CALCULATION OF MASSES OF DARK SOLITONS IN 1D BOSE-EINSTEIN CONDENSATES USING GELFAND YAGLOM METHOD

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Kübra Işık Yıldız

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We certify that we have read this thesis and that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.

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ABSTRACT

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M.S. in Physics
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Nonlinear excitations of Bose-Einstein condensates (BEC) play important role in understanding the dynamics of BECs. Solitons, shape preserving wave packets, are the most fundamental nonlinear excitations of BECs. They exhibit particle-like behaviors since their characteristic features do not change during their oscillations and collisons. Moreover, their effective masses are calculated. We are interested in dark solitons which have their density minima at the center. In literature, the mass of dark soliton is obtained with Gross-Pitaevskii approximation. As a result of the contributions of quantum fluctuations to the ground state energy, a correction term is added to the effective mass. The dispersion relation of these fluctuations are derived from Bogoliubov de Gennes equations. However, with familiar analytical approaches, only a few modes can be taken into account. In order to include all the modes and find an exact expression for ground state energy, we obtain free energy from partition function. The partition function is equivalent to an imaginary-time coherent state Feynman path integral on which periodic boundary conditions are applied. The partition function is in the form of infinite dimensional Gaussian integral, therefore, it is proportional to the determinant of the functional in the integrand. We use Gelfand Yaglom method to calculate the corresponding determinant. Gelfand Yaglom method is a specialized formulation of using zeta functions and contour integrals in calculation of the functional determinant for one-dimensional Schrdinger operators. In this study, we formulate a new technique through this method to calculate ground state energy of stationary dark solitons up to the Bogoliubov order exactly.

Keywords: Mass of dark soliton, path integral, Bogoliubov aproximation, functional determinants, Gelfand Yaglom method.

ÖZET

BOSE-EINSTEIN YOĞUŞMALARINDAKİ KARANLIK SOLİTONLARIN KÜTLELERİNİN GELFAND YAGLOM METODU İLE HESAPLANMASI

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Bose Einstein yoğuşmasının lineer olmayan uyarımları, yoğuşmanın dinamiğini anlamada önemli bir rol oynamaktadır. Şekillerini muhafaza eden dalga paketleri olan solitonlar Bose-Einstein yoğuşmalarının en temel lineer olmayan uyarımlarıdır. Salınımlarda ve çarpışmalarda karakteristik parametreleri değişmediğinden parçacık özelliği de gösterirler ve etkin kütleleri hesaplanabilir. Merkezlerindeki madde yoğunluğu kenarlarına göre daha az olan solitonlara karanlık solitonlar denir. Karanlık solitonların Gross-Pitaevskii yaklaşımıyla hesaplanan taban durum enerjilerine kuantum dalgalanmalarının katkılarını dahil ederek, bu enerji daha ileri bir seviyede hesaplanabilir. Bu dalgalanmaların enerji-momentum ilişkilerini Bogoliubov de Gennes denklemleri verir. Ancak alışılagelmiş analitik yaklaşımlarla, sadece sınırlı sayıdaki modun katkıları hesaplanabilir. Biz, bütün modları dahil ederek taban durum enerjisini analitik olarak elde etmek için, sistemin serbest enerjisini bölüşüm fonksiyonundan türettik. Bölüşüm fonksiyonu, periyodik sınır koullarına sahip bir imajiner zaman koherent durum Feynman yol integrali eklinde yazılabilir. Bu şekilde yazdığımızda sonsuz boyutlu bir Gauss integrali elde ederiz. Bu integralin değeri, integrand içinde üstel fonksiyon halinde bulunan fonksiyonelin determinantı ile orantılıdır. Bu fonksiyonelin determinantını bulmak için fonksiyonel determinantlarının zeta fonksiyonu ve kontur integraller kullanılarak hesaplanmasının bir boyuttaki Schrödinger operatörlerine uyarlanmış hali olan Gelfand Yaglom metodunu kullandık. Böylelikle, karanlık solitonların kütlelerinin Bogoliubov seviyesine kadar kesin analitik hesaplanmasında yeni bir yöntem geliştirdik.

Anahtar sözcükler: Karanlık solitonlar, yol integrali, Bogoliubov yaklaşımı, fonksiyonel determinantlar, Gelfand Yaglom metodu.

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Chapter 1

Introduction

Bose Einstein condensate is a phenomenon signaled by the occupation of the ground state of a system by a macroscopic number of bosons at very low temperatures. In a Bose Einstein condensate (BEC), whole system can be described by a macroscopic wave function therefore, it is possible to observe quantum mechanical phenomena on a macroscopic scale. After its prediction [1] in 1925, observation of a BEC in laboratory was achieved by using ultracold atomic gases in 1995 [2, 3]. One advantage of ultracold gases, is that these systems are highly controlled: one can tune the interactions between atoms or external potential. So, since its observation in cold atoms, BEC has been a growing research area.

Gross-Pitaevskii equation is the governing equation of BEC under the mean field approximation. Uniform Bose gas and solitons, shape maintaining wave packets, are the exact solutions of GP (Gross-Pitaevskii). Solitons are seen in nonlinear systems as a balance of dispersion and nonlinearity [4]. Since nonlinear excitations are important to analyze dynamics of BECs, solitons in BEC are of great interest [5–9].

Solitary waves are seen in many branch of physics, e.g. optics [10, 11], Bose-Einstein condensate, magnetic films [12], etc. They collide [8, 13–15] and oscillate [16–19] in a particle-like manner and also their effective masses can be calculated

[20]. In this thesis, we are interested in calculation of the masses, therefore ground state energies, of dark solitons especially black solitons which are stationary dark solitons. By using Gel'fand Yaglom method, we calculate the ground state energy of black solitons in a Bose Einstein condensate up to the Bogoliubov order.

If density of the Bose gas is uniform, $n(x,t) = n(t)$, ground state energy can be calculated easily within the mean field approximation. This energy is approximate. A correction to this energy can be done by adding ground state energies of elementary excitations whose dispersion relations are derived from Bogoliubov de Gennes (BdG) equations.

If the Bose gas has a single black soliton, first level ground state energy can be calculated again by using the mean field Hamiltonian. Dispersion relation of excitations, however, cannot be obtained since BdG equations for solitons are too complicated and cannot be solved analytically. Several computational works are done to approximate this Bogoliubov-level ground state energy but all of the excitation modes are not included in these works.

Ground state energy is the zero temperature limit of free energy, therefore, can be derived from the partition function. Z, the partition function, can be written as a coherent state path integral on which periodic boundary conditions are applied. And a complicated functional determinant is needed to calculate in order to get partition function of solitons. We calculate this determinant by using Gel'fand Yaglom method [21] and find the ground state energy of black soliton up to Bogoliubov level.

In chapter 2, the physics of Bose Einstein condensates is briefly reviewed. Exact solutions of Gross Pitaevskii equation, namely the uniform solution, dark and bright solitons are mentioned. Then, Bogoliubov approximation is explained.

In the third chapter, Feynman path integral and coherent states are introduced and many body (coherent state) path integral is established. Then, it is showed that if periodic boundary conditions are applied to the imaginary-time coherent state path integral, it becomes the quantum partition function of a many body system. Once we get quantum partition function of the system, the ground state energy can be easily derived.

In chapter 4, we show how to calculate the exact ground state energy of uniform Bose gas. Hamiltonian gives mean field level energy and BdG gives, in principle, Bogoliubov level energy. However, the sum of the ground state energies of elementary excitations of uniform gas diverges. After performing a renormalization, energy is calculated up to the desired accuracy [20, 22].

Chapter 5 is about the ground state energy of dark solitons. First order energy is again calculated with H. Second order corrections cannot be obtained from BdG equations therefore the partition function is used. Z is written in the form of an infinite dimensional Gaussian integral. Such integrals are proportional with the determinant of the corresponding matrix. In our case, we end up with a functional determinant which is the action of dark soliton. To find this determinant we need an advance method and we introduce it in the next chapter.

In chapter 6, first we show how zeta functions and contour integrals are used to find determinants without knowing their eigenvalues. We introduce the Gel'fand Yaglom method which is a 1D formulation of functional determinant calculations by using $\zeta(n)$ and complex algebra. Then we get an expression for the ground state energy of dark soliton by using GY method.

Chapter 2

Solitons in BEC

2.1 Bose-Einstein condensation

While Fermions obey Pauli exclusion principle, Bosons, in principle, can occupy same state. For dilute gases with a large number of particles, around 10^{-9} K [20], the majority of particles occupy the same single particle state and form a Bose-Einstein condensate. This phenomenon was first predicted in 1925 by Einstein after he studied on Bose's paper about statistics of photons, and did some further calculations [1].

If a system is cooled down to the temperatures near absolute zero, it would generally solidify. Bose-Einstein condensate, however, is not a solid phase but instead a weird gas phase in which the wave functions of particles somehow interlaced. Both cooling and the interactions are critical to observe BEC and it was observed experimentally in 1995 [2, 3] for the first time in a cold atom setting. Since then, ultracold gases is a very dynamic area of research [23].

Interactions are very crucial in ultracold gases and give rise to collective behaviors such as superfluidity, vortices, solitons, and solitonic vortices.

2.2 Weakly Interacting Bose gas

In a non-interacting Bose gas, all particles are at their own ground states. When the system is arranged as there is a weak interaction, some particles are excited to more energetic states due to interactions. This interacting many body system is complicated to fully analyzed, so some approximations are made to study on it.

Mean field approach is the most common approach in which all particles are assumed to occupy the same ground state. Mean field approximation allows to make some implications about the system in a quite enough precision for low-energy cases. But it does not explain the quantum and thermal fluctuations of the system. We are interested in the ground state energy and by using mean field we can only have an approximate value for it.

Bogoliubov approximation takes into account, on the other hand, a few number of particles occupying excited states. Since the additional energies of elementary excitations are not neglected like in the mean field, with Bogoliubov approximation we can have a more accurate expression for ground state energy.

2.3 Mean field approach

If the energy of the system is low enough, range of the interactions is small in proportion to mean inter-particle distance. In this limit, effective interaction between the particles can be modeled as a delta function, $U_0\delta(r-r')$, [20] with a strength of

$$U_0 = \frac{4\pi\hbar^2 a}{m} \tag{2.1}$$

where a is s-wave scattering length. With $V(r)$ being the external potential, many body Hamiltonian is then

$$H = \sum_{i=1}^{N}\left[\frac{p_i^2}{2m} + V(r_i)\right] + U_0\sum_{i<j}\delta(r_i - r_j). \tag{2.2}$$

In mean field approach, the condensate state is written as a product of N same normalized symmetric single particle state as

$$\Psi(r_1 \cdots r_N) = \prod_{i=1}^{N} \psi(r_i). \tag{2.3}$$

When we sandwich Hamiltonian between condensate wave function energy functional becomes

$$E[\psi(r)] = \int dr \left[\frac{\hbar^2}{2m} |\nabla \psi(r)|^2 + V(r)|\psi(r)|^2 + \frac{1}{2} U_0 |\psi(r)|^4 \right]. \tag{2.4}$$

By using a Lagrange multiplier, μ, and taking condensate wave function normalized to the particle number N

$$\int dr |\Psi(r)|^2 = N, \tag{2.5}$$

a variational calculation results in

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + V(r) + U_0 |\Psi(r)|^2 \right) \Psi(r) = \mu \Psi(r). \tag{2.6}$$

μ is the chemical potential. This equation is called time independent GP equation and it is the governing equation of BEC under mean field approximation. It is also called nonlinear Schrödinger equation [24].

The time dependent version of the Gross-Pitaevskii equation is

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + V(r) + U_0 |\Psi(r,t)|^2 \right) \Psi(r,t) = i\hbar \frac{\partial \Psi(r,t)}{\partial t}. \tag{2.7}$$

If we take external potential to be zero, or constant equivalently, the homogeneous Bose gas

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + U_0 |\Psi(r)|^2 \right) \Psi(r) = \mu \Psi(r) \tag{2.8}$$

possesses uniform solution

$$U_0 |\Psi(r)|^2 \Psi(r) = \mu \Psi(r) \tag{2.9}$$

$$U_0 |\Psi(r)|^2 = \mu \tag{2.10}$$

$$\Psi_{us} = \sqrt{\frac{\mu}{U_0}} e^{ikr} = \sqrt{n} e^{ikr} \tag{2.11}$$

with an arbitrary phase where $n = |\Psi(r)|^2$ is the particle density. The chemical potential is then nU_0 for uniform Bose gas.

Gross-Pitaevskii equation also have other exact solutions: dark and bright solitons.

2.4 Dark solitons

"Dark" and "bright" comes from the appearance of solitons in an experimental setup. Dark solitons have lower density at its center compared to the background and emerge in BECs under the influence of repulsive interactions ($U_0 > 0$). A bright soliton has a density maxima at its center and is seen in BEC with attractice interaction strength ($U_0 < 0$). Their wavefunctions are

$$\psi_{dark}(x,t) = \sqrt{n_0}\left[i\frac{u}{s} + \sqrt{(1-\frac{u^2}{s^2})}\tanh\left(\frac{x-ut}{\sqrt{2}\xi_u}\right)\right]e^{-i\mu t/\hbar}, \tag{2.12}$$

$$\psi_{bright}(x,t) = \sqrt{\frac{2\mu}{U_0}}\frac{1}{\cosh\left(\sqrt{\frac{2m|\mu|}{\hbar^2}}x\right)}e^{-i\mu t/\hbar} \tag{2.13}$$

respectively [20]. Here n_0 is the density of the condensate when $x \to \pm\infty$, where u is the velocity of soliton. s is the sound velocity in the uniform condensate and given by $(n_0 U_0/m)^{1/2}$.

$$\xi_u = \frac{\xi}{\sqrt{1-\frac{u^2}{s^2}}} \tag{2.14}$$

where ξ is the coherence length which is given by

$$\xi = \frac{\hbar}{\sqrt{2mn_0U_0}}. \tag{2.15}$$

Derivation of ψ_{dark} can be found in Ref. [20]. Here we don't give a detailed calculation but instead focus on a special kind of dark solitons, the stationary ones. They are called black solitons. The density of the center of soliton decreases with decreasing velocity. n_{min} becomes zero for solitons with zero velocity. n_{min}

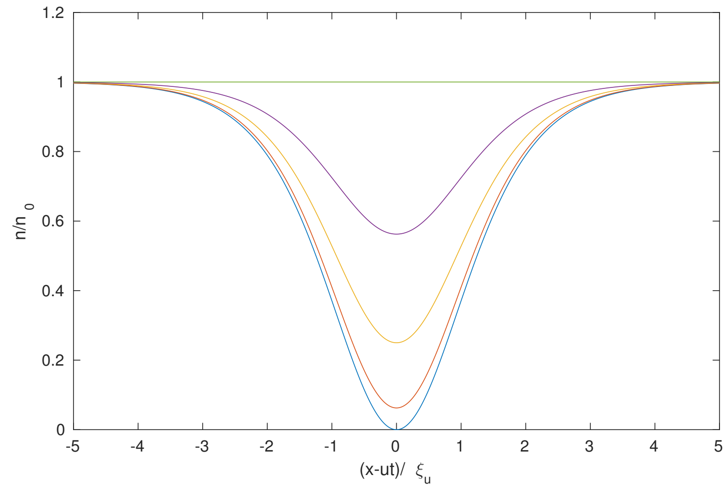

Figure 2.1: The density of a dark soliton for $u^2/s^2 = 0$, 0.25, 0.5, 0.75, and 1

reaches n_0 for solitons moving with the speed of sound, so, solitons dissapear in that limit.

When we put $u = 0$ in ψ_{dark} we get

$$\psi_{black} = \sqrt{n_0}\tanh\left(\frac{x}{\sqrt{2}\xi}\right). \tag{2.16}$$

where we drop the time evolution since black soliton is stationary.

