1;j<=n;j++) sum -= a[i][j]*b[j];</pre>
```

```
b[i] = sum/a[i][i];
}
}
```

```
void gauleg(double x1,double x2,double x[],double w[],int n)
```

```
{int m,j,i;
double z1,z,xm,xl,pp,p3,p2,p1;
m = (n+1)/2;
xm = 0.5*(x2+x1);
xl = 0.5*(x2-x1);
for(i=1;i<=m;i++)
 {z = cos(pi*(i-0.25)/(n+0.5));}
  do
      {p1 = 1.0;}
      p2 = 0.0;
      for(j=1;j<=n;j++)
        {p3 = p2;
        p2 = p1;
        p1 = ((2.0*j-1.0)*z*p2-(j-1.0)*p3)/j;
        }
      pp = n^{(z*p1-p2)/(z*z-1.0)};
      z1 = z;
      z =z1-p1/pp;
       }
  while(fabs(z-z1)>EPS);
  x[i] = xm - xl^* z;
  x[n+1-i] = xm+xl^*z;
  w[i] = 2.0*xl/((1.0-z*z)*pp*pp);
  w[n+1-i] = w[i];
```

} }

```
int fred2(int n, double a, double b, double t[], double t[], double w[],
```

```
double (*g)(double),double (*ak)(double,double))
```

```
{int i,j,far *indx;
```

-

```
double d,* far *omk;
```

```
indx = ivector(n);
omk = matrix(n,n);
gauleg(a,b,t,w,n);
for(i=1;i<=n;i++)
    {for(j=1;j<=n;j++) omk[i][j] = (double)(i == j)-(*ak)(t[i],t[j])*w[j];
    f[i] = (*g)(t[i]);
    }
ludcmp(omk,n,indx);
lubksb(omk,n,indx,f);
farfree(indx);
freematrix(omk);
return 0;
}
```

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```
\{int i, m, ns = 1;
double den, dif, dift, ho, hp, w;
double far *0, far *d;
dif = fat x-xa[1]);
c = vector(n);
d = vector(n);
for(i=1;i<=n;i++)
  {if((dift=fabs(x-xa[i]))<dif)</pre>
      {ns = i;}
      dif = dift;
       }
  c[i] = ya[i];
  d[i] = ya[i];
  }
*y = ya[ns--];
for(m=1;m<n;m++)
  {for(i=1;i<=n-m;i++)
      {ho = xa[i]-x;}
      hp = xa[i+m]-x;
       w = c[i+1]-d[i];
       if((den=ho-hp)==0.0) fatal(5);
       den = w/den;
       d[i] = hp + den;
       c[i] = ho*den;
       }
  *y += (*dy=(2*ns<(n-m) ? c[ns+1] : d[ns--]));
```

void polint(double xa[],double ya[],int n, double x,double *dy)

}

```
}
farfree(d);
farfree(c);
}
```

```
double trapzd(double (*func)(double), double a, double b, int n)
{double x, tnm, sum, del;
static double s;
long int it, j;
if(n==1) return (s = 0.5*(b-a)*(((*func)(a))+((*func)(b))));
else
{for(it=1,j=1;j<n-1;j++) it <<= 1;
tnm = it;
del = (b-a)/tnm;</pre>
```

```
x = a+0.5*del;
for(sum=0.0,j=1;j<=it;j++,x += del) sum += (*func)(x);
s = 0.5*(s+(b-a)*sum/tnm);
return s;
}
```

```
double qromb(double (*func)(double),double a, double b)
{double ss,dss;
  double s[22],h[22];
  int j;
```

```
h[1] = 1.0;
for(j=1;j<=20;j++)
```

_

```
{s[j] = trapzd(func,a,b,j);
if(j>5)
      {polint(&h[j-5],&s[j-5],5,0.0,&ss,&dss);
      if(fabs(dss)<1.0e-6*fabs(ss)) return ss;
      }
    s[j+1] = s[j];
    h[j+1] = 0.25*h[j];
    }
fatal(6);
return 0.0;
}
```

```
double lam;
double far *tt,far *ff,far *ww;
double (*gg)(double),(*akak)(double,double);
int nn;
```

```
double kernel(double t,double s)
{double x,y;
x = s-t;
y = lam/pi/(lam*lam+x*x);
return y;
}
```

```
double gt(double t)
 {return 0.5/pi;
}
```

```
double liebg(double x)
```

{return fredin(x,nn,tt,ff,ww,gg,akak);}

```
double liebe(double x)
{return x*x*liebg(x);}
```

void lieb(double lamda,int n,double *gamma,double *egamma)

{double (*gl)(double); double x;

```
lam = lamda;
nn = n;
gg = gt;
akak = kernel;
tt = vector(n);
ff = vector(n);
ww = vector(n);
fred2(n,-1.0, 1.0, tt, ff, ww, gg, akak);
gl = liebg;
*gamma = lamda/qromb(gl,-1.0,1.0);
gl = liebe;
x = *gamma/lamda;
*egamma = x*x*x*qromb(gl,-1.0,1.0);
farfree(ww);
farfree(ff);
farfree(tt);
}
```

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