2.5 Bogoliubov de Gennes equations

Bogoliubov de Gennes (BdG) equations gives the nature of the elementary excitations of exact solutions of GP. When we write down GP by replacing ψ with $\psi_0 + \delta\psi$ and then linearize it in $\delta\psi$ we find a couple of equations. Those equations possesses both time and space invariance. By using them, we get Bogoliubov de Gennes equations which gives us the dispersion relation of elementary excitations of the ground state of the system.
We will do the calculation for a uniform Bose gas. Same steps can be followed

without specializing $V(x)$ and μ to obtain BdG equations for a general system. The time dependent 1D Gross Pitaevskii equation is

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) + g|\psi|^2\right)\psi = i\hbar\frac{\partial \psi}{\partial t}. \tag{2.17}$$

If we write $\psi = \psi_0 + \delta\psi$ where ψ_0 is an exact solution of GP, $\delta\psi$ is the first order correction to this exact solution, and if we keep the terms up to the second order in $\delta\psi$, we get

$$-\frac{\hbar^2 k^2}{2m}\nabla^2\delta\psi + 2U_0|\psi_0|^2\delta\psi + U_0\psi_0^2\overline{\delta\psi} = i\hbar\frac{\partial\delta\psi}{\partial t}. \tag{2.18}$$

For a uniform Bose gas $\psi_0 = \sqrt{n_0}e^{-i\mu t/\hbar}$, $|\psi_0|^2 = n_0$, $\mu = n_0 U_0$:

$$-\frac{\hbar^2 k^2}{2m}\nabla^2\delta\psi + 2U_0 n_0\delta\psi + U_0 n_0 e^{-i2\mu t/\hbar}\overline{\delta\psi} = i\hbar\frac{\partial\delta\psi}{\partial t}. \tag{2.19}$$

To get rid of the terms with $e^{-i2\cdots}$, we define $\tilde{\delta\psi}$ such that

$$\begin{aligned}
\widetilde{\delta\psi} &\equiv \delta\psi e^{i\mu t/\hbar} \\
\nabla^2\widetilde{\delta\psi} &= \nabla^2\delta\psi e^{i\mu t/\hbar} \\
\frac{\partial\widetilde{\delta\psi}}{\partial t} &= \frac{\partial\delta\psi}{\partial t}e^{i\mu t/\hbar} + \frac{i\mu}{\hbar}e^{i\mu t/\hbar}\delta\psi \\
\frac{\partial\delta\psi}{\partial t} &= \frac{\partial\widetilde{\delta\psi}}{\partial t}e^{-i\mu t/\hbar} - \frac{i\mu}{\hbar}\widetilde{\delta\psi}e^{-i\mu t/\hbar}.
\end{aligned} \tag{2.20}$$

With this substitutions, the linearized GP in terms of $\widetilde{\delta\psi}$ becomes

$$-\frac{\hbar^2 k^2}{2m}\nabla^2\widetilde{\delta\psi} + U_0 n_0\widetilde{\delta\psi} + U_0 n_0\overline{\widetilde{\delta\psi}} = i\hbar\frac{\partial\widetilde{\delta\psi}}{\partial t} \tag{2.21}$$

Equation contains both $\widetilde{\delta\psi}$ and $\overline{\widetilde{\delta\psi}}$, therefore

$$\widetilde{\delta\psi} = A(x)e^{-iwt} + B(x)e^{iwt}. \tag{2.22}$$

As a matter of convention we take it as

$$\widetilde{\delta\psi} = A(x)e^{-iwt} - \overline{B}(x)e^{iwt}. \tag{2.23}$$

After plugging this into the equation above and equate the coefficients of e^{-iwt} and e^{iwt} to zero, since they are linearly independent, we get

$$\begin{aligned}
&-\frac{\hbar^2 k^2}{2m}\nabla^2 A + U_0 n_0 A - U_0 n_0 B - \hbar w A = 0 \\
&-\frac{\hbar^2 k^2}{2m}\nabla^2 B + U_0 n_0 B - U_0 n_0 A + \hbar w B = 0,
\end{aligned} \tag{2.24}$$

the so-called BdG equations for uniform Bose gas. Specializing the x-dependence of $A(x)$ and $\overline{B}(x)$ as

$$A(x) = A_0 e^{ikx} \qquad \overline{B}(x) = \overline{B}_0 e^{-ikx} \tag{2.25}$$

and rewriting the BdG gives the following coupled equaitons

$$\begin{aligned} \left(\frac{\hbar^2 k^2}{2m} + U_0 n_0 - \hbar w\right) A_0 - U_0 n_0 B_0 = 0 \\ -U_0 n_0 A_0 + \left(\frac{\hbar^2 k^2}{2m} + U_0 n_0 + \hbar w\right) B_0 = 0 \end{aligned} \tag{2.26}$$

which gives a nontrivial solution only if

$$\det \begin{bmatrix} \frac{\hbar^2 k^2}{2m} + U_0 n_0 - \hbar w & -U_0 n_0 \\ -U_0 n_0 & \frac{\hbar^2 k^2}{2m} + U_0 n_0 + \hbar w \end{bmatrix} = 0. \tag{2.27}$$

This condition gives, finally, the dispersion relation that we are looking for:

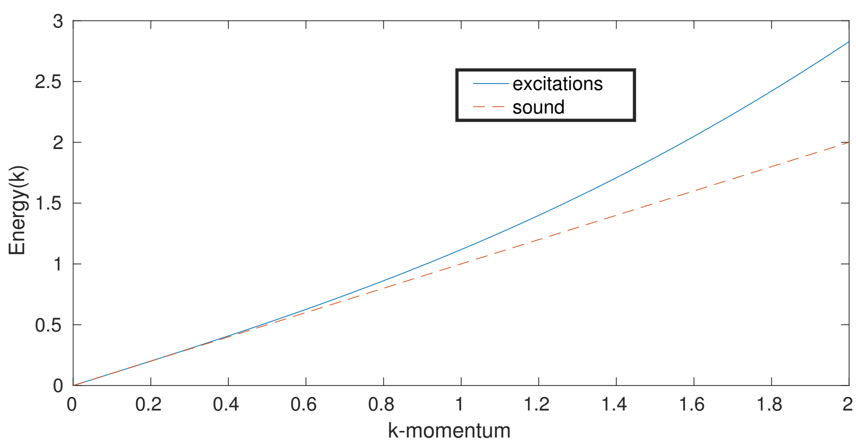

Figure 2.2: Spectrum of Bogoliubov excitations

$$\hbar w = \sqrt{\frac{h^4 k^4}{4m^2} + \frac{n_0 U_0 h^2 k^2}{m}}. \tag{2.28}$$

This dispersion relation displays different features for low energy and high energy limits. For small k's, energy is linear in k,

$$\hbar w \approx \sqrt{\frac{n_0 U_0}{m}} \hbar k = s\hbar k \tag{2.29}$$

where s is the velocity of sound in uniform gas. For large k's, $E = \hbar^2 k^2/2m + n_0 U_0$. Which means the energy-momentum relation of these excitations looks like that of particles in high energy regime, and that of waves in low energy regimes.

Chapter 3

Coherent State Path Integral

3.1 Feynman Path Integral

We use partition function to calculate the ground state energy of solitons. The mathematics of partition function is same with of Feynman path integral, which is an alternate formulation of quantum mechanics, with periodic boundary conditions (PBCs). Therefore, we begin with constructing path integral and mainly follow Ref. [25].

The evolution of a wavefunction in time is determined by the corresponding Hamiltonian,

$$i\hbar\,\partial_t\,|\Psi\rangle = \hat{H}\,|\Psi\rangle\,. \tag{3.1}$$

The wavefunction in a later time is given as $|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar}\,|\Psi(0)\rangle$. If the initial time is set at t rather than zero, then, this relation becomes $|\Psi(t')\rangle = e^{-i\hat{H}(t'-t)/\hbar}\,|\Psi(t)\rangle$. Position space representations are

$$\begin{aligned}\langle x'|\,\Psi(t')\rangle &= \langle x'|\,e^{-i\hat{H}(t'-t)/\hbar}\Psi(t)\rangle \\ \Psi(x',t') &= \langle x'|\,e^{-i\hat{H}(t'-t)/\hbar}\Psi(t)\rangle.\end{aligned} \tag{3.2}$$

When we insert a complete set, wavefunction at t' is

$$\Psi(x',t') = \langle x'| e^{-i\hat{H}(t'-t)/\hbar} \int dx\, |x\rangle \langle x| \Psi(t)\rangle$$
$$\Psi(x',t') = \int dx\, \langle x'| e^{-i\hat{H}(t'-t)/\hbar} |x\rangle \langle x| \Psi(t)\rangle$$
$$\Psi(x',t') = \int dx\, \langle x'| e^{-i\hat{H}(t'-t)/\hbar} |x\rangle\, \Psi(x,t). \tag{3.3}$$

$U(x',t';x,t)$ is called "propagator" or the corresponding Green's function and defined as

$$U(x',t';x,t) \equiv \langle x'| e^{-i\hat{H}(t'-t)/\hbar} |x\rangle\,. \tag{3.4}$$

It gives the probability amplitude. It is hard to calculate propagator for finite $t'-t$ values . The approach is writing the time interval $t'-t$ as $N\Delta t$, evaluating propagator for that infinitesimal time with an approximation, and then merge them again.

Rewriting the propagator as

$$e^{-i\hat{H}(t_f-t_i)/\hbar} = \left[e^{-i\hat{H}\Delta t/\hbar}\right]^N \tag{3.5}$$

and then inserting N-1 resolution of identity gives

$$\begin{aligned} U(x_ft_f,x_it_i) &= \langle x_f| \left[e^{-i\frac{\Delta t}{\hbar}\hat{H}}\right]^N |x_i\rangle \\ &= \int \prod_{k=1}^{N-1} dx_k\, \langle x_f| e^{-i\frac{\Delta t}{\hbar}\hat{H}} |x_{N-1}\rangle \langle x_{N-1}| e^{-i\frac{\Delta t}{\hbar}\hat{H}} |x_{N-2}\rangle \times \\ &\quad \times \langle x_{N-2}| \ldots e^{-i\frac{\Delta t}{\hbar}\hat{H}} |x_1\rangle \langle x_1| e^{-i\frac{\Delta t}{\hbar}\hat{H}} |x_i\rangle\,. \end{aligned} \tag{3.6}$$

In the Hamiltonian, we have $\hat{x}$-terms in potential energy and $\hat{p}$-terms in kinetic energy separately so $\langle p_n| H(\hat{p},\hat{x}) |x_{n-1}\rangle = H(p_n,x_{n-1})$. But in $e^{-i\frac{\Delta t}{\hbar}H}$ there are terms in which $\hat{p}$ and $\hat{x}$ are mixed in order, therefore we can not write

$$\langle x_n| e^{-i\frac{\Delta t}{\hbar}H} |x_{n-1}\rangle = e^{-i\frac{\Delta t}{\hbar}H(p_n,x_{n-1})}$$

directly. For such calculations "normal ordered Hamiltonian" is used to describe in which all $\hat{p}$ s appear on the left of $\hat{x}$ s in each term, so $\hat{x}$ operators act on the right and all $\hat{p}$ operators on the left. Normal ordering is showed as

$$:e^{-i\frac{\Delta t}{\hbar}H}:\,. \tag{3.7}$$

For our calculation converting the exponential in ordered form gives an error order of Δx^2 [25].

We insert another complete set, the set of momentum operator eigenstates,

$$\langle x_n| e^{-i\frac{\Delta t}{\hbar}H(\hat{p},\hat{x})} |x_{n-1}\rangle = \int dp_n \langle x_n| p_n\rangle \langle p_n| : e^{-i\frac{\Delta t}{\hbar}H(\hat{p},\hat{x})} : |x_{n-1}\rangle . \tag{3.8}$$

By using $\langle x|p\rangle = e^{ixp/\hbar}/\sqrt{2\pi\hbar}$, the propagator of Δt becomes

$$\begin{aligned} \langle x_n| e^{-i\frac{\Delta t}{\hbar}H(\hat{p},\hat{x})} |x_{n-1}\rangle &= \int \frac{d^3 p_n}{(2\pi\hbar)^3} \langle x_n| p_n\rangle \langle p_n| : e^{-i\frac{\Delta t}{\hbar}H(\hat{p},\hat{x})} : |x_{n-1}\rangle \\ &= \int d^3 p_n \frac{1}{(2\pi\hbar)^3} e^{ip_n(x_n - x_{n-1})} e^{-i\frac{\Delta t}{\hbar}H(p_n, x_{n-1})}. \end{aligned} \tag{3.9}$$

This integral can be evaluated by writing Hamiltonian as $p^2/2m + V(x)$ and taking the Gaussian integral of p. Inserting this matrix elements into propagator gives

$$U(x_f t_f, x_i t_i) = \lim_{N\to\infty} \int \prod_{k=1}^{N-1} dx_k \left(\frac{m}{2\pi i \Delta t \hbar}\right)^{\frac{3N}{2}} e^{\sum_{k=1}^{N} \frac{i\Delta t}{\hbar}\left\{\frac{m}{2}\left(\frac{x_k - x_{k-1}}{\Delta t}\right)^2 - V(x_{k-1})\right\}}. \tag{3.10}$$

In the continuum limit, we do the following small modifications

$$\sum_{k=1}^{N} \Delta t \to \int_{t_i}^{t_f} dt, \qquad \frac{x_k - x_{k-1}}{\Delta t} \to \partial_t \psi\big|_{t=n\Delta t}, \qquad \prod_{k=1}^{N-1} \to \int D[x(t)] \tag{3.11}$$

and the propagator becomes

$$U(x_f t_f, x_i t_i) = \lim_{N\to\infty} \int D[x(t)] \left(\frac{m}{2\pi i \Delta t \hbar}\right)^{\frac{3N}{2}} e^{\frac{i}{\hbar}\left\{\int_{t_i}^{t_f} dt \frac{m}{2}\left(\frac{dx}{dt}\right)^2 - V(x(t))\right\}}. \tag{3.12}$$

This formulation of time evolution of a quantum state consists all information of a quantum mechanical system and called “path integral formulation” of quantum mechanics.

3.2 Coherent States

To generalize Feynman path integral to many body systems, we need a complete basis. Coherent states form a useful basis that are very easy to handle in second quantized notation. We will only briefly give the relations we are going to use to construct the many body path integral. That is a quite important topic frequently used especially in quantum optics and is discussed in detail in many quantum mechanics and many body textbooks, e.g.Ref. [26, 27].

Coherent states are eigenstates of annihilation operators. Let $|\psi\rangle$ be a bosonic coherent state and $\overline{\psi}$ be the complex conjugate of ψ, then

$$\begin{aligned} a\,|\psi\rangle &= \psi\,|\psi\rangle \\ \langle\psi|\,a^\dagger &= \langle\psi|\,\overline{\psi}. \end{aligned} \tag{3.13}$$

Writing $|\psi\rangle$ in terms of occupying number representation

$$\begin{aligned} |\psi\rangle &= \sum_{n=0}^{\infty} c_n\,|n\rangle \\ \sum_{n=0}^{\infty} \underbrace{c_n a\,|n\rangle}_{c_n\sqrt{n}|n-1\rangle} &= \sum_{n=0}^{\infty} \psi c_n\,|n\rangle \\ \sum_{n=1}^{\infty} c_n\sqrt{n}\,|n-1\rangle &= \sum_{n=0}^{\infty} \psi c_n\,|n\rangle \qquad\qquad m \equiv n-1 \\ \sum_{m=0}^{\infty} c_{m+1}\sqrt{m+1}\,|m\rangle &= \sum_{n=0}^{\infty} \psi c_n\,|n\rangle \end{aligned} \tag{3.14}$$

gives a recursion relation such that $c_{n+1} = c_n\psi/\sqrt{n+1}$.

$$\begin{aligned} c_1 &= \frac{\psi}{\sqrt{1}}c_0 \\ c_2 &= \frac{\psi^2}{\sqrt{2}}c_0 \\ c_n &= \frac{\psi^n}{\sqrt{n!}}c_0 \end{aligned} \tag{3.15}$$

Coherent state is written as

$$|\psi\rangle = c_0 \sum_{n_0}^{\infty} \frac{\psi^n}{\sqrt{n!}}\,|n\rangle \tag{3.16}$$

where the coefficient c_0 comes from normalization

$$\begin{aligned}\langle\psi|\,\psi\rangle &= |c_0|^2\sum_{m,n}\langle m|\,\frac{\overline{\psi}^m}{\sqrt{m!}}\frac{\psi^n}{\sqrt{n!}}\,|n\rangle\\ &= |c_0|^2\sum_n\frac{|\psi|^{2n}}{n!}\\ &= |c_0|^2 e^{|\psi|^2/2}\end{aligned}\tag{3.17}$$

as $c_0 = \exp(-|\psi|^2/2)$.

$$|\psi\rangle = e^{-\frac{\psi^*\psi}{2}}\sum_{n_0}^{\infty}\frac{\psi^n}{\sqrt{n!}}\,|n\rangle\,. \tag{3.18}$$

Their overlap is given by

$$\begin{aligned}\langle\psi|\,\psi'\rangle &= e^{-\frac{|\psi|^2}{2}}e^{-\frac{|\psi'|^2}{2}}\sum_{n,m}\langle n|\,\frac{\overline{\psi}^{*n}}{\sqrt{n!}}\frac{\psi'^m}{\sqrt{m!}}\,|m\rangle\\ &= e^{-\frac{|\psi|^2}{2}}e^{-\frac{|\psi'|^2}{2}}\sum_n\frac{(\overline{\psi}\psi')^n}{n!}\exp\left\{\overline{\psi}\psi' - \frac{|\psi|^2}{2} - \frac{|\psi'|^2}{2}\right\}.\end{aligned}\tag{3.19}$$

Their closure relation is

$$\int\frac{d\psi d\overline{\psi}}{2i\pi}e^{-\overline{\psi}\psi}\,|\psi\rangle\,\langle\psi| = \mathbb{1}. \tag{3.20}$$

In many body systems for clarity we address these relations as

$$\begin{aligned}a_i\,|\psi\rangle &= \psi_i\,|\psi\rangle\\ \langle\psi|\,a_i^\dagger &= \langle\psi|\,\overline{\psi}_i\\ \langle\psi|\,\psi'\rangle &= \exp\left\{\sum_i\overline{\psi_i}\psi_i'\right\}\end{aligned}\tag{3.21}$$

and

$$\int d[\psi^*,\psi]\exp\left\{-\sum_i\psi_i^*\psi_i\right\}|\psi\rangle\,\langle\psi| = \mathbb{1} \tag{3.22}$$

in the non-normalized form.

3.3 Quantum Partition Function of many body Systems

Partition function of a quantum system in grand canonical ensemble is

$$\begin{aligned}
Z &= Tr(e^{-\beta(H-\mu N)}) \\
Z &= \sum_n \langle n| e^{-\beta(H-\mu N)} |n\rangle .
\end{aligned} \tag{3.23}$$

When we insert the closure relation of coherent states into the partition function, we get

$$\begin{aligned}
Z &= \sum_n \langle n| e^{-\beta(H-\mu N)} |n\rangle \\
&= \sum_n \langle n| \int d[\psi^*, \psi] e^{-\sum_i \psi_i^* \psi_i} |\psi\rangle \langle\psi| e^{-\beta(H-\mu N)} |n\rangle \\
&= \int d[\psi^*, \psi] e^{-\sum_i \psi_i^* \psi_i} \sum_n \langle n |\psi\rangle \langle\psi| e^{-\beta(H-\mu N)} |n\rangle \\
&= \int d[\psi^*, \psi] e^{-\sum_i \psi_i^* \psi_i} \sum_n \langle\psi| e^{-\beta(H-\mu N)} |n\rangle \langle n |\psi\rangle \\
&= \int d[\psi^*, \psi] e^{-\sum_i \psi_i^* \psi_i} \langle\psi| e^{-\beta(H-\mu N)} \sum_n |n\rangle \langle n |\psi\rangle \\
&= \int d[\psi^*, \psi] e^{-\sum_i \psi_i^* \psi_i} \langle\psi| e^{-\beta(H-\mu N)} |\psi\rangle .
\end{aligned} \tag{3.24}$$

The integrand of Z looks like the propagator in which the initial state is same with the final state. Therefore, the rest of the formulation is same with that of path integral. We divide β into infinitesimal parts.

$$\begin{aligned}
Z &= \int d[\psi^*, \psi] e^{-\sum_i \psi_i^* \psi_i} \langle\psi| e^{-\Delta\beta(H-\mu N)} e^{-\Delta\beta(H-\mu N)} e^{-\Delta\beta(H-\mu N)} e^{-\Delta\beta(H-\mu N)} |\psi\rangle . \\
&= \int d[\psi_N^*, \psi_N] e^{-\sum_i \psi_{N,i}^* \psi_{N,i}} \int \left(\prod_{n=1}^{N-1} d[\psi_n^*, \psi_n] \right) e^{-\sum_{i,n=1}^{n=N-1} \psi_{n,i}^* \psi_{n,i}} \times \\
&\times \langle\psi_N| e^{-\Delta\beta(H-\mu N)} |\psi_{N-1}\rangle \langle\psi_{N-1}| e^{-\Delta\beta(H-\mu N)} |\psi_{N-2}\rangle \ldots \langle\psi_1| e^{-\Delta\beta(H-\mu N)} |\psi_N\rangle
\end{aligned} \tag{3.25}$$

where we label the coherent state set in the original closure relation as the N^{th} state and we take $\psi_0 = \psi_N$ which corresponds to the periodic boundary conditions.

$$Z = \int \left(\prod_{n=1}^{N} d[\psi_n^*, \psi_n] \right) e^{-\sum_{i,n=1}^{n=N} \psi_{n,i}^* \psi_{n,i}} \left(\prod_{n=1}^{N} \langle \psi_n | \, e^{-\Delta\beta(H-\mu N)} \, | \psi_{n-1} \rangle \right). \quad (3.26)$$

$\Delta\beta$ is too small since we're gonna take the limit $N \to \infty$ as in the case of path integral. Inserting the matrix element

$$\begin{aligned} \langle \psi_n | \, e^{-\Delta\beta(H-\mu N)} \, | \psi_{n-1} \rangle &= \langle \psi_n | \, 1 - \Delta\beta(H - \mu N) + O(\Delta\beta^2) \, | \psi_{n-1} \rangle \\ &= \langle \psi_n \, | \psi_{n-1} \rangle - \Delta\beta \, \langle \psi_n | \, 1 - (H - \mu N) \, | \psi_{n-1} \rangle + O(\Delta\beta^2) \\ &= \langle \psi_n \, | \psi_{n-1} \rangle \left(1 - \Delta\beta \Big[H(\psi_n^*, \psi_{n-1}) - \mu N(\psi_n^*, \psi_{n-1}) \Big] \right). \end{aligned} \quad (3.27)$$

into the partition function results in

$$\begin{aligned} Z = & \int \left(\prod_{n=1}^{N} d[\psi_n^*, \psi_n] \right) e^{-\sum_{i,n=1}^{n=N} \psi_{n,i}^* \psi_{n,i}} \times \\ & \times \prod_{n=1}^{N} \left[\Big(1 - \Delta\beta H(\psi_n^*, \psi_{n-1}) - \Delta\beta\mu N(\psi_n^*, \psi_{n-1}) \Big) \langle \psi_n \, | \psi_{n-1} \rangle \right] \\ = & \int \left(\prod_{n=1}^{N} d[\psi_n^*, \psi_n] \right) e^{-\sum_{i,n=1}^{n=N} \psi_{n,i}^* \psi_{n,i}} e^{\sum_{i,n=1}^{n=N} \psi_{n,i}^* \psi_{n-1,i}} \times \\ & \times e^{-\sum_{n=1}^{n=N} \Delta\beta \left[H(\psi_n^*, \psi_{n-1}) - \mu N(\psi_n^*, \psi_{n-1}) \right]}. \end{aligned} \quad (3.28)$$

In the continuum limit, like in the case of propagator,

$$\Delta\beta \sum_{n=1}^{N} \to \int_0^\beta d\tau, \quad (3.29)$$

where τ can be thought as imaginary time.

$$\frac{\psi_n - \psi_{n-1}}{\Delta\beta} = \partial_\tau \psi \, |_{\tau = n\Delta\beta}, \qquad \prod_{n=1}^{N} d[\psi_n^*, \psi_n] \to D(\psi^*, \psi) \quad (3.30)$$

which make Z looks like

$$
\begin{aligned}
Z &= \int D(\psi^*,\psi) \exp\left\{ \sum_{n=1}^{N} \Delta\beta \left(-\psi_n^* \frac{\psi_n - \psi_{n-1}}{\Delta\beta} - (H-\mu N) \right) \right\} \\
&= \int D(\psi^*,\psi) \exp\left\{ \int_0^\beta d\tau (\psi_n^* \partial_\tau \psi_n + H - \mu N) \right\} \\
&= \int D(\psi^*,\psi) \exp\left\{ \int_0^\beta d\tau (\psi(\tau)^* \partial_\tau \psi(\tau) + H(\psi^*(\tau),\psi(\tau)) - \mu N(\psi^*(\tau),\psi(\tau))) \right\},
\end{aligned}
\tag{3.31}
$$

where the limits of integral are $\psi^*(\beta) = \psi^*(0)$ and $\psi(\beta) = \psi^*(0)$. Here we define $\psi_n^* \equiv \psi^*(\tau)$ and $\psi_{n-1} \equiv \psi(\tau)$.

3.4 Quantum Partition Function for 1D Bose gas

The general many body Hamiltonian for a grand canonical system in second quantized notation is

$$
H - \mu N = \sum_{ij} (h_{ij} - \mu\delta_{ij}) a_i^\dagger a_j + \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_k a_l. \tag{3.32}
$$

For a Bose gas, in mean field approach

$$
h_{ij} = h_{ii}\delta_{ij} \qquad \textit{and} \qquad V_{ijkl} = U_0 \delta_{\substack{i+j,\\ k+l}}, \tag{3.33}
$$

and the exponent in partition function therefore becomes

$$
\begin{aligned}
H\big(\psi^*(\tau),\psi(\tau)) - \mu N(\psi^*(\tau),\psi(\tau))\big) =& \frac{\langle\psi(\tau)|\,(H-\mu N)\,|\psi(\tau)\rangle}{\langle\psi(\tau)|\,\psi(\tau)\rangle} \\
=& \frac{\sum_{ij} \langle\psi(\tau)|\,(h_{ij} - \mu\delta_{ij}) a_i^\dagger a_j\,|\psi(\tau)\rangle}{\langle\psi(\tau)|\,\psi(\tau)\rangle} \\
&+ \frac{\sum_{ijkl} U_0 \delta_{\substack{i+j,\\ k+l}} \langle\psi(\tau)|\, a_i^\dagger a_j^\dagger a_k a_l\,|\psi(\tau)\rangle}{\langle\psi(\tau)|\,\psi(\tau)\rangle}.
\end{aligned}
\tag{3.34}
$$

Here we use

$$a_i \left|\psi(\tau)\right\rangle = \psi_i(\tau) \left|\psi(\tau)\right\rangle \qquad and \qquad \left\langle\psi(\tau)\right| a_j^\dagger = \overline{\psi}_j(\tau) \left\langle\psi(\tau)\right|, \tag{3.35}$$

where $\psi(\tau)$ is the n^{th} coherent state set ($\tau = n\Delta\beta$).

$$\begin{aligned} H\big(\psi^*, \psi) - \mu N(\psi^*, \psi)\big) =& \frac{\sum_{ij}(h_{ij} - \mu\delta_{ij})\bar{\psi}_i(\tau)\psi_j(\tau) \left\langle\psi(\tau)\right|\psi(\tau)\rangle}{\left\langle\psi(\tau)\right|\psi(\tau)\rangle} \\ &+ \frac{\sum_{ijkl} U_0 \delta_{\substack{i+j,\\k+l}} \bar{\psi}_i(\tau)\bar{\psi}_j(\tau)\psi_k(\tau)\psi_l(\tau) \left\langle\psi(\tau)\right|\psi(\tau)\rangle}{\left\langle\psi(\tau)\right|\psi(\tau)\rangle}. \end{aligned} \tag{3.36}$$

Substituting into partition function and converting to x-space with a Fourier transform gives

$$\begin{aligned} Z = \int D[\overline{\psi}, \psi] \exp\Bigg\{ - \int_0^\beta d\tau \int d^d x \Big[& \overline{\psi}(x,\tau)\big(\partial_t + H_0 - \mu\big)\psi(x,\tau) \\ & + \frac{U_0}{2\beta}\big(\overline{\psi}(x,\tau)\psi(x,\tau)\big)^2 \Big]\Bigg\}. \end{aligned} \tag{3.37}$$

3.4.1 Matsubara Frequency Representation

Matsubara frequencies are discrete imaginary frequencies and are used in field theory. To write the action in Matsubara frequency representation, we use the following Fourier transforms

$$\psi(\tau) = \frac{1}{\sqrt{\beta}} \sum_{\omega_n} \psi_n e^{i\omega n \tau}, \qquad \psi_{\omega_n} = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau \psi(\tau) e^{-iw_n\tau} \tag{3.38}$$

where $w_n = 2n\pi/\beta$ for bosons.

$$\begin{aligned} Z = \int D[\overline{\psi}, \psi] \exp\Bigg\{ - \int_0^\beta d\tau \int d^d x \Big[& \frac{1}{\beta}\sum_{w_n} \overline{\psi}_{w_n}(x) e^{-iw_n\tau} \big(\underbrace{\partial_\tau}_{iw_m} + H_0 - \mu\big) \\ \times \frac{1}{\beta}\sum_{w_m} \psi_{w_m}(x) e^{iw_m\tau} + & \frac{U_0}{2\beta}\big(\frac{1}{\beta}\frac{1}{\beta}\frac{1}{\beta}\frac{1}{\beta} \sum_{w_n}\sum_{w_m}\sum_{w_p}\sum_{w_r} \overline{\psi}_{w_n}(x)\overline{\psi}_{w_m}(x)\psi_{w_p}(x) \\ \times \psi_{w_r}(x) e^{-iw_n\tau} e^{-iw_m\tau} e^{iw_p\tau} e^{iw_r\tau}\big) \Big]\Bigg\}, & \end{aligned} \tag{3.39}$$

by using

$$\int_0^\beta d\tau e^{i(w_n - w_m)\tau} = \beta\delta_{w_n,w_m}; \tag{3.40}$$

becomes

$$Z = \int D[\overline{\psi},\psi] \exp\Big\{ -\frac{1}{\beta}\sum_{w_n}\sum_{w_m}\int d^d x \overline{\psi}_{w_n}(x)\psi_{w_m}(x)(iw_m + H_0 - \mu)\times$$
$$\times \underbrace{\int_0^\beta d\tau e^{-iw_n\tau}e^{iw_m\tau}}_{\beta\delta_{w_n,w_m}}\Big\} + exp\Big\{ -\frac{U_0}{2\beta}\frac{1}{\beta^2}\sum_{w_n}\sum_{w_m}\sum_{w_p}\sum_{w_r}\int d^d x \overline{\psi}_{w_n}(x)\times$$
$$\times \overline{\psi}_{w_m}(x)\psi_{w_p}(x)\psi_{w_r}(x)\underbrace{\int_0^\beta d\tau e^{i[(w_p+w_r)-(w_n+w_m)]}}_{\beta\delta_{w_n+w_m,\, w_p+w_r}}\Big\}. \tag{3.41}$$

In terms of the action of Bose gas

$$Z = \int D[\overline{\psi},\psi]\exp\{-S[\overline{\psi},\psi]\}. \tag{3.42}$$

We will use this functional,the action of Bose gas, to obtain free energy of solitons by evaluating Gaussian integral. For this purpose, we write the action in discrete form in x as

$$S[\overline{\psi},\psi] = A\sum_{x=0}^{N}\Delta x\Big\{\sum_{w_n}\overline{\psi}_{n,x}(iw_n - \mu)\psi_{n,x} \tag{3.43}$$

$$+\sum_{w_n} -\frac{\overline{\psi}_{n,x}}{2m\Delta x^2}(\psi_{n,x+1} - 2\psi_{n,x} + \psi_{n,x-1}) \tag{3.44}$$

$$+\frac{g}{2\beta}\sum_{w_{n,m,p,r}}\overline{\psi}_{n,x}\overline{\psi}_{m,x}\psi_{p,x}\psi_{r,x}\delta_{w_n+w_m,\, w_p+w_r}\Big\}. \tag{3.45}$$

The partition function is of the form

$$I = \int dx e^{-s(x)} \tag{3.46}$$

For such integrals, the major contribution comes from $s(x_0)$, where x_0 is the point that makes s minimum. It is called "minimum phase integration". Taylor expansion of $s(x)$ about x_0 is

$$\begin{aligned} s(x) &= s(x_0) + s'(x_0)(x - x_0) + s''(x_0)\frac{(x - x_0)^2}{2} + O(\Delta x^3) + \cdots \\ s(x) &\approx s(x_0) + s''(x_0)\frac{(x - x_0)^2}{2}. \end{aligned} \tag{3.47}$$

If we replace x in $s(x)$ with $x + x'$ and keep only the terms up to the second order in x', we end up with the above relation. Replacing $\psi_{n,x}$ with $\psi^0_{n,x} + \psi^1_{n,x}$ where $\psi^0_{n,x}$ is the solution that gives the minimum action that we can find by taking the derivative of action in Eq. 3.39

$$\begin{aligned} \frac{\partial S}{\partial \overline{\psi}} &= \frac{\partial}{\partial \overline{\psi}} \left\{ \int_0^\beta \int d^d r \left[\overline{\psi}(x,\tau)\big(\partial_t + H_0 - \mu\big)\psi(x,\tau) + \frac{g}{2}\big(\overline{\psi}(x,\tau)\psi(x,\tau)\big)^2 \right] \right\} \\ &= \int_0^\beta \int d^d r \Big[\underbrace{\big(\partial_t + H_0 - \mu\big)\psi(x,\tau) + \frac{g}{2} 2\big(\overline{\psi}(x,\tau)\psi(x,\tau)\big)\psi(x,\tau)}_{=0} \Big] = 0 \end{aligned} \tag{3.48}$$

By taking $\psi(x,\tau)$ τ-independent

$$\begin{aligned} (H_0 - \mu)\psi + g|\psi|^2\psi &= 0 \\ H_0\psi + g|\psi|^2\psi &= \mu\psi \end{aligned} \tag{3.49}$$

is actually time independent Gross-Pitaevskii equation. $\psi^0_{n,x}$ are therefore the exact solutions of GP namely uniform Bose gas and solitons. Replacing ψ with

$\psi^0 + \psi^1$ in the action given in the Eqn.3.45:

$$S = A \sum_{x=0}^{N} \Delta x \Bigg\{ \sum_{w_n} (\overline{\psi}^0_{n,x} + \overline{\psi}^1_{n,x})(iw_n - \mu)(\psi^0_{n,x} + \psi^1_{n,x}) \tag{3.50}$$

$$+ \sum_{w_n} - \frac{\overline{\psi}^0_{n,x} + \overline{\psi}^1_{n,x}}{2m\Delta x^2}(\psi^0_{n,x+1} + \psi^1_{n,x+1} - 2\psi^0_{n,x} - 2\psi^1_{n,x} + \psi^0_{n,x-1} + \psi^1_{n,x-1}) \tag{3.51}$$

$$+ \frac{g}{2\beta} \sum_{w_{n,m,p,r}} (\overline{\psi}^0_{n,x} + \overline{\psi}^1_{n,x})(\overline{\psi}^0_{m,x} + \overline{\psi}^1_{m,x})(\psi^0_{p,x} + \psi^1_{p,x})(\psi^0_{r,x} + \psi^1_{r,x})\delta_{\substack{w_n+w_m,\\ w_p+w_r}} \Bigg\}, \tag{3.52}$$

$$\begin{aligned} S = A \sum_{x=0}^{N} \Delta x \Bigg\{ \sum_{w_n} \big(& i\overline{\psi}^0_{n,x} w_n \psi^0_{n,x} + i\overline{\psi}^0_{n,x} w_n \psi^1_{n,x} + \mu\overline{\psi}^0_{n,x}\psi^0_{n,x} + \mu\overline{\psi}^0_{n,x}\psi^1_{n,x} \\ & + i\overline{\psi}^1_{n,x} w_n \psi^0_{n,x} + i\overline{\psi}^1_{n,x} w_n \psi^1_{n,x} - \mu\overline{\psi}^1_{n,x}\psi^0_{n,x} - \mu\overline{\psi}^1_{n,x}\psi^1_{n,x} \big) \\ + \sum_{w_n} - \frac{1}{2m\Delta x^2} \big(& \overline{\psi}^0_{n,x}\psi^0_{n,x+1} + \overline{\psi}^0_{n,x}\psi^1_{n,x+1} - 2\overline{\psi}^0_{n,x}\psi^0_{n,x} \\ & - 2\overline{\psi}^0_{n,x}\psi^1_{n,x+1} + \overline{\psi}^0_{n,x}\psi^0_{n,x-1} + \overline{\psi}^0_{n,x}\psi^1_{n,x-1} \\ & + \overline{\psi}^1_{n,x}\psi^0_{n,x+1} + \overline{\psi}^1_{n,x}\psi^1_{n,x+1} - 2\overline{\psi}^1_{n,x}\psi^0_{n,x} \\ & - 2\overline{\psi}^1_{n,x}\psi^1_{n,x+1} + \overline{\psi}^1_{n,x}\psi^0_{n,x-1} + \overline{\psi}^1_{n,x}\psi^1_{n,x-1} \big) \\ + \sum_{w_{n,m,p,r}} \frac{g}{2\beta}\delta_{\substack{w_n+w_m,\\ w_p+w_r}} \big(& \overline{\psi}^0_{n,x}\overline{\psi}^0_{m,x}\psi^0_{p,x+1}\psi^0_{r,x+1} + \overline{\psi}^0_{n,x}\overline{\psi}^0_{m,x}\psi^0_{p,x+1}\psi^1_{r,x+1} \\ & + \overline{\psi}^0_{n,x}\overline{\psi}^0_{m,x}\psi^1_{p,x+1}\psi^0_{r,x+1} + \overline{\psi}^0_{n,x}\overline{\psi}^0_{m,x}\psi^1_{p,x+1}\psi^1_{r,x+1} \\ & + \overline{\psi}^0_{n,x}\overline{\psi}^1_{m,x}\psi^0_{p,x+1}\psi^0_{r,x+1} + \overline{\psi}^0_{n,x}\overline{\psi}^1_{m,x}\psi^0_{p,x+1}\psi^1_{r,x+1} \\ & + \overline{\psi}^0_{n,x}\overline{\psi}^1_{m,x}\psi^1_{p,x+1}\psi^0_{r,x+1} + \overline{\psi}^0_{n,x}\overline{\psi}^1_{m,x}\psi^1_{p,x+1}\psi^1_{r,x+1} \\ & + \overline{\psi}^1_{n,x}\overline{\psi}^0_{m,x}\psi^0_{p,x+1}\psi^0_{r,x+1} + \overline{\psi}^1_{n,x}\overline{\psi}^0_{m,x}\psi^0_{p,x+1}\psi^1_{r,x+1} \\ & + \overline{\psi}^1_{n,x}\overline{\psi}^0_{m,x}\psi^1_{p,x+1}\psi^0_{r,x+1} + \overline{\psi}^1_{n,x}\overline{\psi}^0_{m,x}\psi^1_{p,x+1}\psi^1_{r,x+1} \\ & + \overline{\psi}^1_{n,x}\overline{\psi}^1_{m,x}\psi^0_{p,x+1}\psi^0_{r,x+1} + \overline{\psi}^1_{n,x}\overline{\psi}^1_{m,x}\psi^0_{p,x+1}\psi^1_{r,x+1} \\ & + \overline{\psi}^1_{n,x}\overline{\psi}^1_{m,x}\psi^1_{p,x+1}\psi^0_{r,x+1} + \overline{\psi}^1_{n,x}\overline{\psi}^1_{m,x}\psi^1_{p,x+1}\psi^1_{r,x+1} \big) \end{aligned} \tag{3.53}$$

That is a bit lengthy equation but will get simplified when we insert wave-functions of uniform functions of Bose gas and of black soliton in the following chapters to form a calculable Gaussian integral. For now, we leave it here and turn to how to calculate ground state energy of 1D Bose gas.

Chapter 4

Energy of uniform solution

In the case of uniform solution of Gross Pitaevskii, the total energy of 1D BEC can be calculated via the usual procedure. We can get the first order energy by using exact solutions of GP equations and the second order correction to this energy by summing up the ground state energies of the excitations.

4.1 First order energy

First order energy of the uniform solution is simply $\langle\psi| H |\psi\rangle$ where $\psi = \sqrt{n}\exp(i\mu t/\hbar)$, $n = N/V$. Hamiltonian is written with Gross Pitaevskii,

$$\begin{aligned} \langle\psi| H |\psi\rangle = E(\psi) &= \int dr \left[\frac{\hbar^2}{2m}|\nabla\psi(r)|^2 + V(r)|\psi(r)|^2 + \frac{1}{2}U_0|\psi(r)|^4\right] \\ &= \frac{U_0 N^2}{2V} \end{aligned} \tag{4.1}$$

4.2 Second order energy

As it is mentioned above, in GP approximation, all the particles are assumed to be in the condensate ground state. In order to describe the behaviour of condensate better, we can use Bogoliubov approximation which corresponds to allowing a few particles to occupy excited states while the majority of them still remain in the condensate state.

In chapter 2, we find the spectrum of the quantum fluctuations on the background of uniform gas as

$$\hbar w = \sqrt{\frac{h^4 k^4}{4m^2} + \frac{n_0 U_0 h^2 k^2}{m}}. \tag{4.2}$$

We can,in principle, find the contribution of these elementary excitations to the ground state energy by summing up the ground state energies of these excitations, $\sum_{k=0}^{\infty} \hbar w/2$, however this sum does not converge. To find that contribution a more detailed examination [20, 22] in which 2^{nd} order Born approximation is needed.

The Hamiltonian of weakly interacting Bose gas in second quantized notation is

$$\hat{H} = \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k + \frac{1}{2V} \sum_{k,k',q} V(q) a_{k+q}^\dagger a_{k'}^\dagger a_k a_{k'+q}. \tag{4.3}$$

In a condensate

$$\hat{N}_0 = a_0^\dagger a_0, \qquad \frac{N_0}{N} = O(1). \tag{4.4}$$

One of the mathematical differences between operators acting on a function and coefficients is the commutation relation. Since operators may not commute, we should respect their orders. Consider the operators $a_0^\dagger$ and a_0. They obey the commutation rule $a_0 a_0^\dagger - a_0^\dagger a_0 = 1$ but their non commuting nature is negligible since $a_0 \propto \sqrt{N_0} \gg 1$. This point is the starting point of Bogoliubov approximation. We consider a_0 as a coefficient instead of an operator and take $\sqrt{N_0}$.

In the sum, if we take $V(q)$ constant, U_0, the second part of the Hamiltonian is

$$H_I = \frac{1}{2V} U_0 \sum_{k,k',q} a^\dagger_{k+q} a^\dagger_{k'} a_k a_{k'+q}. \tag{4.5}$$

This four fold sum represents the momentums of 2 incoming and 2 outgoing particles, daggered ones represent momentums of particles after collision and the others correspond to the momentums of particles before collision. In this sum, there are small terms including a_k and $a^\dagger_k$ and greater terms including a_0. The greatest term is the one with 4 a_0s. Next greater terms have 3 a_0. But such interactions are not possible they do not satisfy momentum conservation. Therefore $3a_0$ terms do not exist at all. The second greatest terms are then the ones with $2a_0$s. The remaining terms are negligible.

There are six possibilities for a collision possess two of zero momentum. If the first and second ones are a_0, then $k+q=0$ and $k'=0$ results in $a^\dagger_0 a^\dagger_0 a_k a_q = a^\dagger_0 a^\dagger_0 a_k a_{-k}$. Other five possibilities are

$$\begin{array}{llrl}
1,3=0 & k+q=0 & k=0 \rightarrow & a^\dagger_0 a^\dagger_{k'} a_0 a_{k'} = a^\dagger_0 a^\dagger_k a_0 a_k \\
1,4=0 & k+q=0 & k'+q=0 \rightarrow & a^\dagger_0 a^\dagger_k a_k a_0 = a^\dagger_0 a^\dagger_k a_k a_0 \\
2,3=0 & k'=0 & k=0 \rightarrow & a^\dagger_q a^\dagger_0 a_0 a_q = a^\dagger_k a^\dagger_0 a_0 a_k \\
2,4=0 & k'=0 & k'+q=0 \rightarrow & a^\dagger_k a^\dagger_0 a_k a_0 = a^\dagger_k a^\dagger_0 a_k a_0 \\
3,4=0 & k=0 & k'+q=0 \rightarrow & a^\dagger_q a^\dagger_{-q} a_0 a_0 = a^\dagger_k a^\dagger_{-k} a_0 a_0.
\end{array} \tag{4.6}$$

The interaction part of H becomes

$$\hat{H}_I = \frac{U_0}{2V} N_0^2 + \frac{U_0}{V} N_0 \sum_{k \neq 0} \left[a^\dagger_k a_k + a^\dagger_{-k} a_{-k} + \frac{1}{2}(a_{-k} a_k + a^\dagger_k a^\dagger_{-k}) + O(N_0^0) \right]. \tag{4.7}$$

Here a_0 represents the particles in the condensate and a_k represents the excited particles. With this, the physical interpretation of $a^\dagger_k a_k$ term is the interaction between excited particles with the condensate. $a_{-k} a_k, a^\dagger_k a^\dagger_{-k}$ is for the particle annihilation and creation from the condensate to the excited states. Note that in this approximation the total number of excited particles is not conserved.

By writing the Hamiltonian in terms of the total particle number, $N = N_0 +$

$\sum a_k^\dagger a_k$,

$$\hat{H} = \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k + \frac{U_0}{2V}(N - \sum_{k\neq 0} a_k^\dagger a_k)^2 +$$
$$\frac{U_0}{V}(N - \sum_{k\neq 0} a_k^\dagger a_k) \sum_{k\neq 0} \left[a_k^\dagger a_k + a_{-k}^\dagger a_{-k} + \frac{1}{2}(a_{-k} a_k + a_k^\dagger a_{-k}^\dagger) \right] + O(N_0^0), \tag{4.8}$$

and neglecting the N_k^2 in the second term gives

$$\begin{aligned}
\hat{H} &= \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k + \frac{U_0}{2V} N^2 - \frac{2U_0}{2V} N \sum_{k\neq 0} a_k^\dagger a_k \\
&+ \left(\frac{U_0}{V} N - \frac{U_0}{V} \sum_{k\neq 0} a_k^\dagger a_k \right) [\cdots] + O(N_0^0) \\
&= \frac{U_0 N^2}{2V} + \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k + \sum_{k\neq 0} \left[-\frac{U_0 N}{V} + \frac{U_0 N}{V} [\cdots] + \underbrace{\frac{U_0}{V} \sum_{k\neq 0} a_k^\dagger a_k [\cdots]}_{=O(N_k)\cdot O(N_k)} \right]^0 \\
&= \frac{U_0 N}{2V} + \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k + \frac{U_0 N}{2V} \sum_{k\neq 0} (a_k a_{-k} + a_k^\dagger a_{-k}^\dagger + 2 a_k^\dagger a_k)
\end{aligned} \tag{4.9}$$

In Gross Pitaevskii approximation, we take U_0 as $4\pi\hbar^2 a/m$. For the ongoing calculation, however, that expression does not have enough accuracy. We need to replace the interaction potential between the particles from delta function to a Gaussian which is done by taking into account the second Born approximation.

4.2.1 Second Order Born Approximation

We may take the interaction as a perturbation if U_0 is small enough. In the perturbation theory, the energy correction to the nth energy state due to the interaction is given by

$$\Delta E = \langle \psi_n^0 | H' | \psi_n^0 \rangle + \sum_{m\neq n} \frac{| \langle \psi_m^0 | H' | \psi_n^0 \rangle |^2}{E_n^0 - E_m^0}. \tag{4.10}$$

The correction to the ground state energy, therefore, is

$$\Delta E = U_{00} + \sum_{m \neq 0} \frac{U_{0n} U_{n0}}{E_0 - E_n}. \tag{4.11}$$

The matrix element for a general case can be written as explained in Ref. [22]

$$U_{mn} = \langle k_1', k_2' | \, U \, | k_1, k_2 \rangle = \frac{1}{V} \int U(x) e^{-i\vec{k}\cdot\vec{x}} d^3x \tag{4.12}$$

where k_1, k_2 refers to the momentum of the particles before the collision, k_1', k_2' after the collision. $\vec{k} = \vec{k_2'} - \vec{k_2}$. In our case $k_1 = k_2 = 0$ since we look for the corrections to the ground state. Here U_{00} refers to the U_0 which is defined as $\int U(x) d^3x$. The major contribution to the integrand comes from the zero momenta terms and we neglect the others tiny corrections. That means $|U_{n0}|^2 = U_0^2$ and the interaction strength having the desired accuracy is

$$\begin{aligned}
U_{0,new} &= U_{0,old} + \frac{U_{old}^2}{V} \sum_{k \neq 0} \frac{2m}{\hbar^2(-2k^2)} \\
&= \frac{4\pi\hbar^2 a_{old}}{m} \left[1 + \frac{4\pi\hbar^2 a_{old}}{mV} \sum_{k \neq 0} \frac{2m}{\hbar^2(-2k^2)} \right].
\end{aligned} \tag{4.13}$$

When we substitute U_0 in H

$$\begin{aligned}
\hat{H} = {}& \frac{4\pi\hbar^2 a}{m} \left[1 + \frac{4\pi a}{V} \sum_{k \neq 0} \frac{1}{k^2} \right] \frac{N^2}{2V} + \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k \\
&+ \frac{4\pi\hbar^2 a}{m} \left[1 + \frac{4\pi a}{V} \sum_{k \neq 0} \frac{1}{k^2} \right] \frac{N}{2V} \sum_{k \neq 0} (a_k a_{-k} + a_k^\dagger a_{-k}^\dagger + 2 a_k^\dagger a_k)
\end{aligned} \tag{4.14}$$

we should neglect the correction of U_0 in the third term and keep it in the first term to achieve the consistency in precision,

$$\begin{aligned}
\hat{H} = {}& \frac{4\pi\hbar^2 a}{m} \left[1 + \frac{4\pi a}{V} \sum_{k \neq 0} \frac{1}{k^2} \right] \frac{N^2}{2V} + \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k \\
&+ \frac{4\pi\hbar^2 a}{m} \frac{N}{2V} \sum_{k \neq 0} (a_k a_{-k} + a_k^\dagger a_{-k}^\dagger + 2 a_k^\dagger a_k).
\end{aligned} \tag{4.15}$$

With this Hamiltonian, we aimed to calculate the corrected ground state energy. But, this expression of the Hamiltonain does not allow this since it has off-diagonal elements. To obtain the energy levels from H, we apply a linear transformation, Bogoliubov transformation, to diagonalize it. At the end, we will have a H in the form of $E_G + \sum_k E(K)\alpha_k^\dagger \alpha_k$ where $E(k)$ is the dispersion relation that we have found from BdG equations.

4.2.2 Bogoliubov Transformation

Hamiltonian is

$$H = H_1 + H_2 = H_0 + \sum_{k\neq 0}(A a_k a_{-k} + A a_k^\dagger a_{-k}^\dagger + C a_k^\dagger a_k) \tag{4.16}$$

where

$$H_1 = \frac{2\pi\hbar^2 a N^2}{mV}\left[1 + \frac{4\pi\hbar^2 a}{V\hbar^2}\sum_{k\neq 0}\frac{1}{k^2}\right] \tag{4.17}$$

$$A = \frac{2\pi\hbar^2 a N^2}{mV} \tag{4.18}$$

$$C = \frac{4\pi\hbar^2 a N^2}{mV} + \frac{\hbar^2 k^2}{2m}. \tag{4.19}$$

We replace the $\sum_k$ with $\sum_{k\neq 0}$ in the second term of H since $k=0$ contribution is already zero. We perform a linear transformation, L, on H_2 by defining new creation and anihilaiton operators α_k and $\alpha_k^\dagger$ such that

$$a_k = \frac{\alpha_k + L\alpha_{-k}^\dagger}{\sqrt{1-L^2}}, \qquad a_k^\dagger = \frac{\alpha_k^\dagger + L\alpha_{-k}}{\sqrt{1-L^2}}. \tag{4.20}$$

α_k and $\alpha_k^\dagger$ are the annihilation and creation operators of the elementary excitations rather then of particles, a_k and $a_k^\dagger$. They obey the same commutation relations,

$$\alpha_k \alpha_{k'} - \alpha_{k'}\alpha_k = 0 \tag{4.21}$$

$$\alpha_k \alpha_{k'}^\dagger - \alpha_{k'}\alpha_k^\dagger = \delta_{kk'}. \tag{4.22}$$

By writing the Hamiltonian in terms of α_k and $\alpha_k^\dagger$

$$
\begin{aligned}
H_2 &= \sum_{k\neq 0}(Aa_k a_{-k} + Aa_k^\dagger a_{-k}^\dagger + Ca_k^\dagger a_k) \\
&= \sum_{k\neq 0}\frac{1}{1-L^2}\Big[A(\alpha_k + L\alpha_{-k}^\dagger)(\alpha_{-k} + L\alpha_k^\dagger) + A(\alpha_k^\dagger + L\alpha_{-k})(\alpha_{-k}^\dagger + L\alpha_k) \\
&\qquad\qquad + C(\alpha_k^\dagger + L\alpha_{-k})(\alpha_k + L\alpha_{-k}^\dagger)\Big] \\
&= \sum_{k\neq 0}\frac{1}{1-L^2}\Big[\underbrace{(A + AL^2 + CL)\alpha_k\alpha_{-k} + (A + AL^2 + CL)\alpha_k^\dagger\alpha_{-k}^\dagger}_{\substack{\text{non-diagonal terms}\\ \text{should vanish}}} \\
&\qquad\qquad + \underbrace{(2AL + C)\alpha_k^\dagger\alpha_k + (2AL + CL^2)(1 + \alpha_k^\dagger\alpha_k)}_{\substack{\text{diagonal terms}\\ \text{+a constant}}}\Big],
\end{aligned}
\tag{4.23}
$$

we get the terms which should vanish. This, actually the condition that determines what L is:

$$A(1 + L^2) + CL = 0 \tag{4.24}$$

$$L = \frac{\pm\sqrt{C^2 - 4A^2} - C}{2A} \qquad \text{take} L = \frac{\sqrt{C^2 - 4A^2} - C}{2A}. \tag{4.25}$$

Plugging L into the remaining terms in the H_2 gives

$$H_2 = \sum_{k\neq 0}\left\{\frac{2AL + CL^2}{1 - L^2} + \frac{(4AL + C + CL^2)}{1 - L^2}\alpha_k^\dagger\alpha_k)\right\}. \tag{4.26}$$

First term contributes to the ground state energy together with H_1 and the second term is the dispersion relation.

$$
\begin{aligned}
E(k) &= \frac{4AL + C + CL^2}{1 - L^2} \\
&= \frac{4AL - C^2/LA}{1 + CL/A - 1} = \frac{4AL - C^2L/A}{2 + CL/A} = \frac{4A^2L - C^2L}{2A + CL}.
\end{aligned}
\tag{4.27}
$$

We define D as $C^2 - 4A^2$,

$$
\begin{aligned}
E(k) &= \frac{(\sqrt{D} - C)(4A^2 - C^2)}{2A} \Bigg/ \frac{4A^2 + C(\sqrt{D} - C)}{2A} \\
&= \frac{-D(\sqrt{D} - C)}{2A} \frac{4A^2 + C\sqrt{D} - C^2}{2A} \\
&= \frac{-D(\sqrt{D} - C)}{C\sqrt{D} - D} = \sqrt{D} = \sqrt{C^2 - 4A^2} \\
&= \sqrt{\left(\frac{4\pi\hbar^2 aN}{mV} + \frac{\hbar^2 k^2}{2m}\right)^2 - 4\left(\frac{2\pi\hbar^2 aN}{mV}\right)^2} \\
&= \sqrt{\frac{\hbar^4 k^4}{4m^2} + \frac{4\hbar^4 k^2 \pi a N}{m^2 V}} \\
&= \sqrt{\frac{\hbar^4 k^4}{4m^2} + \frac{nU_0 \hbar^2 k^2}{m}}
\end{aligned}
\tag{4.28}
$$

is same with the one we have found via BdG equations. The constant term that contributes to the ground state energy is

$$
\begin{aligned}
E'_G &= \frac{2AL + CL^2}{1 - L^2} = \frac{2AL - C^2 L/A - C}{2 + CL/A} \\
&= \frac{(2A^2 - C^2)(\sqrt{D} - C)/2A - CA}{2A + C(\sqrt{D} - C)/2A} = \frac{2A^2\sqrt{D} - 2A^2 C - C^2 D + C^3 - 2CA^2}{C\sqrt{D} - D} \\
&= \frac{-C^2\sqrt{D} + CD}{C\sqrt{D} - D} + \frac{2A^2 D}{C\sqrt{D} - D} = -C + \frac{2A^2 D}{C\sqrt{D} - D} \\
&= -\frac{C}{2} - \frac{C}{2} + \frac{2A^2 D}{C\sqrt{D} - D} = -\frac{C}{2} + \frac{1}{2}\left[\frac{-C^2\sqrt{D} + CD + 4A^2\sqrt{D}}{C\sqrt{D} - D}\right] \\
&= -\frac{C}{2} + \frac{\sqrt{D}}{2}\left[\frac{-D + C\sqrt{D}}{C\sqrt{D} - D}\right] = \frac{\sqrt{D} - C}{2} = \frac{\sqrt{C^2 - 4A^2} - C}{2} \\
&= \frac{1}{2}\sqrt{\frac{\hbar^4 k^4}{4m^2} + \frac{nU_0 \hbar^2 k^2}{m}} - \frac{1}{2}\frac{4\pi\hbar^2 aN}{mV} - \frac{1}{2}\frac{\hbar^2 k^2}{2m}.
\end{aligned}
\tag{4.29}
$$

With this linear transformation, Hamiltonian is diagonalized,

$$\begin{aligned}\hat{H} &= \frac{4\pi\hbar^2 a}{m}\left[1+\frac{4\pi\hbar^2 a}{V\hbar^2}\sum_{k\neq 0}\frac{1}{k^2}\right]\frac{N^2}{2V} \\ &+\sum_{k\neq 0}\left[\frac{1}{2}\sqrt{\frac{\hbar^4k^4}{4m^2}+\frac{nU_0\hbar^2k^2}{m}}-\frac{1}{2}\frac{4\pi\hbar^2 aN}{mV}-\frac{1}{2}\frac{\hbar^2k^2}{2m}\right] \\ &+\sqrt{\frac{\hbar^4k^4}{4m^2}+\frac{nU_0\hbar^2k^2}{m}}\alpha_k^\dagger\alpha_k\end{aligned} \tag{4.30}$$

We define v as

$$v=\sqrt{\frac{4\pi\hbar^2 aN}{m^2V}}=\sqrt{\frac{U_0N}{mV}} \tag{4.31}$$

. H is

$$\hat{H}=\underbrace{\frac{Nmu^2}{2}+\frac{1}{2}\sum_{k\neq 0}\left[\frac{m^3v^4}{\hbar^2k^2}+E(k)-\frac{\hbar^2k^2}{2m}-mv^2\right]}_{\text{corrected ground state energy}}+\underbrace{\sum_{k\neq 0}E(k)\alpha_k^\dagger\alpha_k}_{\text{spectrum of excitations}} \tag{4.32}$$

where E(k) in terms v is $\sqrt{\hbar^2k^2v^2+(\hbar^2k^2/2m)^2}$. Finally, second order grund state energy can be calculated

$$\begin{aligned}E_G &= \frac{1}{2}Nmv^2+\frac{1}{2}\sum_{k\neq 0}\left\{\sqrt{\hbar^2k^2v^2+\frac{\hbar^4k^4}{4m^2}}-\frac{\hbar^2k^2}{2m}-mv^2+\frac{m^3v^4}{\hbar^2k^2}\right\} \\ &= \frac{1}{2}Nmv^2+\frac{1}{2}\frac{4\pi V}{(2\pi\hbar)^3}\int p^2dp\left[\underbrace{\sqrt{p^2v^2+\frac{p^4}{4m^2}}}_{\to I_1}-\frac{p^2}{2m}-mv^2+\frac{m^3v^4}{p^2}\right].\end{aligned} \tag{4.33}$$

First we evaluate I_1,

$$\begin{aligned}I_1 &= \int p^2dp\frac{p}{2m}\sqrt{4m^2v^2+p^2}; \qquad z\equiv 4m^2v^2+p^2; \qquad \frac{dz}{dp}=2p \\ &= \int(z-4m^2v^2)\frac{dz}{2}\frac{1}{2m}\sqrt{z}=\frac{1}{4m}\int z^{3/2}dz-\frac{1}{4m}4m^2v^2\int\sqrt{z}dz \\ &= \frac{1}{4m}\frac{z^{5/2}2}{5}-\frac{mv^2z^{3/2}2}{3}=\left[\frac{1}{10m}z^{5/2}-\frac{2mv^2}{3}z^{3/2}\right]_{4m^2v^2}^{4m^2v^2+p_f^2}\end{aligned} \tag{4.34}$$

and substitute in E_G

$$\begin{aligned}
E_G = \frac{1}{2}Nmv^2 + \frac{2\pi V}{(2\pi\hbar)^3}\Bigg[& \frac{(4m^2v^2+p_f^2)^{5/2}}{10m} - \frac{(4m^2v^2)^{5/2}}{10m} \\
& - \frac{2mv^2}{3}(4m^2v^2+p_f^2)^{3/2} + \frac{2mv^2}{3}(4m^2v^2)^{3/2} \\
& - \frac{p_f^5}{10m} - \frac{mv^2p_f^3}{3} + m^3v^4p_f\Bigg] \\
= \frac{1}{2}Nmv^2 + \frac{2\pi V}{(2\pi\hbar)^3}\Bigg[& \frac{p_f^5}{10m}\left(1+\frac{4m^2v^2}{p_f^2}\right)^{5/2} - \frac{2mv^2p_f^3}{3}\left(1+\frac{4m^2v^2}{p_f^2}\right)^{3/2} \\
& - \frac{(2mv)^5}{10m} - \frac{2mv^2p_f^3}{3}8m^3v^3 - \frac{p_f^5}{10m} - \frac{mv^2p_f^3}{3} + m^3v^4p_f\Bigg] \\
= \frac{1}{2}Nmv^2 + \frac{2\pi V}{(2\pi\hbar)^3}\Bigg[& \frac{p_f^5}{10m}\left(1+\frac{5}{2}\frac{4m^2v^2}{p_f^2}+\frac{5}{2}\frac{3}{2}\frac{16m^4v^4}{2p_f^4}\right) - \frac{(2mv)^5}{10m} \\
& - \frac{2mv^2p_f^3}{3}\left(1+\frac{3}{2}\frac{4m^2v^2}{p_f^2}\right) - \frac{2mv^2p_f^3}{3}8m^3v^3 \\
& - \frac{p_f^5}{10m} - \frac{mv^2p_f^3}{3} + m^3v^4p_f\Bigg] \\
= \frac{1}{2}Nmv^2 + \frac{2\pi V}{(2\pi\hbar)^3}\Bigg[& \frac{p_f^5}{10m} + mv^2p_f^3 + 3m^3v^4p_f - \frac{(2mv)^5}{10m} - \frac{2mv^2p_f^3}{3} \\
& - 4m^3v^4p_f - \frac{16m^4v^5}{3} - \frac{p_f^5}{10m} - \frac{mv^2p_f^3}{3} + m^3v^4p_f\Bigg] \\
= \frac{1}{2}Nmv^2 + \frac{2\pi V}{(2\pi\hbar)^3}\Bigg[& -\frac{128}{15}m^4v^5\Bigg].
\end{aligned} \tag{4.35}$$

E_G in terms of the original parameters is

$$E_G = \frac{2\pi\hbar^2aN^2}{mV}\left[1+\frac{128}{15}\sqrt{\frac{a^3N}{\pi V}}\right]. \tag{4.36}$$

Chapter 5

Energy of a Black Soliton

In this chapter we first calculate first order ground state energy of black soliton with mean field Hamiltonian. Then we recalculate this first order energy with partition function. To do so we only take S_0 term. We are interested in Bogoliubov level ground state energy of soliton but BdG equations can not be solved analytically for soliton as it is shown at the end of this chapter. That is why, there is not an analytical expression for this energy. We, then use partition function to calculate this second order energy by taking into account S_2 term in the action.

5.1 First order energy by variational calculus

Energy of soliton with mean-field approximation is calculated in e.g. Ref [20]. Here, we follow those calculations. Energy of the system can be written as

$$\langle\psi| H |\psi\rangle = E(\psi) = \int dr \left[\frac{\hbar^2}{2m}|\nabla\psi(r)|^2 + V(r)|\psi(r)|^2 + \frac{1}{2}U_0|\psi(r)|^4\right]. \quad (5.1)$$

Since the number of particles is not conserved in general, $E - \mu N$ sholud be considered instead of E itself. $V(x) = 0$ and $N = \int dr|\psi(r)|^2$. Moreover the system is quasi-one dimensional therefore $\int dr = A\int dx$ where A is the area.

This equation gives us the energy of the whole system: soliton+background. We get soliton energy if we subtract the energy of the system with soliton from the energy of the system without soliton,

$$(E-\mu N)_w = A\int dx\left[\frac{\hbar^2}{2m}\left|\frac{d\psi}{dx}\right|^2+\frac{1}{2}U_0|\psi|^4-\mu|\psi|^2\right] \tag{5.2}$$

$$(E-\mu N)_{w/o} = A\int dx\left(\frac{U_0}{2}|\psi^4|-\mu|\psi|^2\right) \tag{5.3}$$

$$\Delta(E-\mu N) = A\int dx\left[\frac{\hbar^2}{2m}\left|\frac{d\psi}{dx}\right|^2+\frac{1}{2}U_0(|\psi|^4-n_0^2)-\mu(|\psi|^2-n_0)\right]. \tag{5.4}$$

Chemical potential is U_0n_0 in the case of uniform Bose gas. For infinite-sized systems including finite number of solitons, the chemical potential can be taken U_0n_0 as well and we also consider such a system. The soliton energy then becomes

$$\Delta(E-\mu N) = \underbrace{A\int dx\left[\frac{\hbar^2}{2m}\left|\frac{d\psi}{dx}\right|^2\right]}_{I_1}+\underbrace{A\int dx\left[\frac{U_0}{2}(|\psi|^2-n_0)^2\right]}_{I_2}. \tag{5.5}$$

We are interested in black solitons but the following calculations are simple enough to consider more general case, dark solitons. The integrals I_1 and I_2,

$$\begin{aligned}
I_1 &= A\int dx\left[\frac{\hbar^2}{2m}\left|\sqrt{n_0}e^{-i\mu t/\hbar}\sqrt{1-\frac{u^2}{s^2}}\frac{1}{\cosh^2(\frac{x-ut}{\sqrt{2}\xi u})}\frac{1}{\sqrt{2}\xi u}\right|^2\right]\\
&= An_0\left(1-\frac{u^2}{s^2}\right)\frac{1}{2\xi_u^2}\frac{\hbar^2}{2m}\underbrace{\int d\tilde{x}\frac{1}{\cosh^4\tilde{x}}}_{\int_{-\infty}^{\infty}dx\frac{1}{\cosh^4 x}=\frac{4}{3}}\sqrt{2}\xi u\\
&= An_0\left(1-\frac{u^2}{s^2}\right)\frac{1}{\sqrt{2}\xi}\sqrt{1-u^2/s^2}\frac{\hbar^2}{2m}\frac{4}{3},
\end{aligned} \tag{5.6}$$

per unit area

$$\begin{aligned}
\frac{I_1}{A} &= \left(1-\frac{u^2}{s^2}\right)^{3/2} n_0\frac{2\hbar^2}{3m}\frac{1}{\sqrt{2}}\frac{\sqrt{2}\sqrt{mn_0U_0}}{\hbar}\\
&= \left(1-\frac{u^2}{s^2}\right)^{3/2} n_0\hbar\underbrace{\sqrt{\frac{n_0U_0}{m}}}_{S}\frac{2}{3};
\end{aligned} \tag{5.7}$$

and

$$I_2 = \frac{AU_0}{2} \int d\tilde{x} \left[n_0 - n_0 \left(1 - \frac{u^2}{s^2}\right) \frac{1}{\cosh^2 \tilde{x}} - n_0 \right]^2 \sqrt{2}\xi_u \tag{5.8}$$

$$= \frac{AU_0}{2} n_0^2 \left(1 - \frac{u^2}{s^2}\right)^2 \underbrace{\int d\tilde{x} \frac{1}{\cosh^4 \tilde{x}}}_{4/3} \sqrt{2}\xi_u, \tag{5.9}$$

per unit area

$$\frac{I_2}{A} = \frac{n_0^2 U_0}{2} \left(1 - \frac{u^2}{s^2}\right)^2 \frac{4}{3} \frac{\sqrt{2}\xi}{\sqrt{1 - \frac{u^2}{s^2}}} \tag{5.10}$$

$$= \left(1 - \frac{u^2}{s^2}\right)^{3/2} \frac{2n_0}{3} \frac{n_0 U_0 \sqrt{2}\hbar}{\sqrt{2 m n_0 U_0}} \tag{5.11}$$

$$= \left(1 - \frac{u^2}{s^2}\right)^{3/2} n_0 \hbar \underbrace{\sqrt{\frac{n_0 U_0}{m}}}_{s} \frac{2}{3}. \tag{5.12}$$

Finally the energy of a single soliton per unit area is obtained as

$$\frac{E}{A} = \frac{4}{3} n_0 \hbar s \left(1 - \frac{u^2}{s^2}\right)^{3/2}. \tag{5.13}$$

This equation possesses an interesting feature, energy is inversely proportional to the velocity which correspondsn to negative effective mass.

This energy can also be expressed as

$$E = \frac{4}{3} n_0 \hbar s \left(1 - \frac{u^2}{s^2}\right) \tag{5.14}$$

$$= \frac{4}{3} n_0 \hbar \frac{\sqrt{n_0 U_0}}{\sqrt{m}} \left(1 - \frac{u^2 m}{\underbrace{n_0 U_0}_{\mu}}\right)^{3/2} \tag{5.15}$$

$$= \frac{4\hbar}{3\sqrt{m} U_0} \left(\mu - m u^2\right)^{3/2}. \tag{5.16}$$

For black solitons

$$\begin{aligned} E &= \frac{4\hbar}{3\sqrt{m}U_0}\mu^{3/2} \\ &= \frac{4\hbar\sqrt{U_0}}{3\sqrt{m}}|\psi_0|^2\psi_0. \end{aligned} \tag{5.17}$$

5.2 First order energy from partition function

In this section we reevaluate the previous result, energy of black soliton, from partition function. We have written the lengthy expression of the action after performing the saddle point analysis. Plugging the wavefunction of black soliton, which is

$$\psi_{black} = \sqrt{\beta}\psi_0 \tanh\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)\delta_{w_n,0}$$

in Matsubara frequnecy domain, into the open form of the general action gives

$$\begin{aligned} S =& A\sum_{x=0}^{N}\Delta x\Bigg\{\sum_{w_n}(iw_n-\mu)\beta|\psi_0|^2\tanh^2\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)\delta_{w_n,0}\delta_{w_n,0} \\ &+\sum_{w_n}\frac{-1}{2m\Delta x^2}\sqrt{\beta}\psi_0\tanh\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)\delta_{w_n,0}\Bigg[\sqrt{\beta}\psi_0\tanh\left(\frac{(x+1)\Delta x}{\sqrt{2}\xi}\delta_{w_n,0}\right. \\ &-2\sqrt{\beta}\psi_0\tanh\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)\delta_{w_n,0}+\sqrt{\beta}\psi_0\tanh\left(\frac{(x-1)\Delta x}{\sqrt{2}\xi}\delta_{w_n,0}\right.\Bigg] \\ &+\sum_{\substack{w_n,w_m\\w_p,w_r}}\frac{U_0}{2\beta}\delta_{\substack{w_n+w_m\\w_p+w_r}}\left(\beta^2|\psi_0|^4\tanh^4\left(\frac{x\Delta x}{\sqrt{2}\eta}\right)\delta_{w_n,0}\delta_{w_m,0}\delta_{w_p,0}\delta_{w_r,0}\right)\Bigg\} \\ &+A\sum_{x=0}^{N}\Delta x\Bigg\{\sum_{w_n}\sqrt{\beta}\psi_0\tanh\left(\frac{(x-1)\Delta x}{\sqrt{2}\xi}\right)\delta_{w_n,0}\left[(iw_n-\mu)(\psi^1_{n,x}+\bar{\psi}^1_{n,x})\right] \\ &+\sum_{w_n}\frac{-1}{2m\Delta x^2}\Bigg(\sqrt{\beta}\psi_0\tanh\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)\left[\psi^1_{n,x+1}-2\psi^1_{n,x}+\psi^1_{n,x-1}-\bar{\psi}^1_{n,x}\right] \\ &+\sqrt{\beta}\psi_0\tanh\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)(\bar{\psi}^1_{n,x})\Bigg) \\ &+\sum_{\substack{w_n,w_m\\w_p,w_r}}\frac{U_0}{2\beta}\delta_{\substack{w_n+w_m,\\w_p,w_r}}\beta^{3/2}|\psi_0|^3\tanh^3\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)\left[\delta_{w_n,0}\delta_{w_m,0}\delta_{w_p,0}\psi^1_{r,x}\right. \end{aligned}$$

$$
\begin{aligned}
&+ \delta_{w_n,0}\delta_{w_m,0}\delta_{w_r,0}\psi^1_{p,x} + \delta_{w_n,0}\delta_{w_p,0}\delta_{w_r,0}\overline{\psi}^1_{m,x} + \delta_{w_m,0}\delta_{w_p,0}\delta_{w_r,0}\overline{\psi}^1_{n,x}\Big]\Bigg\} \\
&+A\sum_{x=0}^{N}\Delta x\Bigg\{\sum_{w_n}\overline{\psi}^1_{n,x}(iw_n - \mu + \frac{1}{m\Delta x^2})\psi^1_{n,x} + \sum_{w_n}\overline{\psi}^1_{n,x}(\frac{-1}{2m\Delta x^2})\psi^1_{n,x+1} \\
&\quad + \sum_{w_n}\overline{\psi}^1_{n,x}(\frac{-1}{2m\Delta x^2})\psi^1_{n,x-1} + \sum_{\substack{w_n,w_m \\ w_p,w_r}}\frac{U_0}{2\beta}\delta_{\substack{w_n+w_m, \\ w_p,w_r}}\beta|\psi_0|^2\tanh^2(\frac{x\Delta x}{\sqrt{2}\xi})\times \\
&\quad \underbrace{\times\Big[\delta_{w_n,0}\delta_{w_m,0}\psi^1_{p,x}\psi^1_{r,x} + \delta_{w_n,0}\delta_{w_p,0}\overline{\psi}^1_{m,x}\psi^1_{r,x} + \delta_{w_n,0}\delta_{w_r,0}\overline{\psi}^1_{p,x}\psi^1_{r,x} + \delta_{w_m,0}\delta_{w_p,0}\overline{\psi}^1_{n,x}\psi^1_{r,x} + \delta_{w_m,0}\delta_{w_r,0}\overline{\psi}^1_{n,x}\psi^1_{p,x} + \delta_{w_p,0}\delta_{w_r,0}\overline{\psi}^1_{m,x}\overline{\psi}^1_{n,x}\Big]}_{\frac{U_0}{2}|\psi_0|^2\tanh^2\left(\frac{x\Delta x}{\sqrt{2}\eta}\right)\left[\psi^1_{n,x}\psi^1_{-n,x}+4\overline{\psi}^1_{n,x}\psi^1_{n,x}+\overline{\psi}^1_{n,x}\overline{\psi}^1_{-n,x}\right]}\Bigg\}
\end{aligned}
\tag{5.18}
$$

We only take S_0 term for now. After taking Matsubara sums with the help of Kronocker delta,

$$
\begin{aligned}
S_{0,bs} =& A\sum_{x=0}^{N}\Delta x\Bigg\{\mu\beta|\psi_0|^2\tanh^2(\frac{x\Delta x}{\sqrt{2}\xi}) \\
&- \frac{1}{2m\Delta x^2}\sqrt{\beta}\psi_0\tanh(\frac{x\Delta x}{\sqrt{2}\xi})\sqrt{\beta}\psi_0\Big[\tanh(\frac{(x+1)\Delta x}{\sqrt{2}\xi} \\
&- 2\tanh(\frac{x\Delta x}{\sqrt{2}\xi}) + \tanh(\frac{(x-1)\Delta x}{\sqrt{2}\xi}\Big] \\
&+ \frac{U_0}{2\beta}(\beta^2|\psi_0|^4\tanh^4(\frac{x\Delta x}{\sqrt{2}\xi}))\Bigg\}.
\end{aligned}
\tag{5.19}
$$

After converting the summation to the integral, by using $\mu = g|\psi_0|^2$,

$$
\begin{aligned}
S_{0,bs} = A\int dx\Big[&\underbrace{\mu\beta|\psi_0|^2\tanh^2(\frac{x}{\sqrt{2}\xi})}_{\to I_1} - \underbrace{\frac{\beta|\psi_0|^2}{2m}\tanh(\frac{x}{\sqrt{2}\xi})\frac{\partial^2}{\partial x^2}\tanh(\frac{x}{\sqrt{2}\xi})}_{\to I_2} \\
&+ \underbrace{\frac{U_0\beta|\psi_0|^4}{2}\tanh^4(\frac{x}{\sqrt{2}\xi})}_{\to I_3}\Big].
\end{aligned}
\tag{5.20}
$$

There are three integrals of $\tanh^2 x$,$\tanh^2 x\ \text{sech}^2 x$,and $\tanh^4 x$ respectively. The system is inifinite-sized and dx integral goes from $-\infty$ to ∞.For such a system

$$
\begin{aligned}
&\int \tanh^2 x dx = x - \tanh x \\
&\int \tanh^2 x \operatorname{sech}^2 x dx = \frac{\tanh^3 x}{3} \\
&\int \tanh^4 x dx = x - \frac{4\tanh x}{3} + \frac{1}{3}\tanh \cancelto{0}{x \operatorname{sech}^2} x.
\end{aligned}
\tag{5.21}
$$

The integrals are then evaluated easily:

$$
\begin{aligned}
I_1 &= A\int dx \left[-\mu\beta|\psi_0|^2 \tanh^2\left(\frac{x}{\sqrt{2}\xi}\right)\right] \\
&= -A\mu\beta|\psi_0|^2 \left[x - \sqrt{2}\tanh\left(\frac{x}{\sqrt{2}\xi}\right)\xi\right]_{-\infty}^{\infty} \\
&= -A\mu\beta|\psi_0|^2 x|_{-\infty}^{\infty} + 2\sqrt{2}\xi A\mu\beta|\psi_0|^2, \\
I_2 &= A\int dx \frac{-\beta|\psi_0|^2}{2m}\tanh\left(\frac{x}{\sqrt{2}\xi}\right)\frac{\partial^2}{\partial x^2}\tanh\left(\frac{x}{\sqrt{2}\xi}\right) \\
&= -\frac{A\beta|\psi_0|^2}{2m}\int dx \tanh\left(\frac{x}{\sqrt{2}\xi}\right)\left(\frac{-2}{2\xi^2}\right)\operatorname{sech}^2\left(\frac{x}{\sqrt{2}\xi}\right)\tanh\left(\frac{x}{\sqrt{2}\xi}\right) \\
&\frac{A\beta|\psi_0|^2}{\xi^2 2m}\frac{\sqrt{2}\xi}{3}\tanh^3\left(\frac{x}{\sqrt{2}\xi}\right)\Bigg|_{-\infty}^{\infty} \\
&= \frac{\sqrt{2}A\beta|\psi_0|^2}{3\xi m}, \\
I_3 &= A\int dx \frac{g\beta|\psi_0|^4}{2}\tanh^4\left(\frac{x}{\sqrt{2}\xi}\right) \\
&= \frac{Ag\beta|\psi_0|^4}{2}\left[\frac{-4\sqrt{2}\xi}{3}\tanh\left(\frac{x}{\sqrt{2}\xi}\right) + \frac{\sqrt{2}\xi}{3}\tanh\left(\frac{x}{\sqrt{2}\xi}\right)\operatorname{sech}^2\left(\frac{x}{\sqrt{2}\xi}\right) + x\right]_{-\infty}^{\infty} \\
&= -\frac{Ag\beta|\psi_0|^4}{2}\frac{8\sqrt{2}\xi}{3} + \frac{Ag\beta|\psi_0|^4}{2}x\Big|_{-\infty}^{\infty}.
\end{aligned}
\tag{5.22}
$$

S_0 becomes

$$
S_{0,bs} = A|\psi_0|^2\beta\left(\frac{g|\psi_0|^2}{2} - \mu\right)x\Big|_{-\infty}^{\infty} + A|\psi_0|^2\beta\xi\left(2\sqrt{2}\mu + \frac{\sqrt{2}}{3m\xi^2} - \frac{4\sqrt{2}g|\psi_0|^2}{3}\right).
\tag{5.23}
$$

S_0 is constant therefore it goes out of the integral

$$
Z = e^{S_0}\int \cdots .
\tag{5.24}
$$

The remaining in the integral are the higher order contributions. Free energy is

$$A = -\frac{1}{\beta}\ln Z = -\frac{1}{\beta}\ln\big(e^{S_0}\cdots\big) = -\frac{1}{\beta}S_0 + \cdots . \tag{5.25}$$

The first order energy of black soliton is

$$-\frac{1}{\beta}S_0 = -A|\psi_0|^2\left(\frac{g|\psi_0|^2}{2} - \mu\right)x\Big|_{-\infty}^{\infty} - A|\psi_0|^2\xi\left(2\sqrt{2}\mu + \frac{\sqrt{2}}{3m\xi^2} - \frac{4\sqrt{2}g|\psi_0|^2}{3}\right). \tag{5.26}$$

First term is the background energy, $nU_0V/2$, which we have obtained in the previous chapter. The second term is just

$$-\frac{1}{\beta}S_0 = -A|\psi_0|^2\xi\left(2\sqrt{2}\mu + \frac{\sqrt{2}}{3m\xi^2} - \frac{4\sqrt{2}g|\psi_0|^2}{3}\right) = \frac{4}{3}|\psi_0|^2\psi_0\sqrt{U_0}A, \tag{5.27}$$

the same with the first order energy coming from the variational calculation.

5.3 Second order energy from BdG equation

By linearizing Gross Pitaevskii equation for homogeneous Bose gas, we get

$$-\frac{\hbar^2}{2m}\nabla^2\psi^1 + 2U_0|\psi^0|^2\psi^1 + U_0{\psi^0}^2\overline{\psi^1} = i\hbar\frac{\partial\psi^1}{\partial t}. \tag{5.28}$$

To find the excitations on a black soliton background, we plug soliton wavefunction, $\psi_0\tanh\big(x/\sqrt{2}\xi\big)$ into this equation,

$$-\frac{\hbar^2}{2m}\nabla^2\psi^1 + 2U_0|\psi_0|^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)\psi^1 + U_0\psi_0^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)e^{-i2\mu t/\hbar}\overline{\psi^1} = i\hbar\frac{\partial\psi^1}{\partial t}. \tag{5.29}$$

To get rid of $e^{-i2\cdot\cdot}$ term, we define

$$\widetilde{\psi^1} = \psi^1 e^{i\mu t/\hbar}. \tag{5.30}$$

The equation

$$
\begin{aligned}
&-\frac{\hbar^2}{2m}\nabla^2\widetilde{\psi^1}e^{-i\mu t/\hbar}+2U_0|\psi_0|^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)\widetilde{\psi^1}e^{-i\mu t/\hbar}\\
&+U_0\psi_0^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)e^{-i2\mu t/\hbar}\overline{\widetilde{\psi^1}}e^{i\mu t/\hbar}=i\hbar\frac{\partial\widetilde{\psi^1}}{\partial t}e^{-i\mu t/\hbar}+\frac{i\hbar(-i\mu)}{\hbar}\widetilde{\psi^1}e^{-i\mu t/\hbar}.
\end{aligned}
\tag{5.31}
$$

simplifies to

$$
\begin{aligned}
&-\frac{\hbar^2}{2m}\nabla^2\widetilde{\psi^1}+\left[2U_0|\psi_0|^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)-\mu\right]\widetilde{\psi^1}\\
&+U_0\psi_0^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)\overline{\widetilde{\psi^1}}=i\hbar\frac{\partial\widetilde{\psi^1}}{\partial t}.
\end{aligned}
\tag{5.32}
$$

We use the time invariance of the system in order to write

$$
\widetilde{\psi^1}=A(x)e^{-iwt}-\overline{B}(x)e^{iwt}
\tag{5.33}
$$

which gives

$$
\begin{aligned}
&-\frac{\hbar^2}{2m}\nabla^2A(x)e^{-iwt}+\frac{\hbar^2}{2m}\nabla^2\overline{B}(x)e^{iwt}\\
&+\left[2U_0|\psi_0|^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)-\mu\right]\left[A(x)e^{-iwt}-\overline{B}(x)e^{iwt}\right]\\
&+U_0\psi_0^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)\left[\overline{A}(x)e^{iwt}-B(x)e^{-iwt}\right]\\
&=i\hbar A(x)(-iw)e^{-iwt}-i\hbar\overline{B}(x)(iw)e^{iwt}.
\end{aligned}
\tag{5.34}
$$

Since $\exp(-iwt)$ and $\exp(iwt)$ are linearly independent, we can equate their coefficients to zero.

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\nabla^2A+\left[2U_0|\psi_0|^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)-\mu\right]A-U_0\psi_0^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)B&=\hbar wA\\
\frac{\hbar^2}{2m}\nabla^2\overline{B}-\left[2U_0|\psi_0|^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)-\mu\right]\overline{B}+U_0\psi_0^2\tanh^2\big(\frac{x}{\sqrt{2}\xi}\big)\overline{A}&=\hbar w\overline{B}.
\end{aligned}
\tag{5.35}
$$

These are the BdG equations for dark solitons. Since they are not analytically solvable, the contributions of all modes are not known. With numerical calculation contributions coming from a few modes are analyzed but to include all the modes, a different approach should be used.

5.4 Second order energy from partition function

After performing Matsubara sums, the second part of the action becomes

$$\begin{aligned}
S_{2,bs} = A\sum_{x=0}^{N}\Delta x\sum_{n}\Bigg\{&\overline{\psi^1}_{n,x}\left(iw_n - \mu + \frac{1}{m\Delta x^2} + 2U_0|\psi_0|^2\tanh^2\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)\right)\psi^1_{n,x}\\
&+\overline{\psi^1}_{n,x}\left(\frac{-1}{2m\Delta x^2}\right)\psi^1_{n,x+1}\\
&+\overline{\psi^1}_{n,x}\left(\frac{-1}{2m\Delta x^2}\right)\psi^1_{n,x-1}\\
&+\psi^1_{n,x}\left(\frac{U_0}{2}|\psi_0|^2\tanh^2\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)\right)\psi^1_{-n,x}\\
&+\overline{\psi^1}_{n,x}\left(\frac{U_0}{2}|\psi_0|^2\tanh^2\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)\right)\overline{\psi^1}_{-n,x}\Bigg\}. \qquad (5.36)
\end{aligned}$$

If we define $S^n_{2,bs}$ as

$$S_{2,bs} = \sum_n S^n_{2,bs},$$

$S^n_{2,bs}$ can be written as an infinite dimensional integral.

$$S^n_{2,bs} = A\sum_{\substack{x=1\\y=1}}^{N}\Delta x\left[\overline{\psi}^1_{n,x}K^n_1\psi^1_{n,y} + \psi^1_{n,x}K^n_2\psi^1_{-n,y}\overline{\psi}^1_{n,x}K^n_3\overline{\psi}^1_{-n,y}\right] \qquad (5.37)$$

where K^n_1, K^n_2, and K^n_3 are the matrices respectively given by

$$K^n_1 = \begin{bmatrix} \tilde{f}(n,x) & \tilde{c} & 0 & \dots & 0\\ \tilde{c} & \tilde{f}(n,x) & \cdots & \dots & 0\\ 0 & \tilde{c} & \tilde{f}(n,x) & \tilde{c} & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & \dots & 0 & \tilde{c} & \tilde{f}(n,x) \end{bmatrix} \qquad (5.38)$$

$$K^n_2 = \begin{bmatrix} \tilde{h}(x) & 0 & 0 & \dots & 0\\ 0 & \tilde{h}(x) & 0 & \dots & 0\\ 0 & 0 & \tilde{h}(x) & \dots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & \dots & \vdots & 0 & \tilde{h}(x) \end{bmatrix} \qquad (5.39)$$

$$K^n_3 = K^n_2 \qquad (5.40)$$

$$K^n_4 = K^n_1 \qquad (5.41)$$

where

$$\tilde{f}(n,x) = \frac{1}{2}\left(iw_n - \mu + \frac{1}{m\Delta x^2} + 2U_0|\psi_0|^2\tanh^2\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)\right)$$
$$\tilde{h}(x) = \left(\frac{U_0}{2}|\psi_0|^2\tanh^2\left(\frac{x\Delta x}{\sqrt{2}\xi}\right)\right)$$
$$\tilde{c} = \left(\frac{-1}{2m\Delta x^2}\right). \tag{5.42}$$

We have an integral of the form

$$Z = \exp\{-S_{0,bs}\}\prod_n\left[\int\frac{1}{N}d\psi d\overline{\psi}\right]\exp\Bigg\{-A\sum_{\substack{x=1\\y=1}}^{N}\Delta x\,[\overline{\psi}^1_{n,x}K_1^n\psi^1_{n,y} + \psi^1_{n,x}K_2^n\psi^1_{-n,y} + \overline{\psi}^1_{n,x}K_3^n\overline{\psi}^1_{-n,y} + \psi^1_{n,x}K_{14}^n\overline{\psi}^1_{n,y}]\Bigg\}. \tag{5.43}$$

It looks like infinite dimensional Gaussian integrals. It has off-diagonal terms. Gaussian integrals of different dimensions can be evaluated.

$\longrightarrow$ **One dimension case:** It is well known that

$$\int_{-\infty}^{\infty}dxe^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}} \tag{5.44}$$

$\longrightarrow$ **Two dimensions case:** It is easy to show that

$$\int_{-\infty}^{\infty}d\vec{x}e^{-\frac{1}{2}\vec{x}^T\mathbf{M}\vec{x}} = (2\pi)^{D/2}\frac{1}{\sqrt{\det\mathbf{M}}} \tag{5.45}$$

where D is the dimension of the matrix $\mathbf{M}$. Its proof can be found in Ref. [28]

$\longrightarrow$ **Infinite dimensions case:** In the case of infinitely many dimensions, the formula is given as

$$\lim_{N\to\infty}\left[\int\frac{1}{\mathbb{N}}\left(\prod_{k=1}^{N}d\overline{\psi}_k d\psi_k\right)e^{-\sum_{i,j=1}^{N}\overline{\psi_i}\mathbf{M}_{ij}\psi_j}\right] = \lim_{N\to\infty}\frac{1}{\det\mathbf{M}} \tag{5.46}$$

where $\mathbb{N}$ is normailzation constant.

The partition function of Bose gas is not exactly of the form of this but it can be transformed to by defining a new variable Φ^1 such that

$$\Phi^1 = \begin{bmatrix}\psi^1\\ \overline{\psi}^1\end{bmatrix}. \tag{5.47}$$

With this new definition

$$\overline{\Phi}^1 \mathbb{K} \Phi^1 = \begin{bmatrix} \overline{\psi}^1 & \psi^1 \end{bmatrix} \begin{bmatrix} K_1 & K_2 \\ K_3 & K_4 \end{bmatrix} \begin{bmatrix} \psi^1 \\ \overline{\psi}^1 \end{bmatrix} = \begin{bmatrix} \overline{\psi}^1 & \psi^1 \end{bmatrix} \begin{bmatrix} K_1 \psi^1 & K_2 \overline{\psi}^1 \\ K_3 \psi^1 & K_4 \overline{\psi}^1 \end{bmatrix}$$
$$= \overline{\psi}^1 K_1 \psi^1 + \overline{\psi}^1 K_2 \overline{\psi}^1 + \psi^1 K_3 \psi^1 + \psi^1 K_4 \overline{\psi}^1. \tag{5.48}$$

This new definition allows us to write the action in the form of a Gaussian

$$S^n_{u,2} = A \sum_{x=1,y=1}^{2N} \Delta x \bar{\Phi}^1 \mathbb{K}^n_{xy} \Phi^1 \tag{5.49}$$

and the second order contribution to the free energy can be calculated from the partition function,

$$Z = \exp\{-S_{0,bs}\} \prod_n \left[\int \frac{1}{N} d\psi d\overline{\psi} \exp\left\{ -A \sum_{x=1,y=1}^{2N} \Delta x \bar{\Phi}^1 \mathbb{K}^n_{xy} \Phi^1 \right\} \right]$$
$$= \exp\{-S_{0,bs}\} \prod_n \frac{1}{\det \mathbb{K}^n}. \tag{5.50}$$

Evaluating the corresponding determinant, however, is not straightforward. We need to use Gel'fand Yaglom method which is explained in the following chapter.

Chapter 6

Gelfand Yaglom method

6.1 Functional Determinants

Evaluating functional determinants are crucial in many areas of physics. Although they are hard to evaluate, they possess important information. Several methods have been developed to evaluate functional determinants exactly or approximately. [29]. Using zeta functions and contour integrals is one of these methods which allows to find determinant of an operator without explicitly calculating its eigenvalues [30].

Zeta functions are widely used in quantum field theory [31–33] to calculate functional determinants. Riemann zeta functions are generally associated with a set of λ_n as

$$\zeta_R(s) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n^s} \tag{6.1}$$

where λ_ns can be considered as eigenvalues of a finite dimensional matrix M. $\zeta_R(s)$ is convergent when real part of s is greater than 1 [30].

The derivative of $\zeta_R(s)$ is

$$\frac{d\zeta(s)}{ds} = \frac{d}{ds} \sum_{n=1} \frac{1}{\lambda_n^s} = \sum_{n=1} \frac{-1}{\lambda_n^s} \ln \lambda_n. \tag{6.2}$$

At $s = 0$

$$\left.\frac{d\zeta_R(s)}{ds}\right|_{s=0} = -\sum_n \ln \lambda_n = -\ln \prod_n \lambda_n \tag{6.3}$$

gives the determinant of M

$$\boxed{\det M = \exp\{-\zeta_R'(0)\}}. \tag{6.4}$$

We define a function $F(\lambda)$ such that

$$F(\lambda) = 0 \qquad \forall \lambda = \lambda_n. \tag{6.5}$$

The contour integral

$$I = \frac{1}{2\pi i}\int_\gamma d\lambda \lambda^{-s} \frac{d \ln F(\lambda)}{d\lambda} = \frac{1}{2\pi i}\int_\gamma d\lambda \lambda^{-s} \frac{F'(\lambda)}{F(\lambda)} \tag{6.6}$$

has poles at exactly each λ_n.

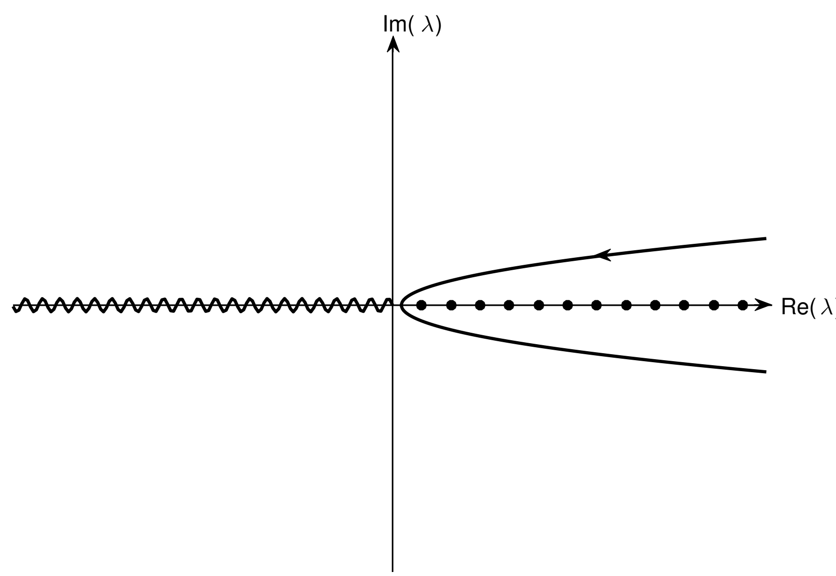

Figure 6.1: Contour in the complex λ plane and the branch cut

The residues of the integrand at these poles can be calculated by expanding the integrand in Taylor series,

$$\mathbf{res}_{\lambda_n} = \lambda^{-s}\frac{F'(\lambda)}{F(\lambda)}(\lambda-\lambda_n)\Big|_{\lambda=\lambda_n} = \lambda_n^{-s}\frac{F'(\lambda_n)(\lambda-\lambda_n)}{F(\lambda_n)+F'(\lambda_n)(\lambda-\lambda_n)+O(\lambda_n)^2} = \lambda_n^{-s}. \tag{6.7}$$

Writing the contour integral as the sum of residues shows that this integral equals to $\zeta_R(s)$.

$$I = \frac{1}{2\pi i}\int_\gamma d\lambda \lambda^{-s}\frac{d\ln F(\lambda)}{d\lambda} = \frac{1}{2\pi i}2\pi i\sum \mathbf{res} = \sum \lambda_n^{-s} = \zeta_R(s). \tag{6.8}$$

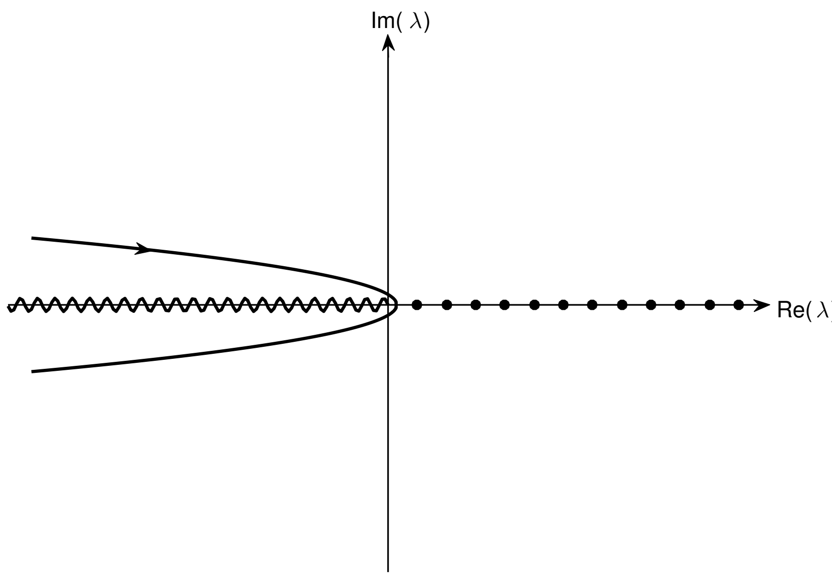

Figure 6.2: Deformed contour

After deforming the contour as in Figure 6.2, the integral can be written as

$$\begin{aligned}\zeta(s) &= \frac{1}{2\pi i}\left\{\int_{-\infty}^{0} d\lambda\frac{1}{e^{i\pi s}}\frac{1}{\lambda^s}\frac{d\ln F(\lambda)}{d\lambda} + \int_0^{-\infty} d\lambda\frac{1}{e^{-i\pi s}}\frac{1}{\lambda^s}\frac{d\ln F(\lambda)}{d\lambda}\right\}\\ &= \frac{\sin\pi s}{\pi}\int_0^{-\infty} d\lambda\frac{1}{\lambda^s}\frac{d\ln F(\lambda)}{d\lambda}\end{aligned} \tag{6.9}$$

We find an expression that relates the desired determinant with $\zeta_R'(0)$. We can, now, find another expression for $\zeta_R'(0)$

$$\begin{aligned}\frac{d\zeta}{ds}\Big|_{s=0} &= \frac{\pi\cos(\pi s)}{\pi}\int_0^{\infty} d\lambda \frac{1}{\lambda^s}\frac{d\ln F(\lambda)}{d\lambda}\Big|_{s=0} \\ &\quad + \frac{\sin(\pi s)}{\pi}\int_0^{infty} d\lambda \frac{1}{\lambda^s}\frac{d\ln F(\lambda)}{d\lambda}(-\ln\lambda)\Big|_{s=0} \qquad (6.10)\\ &= \int_0^{-\infty} d\ln F(\lambda) + 0\cdot\int_0^{-\infty} -\ln\lambda d\ln F(\lambda) \qquad (6.11)\\ &= \ln F(-\infty) - \ln F(0) \qquad (6.12)\end{aligned}$$

which does not require an information of eigenvalues. With this equality, $\det M$ can be written in terms of $F(\lambda)$ only,

$$\begin{aligned}\zeta'(0) &= -\ln\det M \\ \zeta'(0) &= \ln F(-\infty) - \ln F(0) \\ -\ln\det M &= \ln F(-\infty) - \ln F(0) \\ \det M &= \frac{F(0)}{F(-\infty)}. \qquad (6.13)\end{aligned}$$

$\ln F(-\infty)$ is an issue and not allowing us to evaluate the determinant itself. But we still can determine the ratio of two operators; M and M_{free}. To do this, we first define M_{free} as it describes the same system with M when $V_{ext} = 0$. Second, it is assumed that the behaviors of the two functions, $F(\lambda)$ and $F_{free}(\lambda)$ are same at $-\infty$ [29].

$$\begin{aligned}\det M &= \frac{F(0)}{F(-\infty)} \\ \det M_{free} &= \frac{F_{free}(0)}{F_{free}(-\infty)} \qquad (6.14)\end{aligned}$$

With this assumption, we end up with a magnificent relation

$$\boxed{\frac{\det M}{\det M_{free}} = \frac{F(0)}{F_{free}(0)}}. \qquad (6.15)$$

6.2 Gelfand Yaglom method

Contour integral method allows to find the ratio of functional determinants whose eigenvalues are not explicitly known if functions $F(\lambda)$ and $F_{free}(\lambda)$ are given. Gel'fand Yaglom method is used to find these functions for 1D Schrödinger operators.

We write a one dimensional Hamiltonian of which we want to find determinant.

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \tag{6.16}$$

where the system is defined in the interval $[0,1]$. And H_{free} is the Hamiltonian of uniform system as

$$H_{free} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}. \tag{6.17}$$

Let

$$H\Phi_{\lambda_n} = \lambda_n \Phi_{\lambda_n} \tag{6.18}$$

be the eigenvalue equation on which Dirichlet boundary conditions are applied; $\Phi(0) = 0$, $\Phi(1) = 0$. We write also an initial value equation with the same operator,

$$H\Phi_\lambda = \lambda \Phi_\lambda \tag{6.19}$$

with the initial conditions $\Phi_\lambda(0) = 0$ and $\Phi'_\lambda(0) = 1$. When $\lambda = \lambda_n$, the second boundary condition of the eigenvalue equation is satisfied as

$$\Phi_{\lambda_n}(1) = 0 \tag{6.20}$$

If we consider $\Phi_\lambda(1)$ as a function of λ, $F(\lambda)$, then

$$F(\lambda) = 0 \qquad \forall \lambda = \lambda_n. \tag{6.21}$$

That means, we can find the required function, $F(\lambda)$, by writing an initial value equation with the operator which determinant is of interest.

$$\frac{\det H}{\det H_{free}} = \frac{\Phi_{\lambda=0}(1)}{\Phi_\lambda^{free}(1)} \tag{6.22}$$

.

To sum up the method, we have a 1D Schrödinger operator M. It is defined in the interval $[0, L]$. We want to find its determinant but we can not calculate its eigenvalues. Then we write two differential equations; one for M and one for M_{free},

$$\begin{aligned} M\Phi(x) &= 0 \\ M_{free}\Phi_{free}(x) &= 0. \end{aligned} \tag{6.23}$$

Boundary conditions are $\Phi(0), \Phi_{free}(0) = 0$ and $\Phi'(0), \Phi'_{free}(0) = 1$. Then

$$\frac{\det M}{\det M_{free}} = \frac{\Phi(L)}{\Phi_{free}(L)}. \tag{6.24}$$

.

6.3 Calculation of the free energy with GY method

Helmholtz Free energy, A, of uniform Bose gas and of black soliton are

$$A_{bs} = -\frac{1}{\beta} \ln Z_{bs} = -\frac{1}{\beta} \ln \left(e^{-S_{0,bs}} \prod_n \frac{1}{\det S^n_{2,bs}} \right) \tag{6.25}$$

$$A_{us} = -\frac{1}{\beta} \ln Z_{us} = -\frac{1}{\beta} \ln \left(e^{-S_{0,us}} \prod_n \frac{1}{\det S^n_{2,us}} \right) \tag{6.26}$$

respectively where the subscript us is for uniform solution and bs is for black soliton. We can calculate the difference between

$$A_{bs} = -\frac{1}{\beta} \left(-S_{0,bs} + \sum_n \ln \frac{1}{\det S^n_{2,bs}} \right) = A_{0,bs} - \frac{1}{\beta} \sum_n \ln \frac{1}{\det S^n_{2,bs}} \tag{6.27}$$

$$A_{us} = -\frac{1}{\beta} \left(-S_{0,us} + \sum_n \ln \frac{1}{\det S^n_{2,us}} \right) = A_{0,us} - \frac{1}{\beta} \sum_n \ln \frac{1}{\det S^n_{2,us}} \tag{6.28}$$

as

$$A_{bs} - A_{us} = A_{0,bs} - A_{0,us} - \frac{1}{\beta} \left[\sum_n \ln \frac{1}{\det S^n_{2,bs}} - \sum_n \ln \frac{1}{\det S^n_{2,us}} \right] \tag{6.29}$$

where $A_{0,us}$ and $A_{0,bs}$ are the ground state energies of uniform Bose gas and of black soliton respectively which we have calculated in Chapter 4 and Chapter 5 as

$$\begin{aligned} A_{0,us} &= \frac{U_0 N^2}{2V} \\ A_{0,bs} &= \frac{U_0 N^2}{2V} + \frac{4\hbar}{3\sqrt{m U_0}} \mu^{3/2}. \end{aligned} \tag{6.30}$$

The difference is then

$$\begin{aligned} A_{bs} - A_{us} &= \frac{4\hbar}{3\sqrt{m U_0}} \mu^{3/2} - \frac{1}{\beta} \sum_n \ln \left(1/\det S^n_{2,bs} \Big/ 1/\det S^n_{2,us} \right) \\ &= \frac{4\hbar}{3\sqrt{m U_0}} \mu^{3/2} - \frac{1}{\beta} \sum_n \ln \left(\frac{\det S^n_{2,us}}{\det S^n_{2,bs}} \right). \end{aligned} \tag{6.31}$$

We can think $S_{2,us}$,the action of uniform solution, as the normalized functional of the free system, $V(x) = 0$, and $S_{2,bs}$ as the desired one. Then we can perform GY method.

$$\frac{\det M}{\det M_{free}} = \frac{\det S^n_{2,bs}}{\det S^n_{2,us}} = \frac{\Phi^n_{bs}(2L)}{\Phi^n_{us}(2L)} \tag{6.32}$$

where $\Phi^n_{bs}(2L)$ and $\Phi^n_{us}(2L)$ are the solutions of the corresponding initial value problems. We calculate $\Phi^n_{us}(2L)$ analytically and $\Phi^n_{bs}(2L)$ numerically. The exact second order ground state energy can be found then with

$$E_{bs} - E_{us} = \lim_{T\to 0} A_{bs} - A_{us} = \lim_{T\to 0} \left\{ \frac{4\hbar}{3\sqrt{m U_0}} \mu^{3/2} - \frac{1}{\beta} \sum_n \ln \left(\frac{\Phi^n_{us}(2L)}{\Phi^n_{bs}(2L)} \right) \right\}. \tag{6.33}$$

We see how to write the partition function in terms of the determinant of S_2 in Chapter 5, for black soliton. We follow the same way to obtain it for uniform Bose gas. For uniform gas we do not need to do that calculation since we calculate the second order energy of Bose gas without referring GY method. But we need that to determine the energy of soliton since GY method does not provide a determinant itself rather a ratio of two.

6.3.1 Partition function of uniform Bose gas

The general open form of action is written in Chapter 3. When we plug the wavefunciton of uniform solution, $\sqrt{n_0}\delta_{n,0}\sqrt{\beta}$, (in Matsubara frequancy domain) into this general form of action we get rather a long equation. It will be in the form

$$\begin{aligned} S = \quad & S_0 \\ & + S_1 \\ & + S_2. \end{aligned} \tag{6.34}$$

where S_0 goes for zeroth order action in fluctuation ψ^1, S_1 for first order action in ψ^1, and lastly S_2 for the second order:

$$\begin{aligned} S = \quad & A \sum_{s=0}^{N} \Delta x \Bigg(\sum_{w_n} (iw_n - \mu) n_0 \delta_{w_n,0} \delta_{w_n,0} \beta + \sum_{w_n} \frac{-1}{2m\Delta x^2} n_0 \delta_{w_n,0} \delta_{w_n,0} \beta (1 - 2 + 1) \\ & \quad + \frac{U_0}{2\beta} \sum_{w_{n,m,p,r}} \delta_{\substack{w_n+w_m,\\ w_p+w_r}} n_0^2 \beta^2 \delta_{w_n,0} \delta_{w_m,0} \delta_{w_p,0} \delta_{w_r,0} \Bigg) \\ & + A \sum_{s=0}^{N} \Delta x \Bigg(\sum_{w_n} (iw_n - \mu)(\sqrt{n_0}\delta_{w_n,0})(\psi^1_{n,x} + \overline{\psi}^1_{n,x}) \\ & \quad + \sum_{w_n} \frac{-1}{2m\Delta x^2} (\sqrt{n_0}\delta_{w_n,0})(\psi^1_{n,x+1} - 2\psi^1_{n,x} + \psi^1_{n,x-1} + \overline{\psi}^1_{n,x} - 2\overline{\psi}^1_{n,x} + \overline{\psi}^1_{n,x}) \\ & \quad + \frac{U_0}{2\beta} \sum_{w_{n,m,p,r}} \delta_{\substack{w_n+w_m,\\ w_p+w_r}} \times \\ & \qquad\qquad \times \Big[n_0\sqrt{n_0}\delta_{w_n,0}\delta_{w_m,0}\delta_{w_p,0}\psi^1_{r,x} + n_0\sqrt{n_0}\delta_{w_m,0}\delta_{w_n,0}\delta_{w_r,0}\psi^1_{p,x} \\ & \quad + n_0\sqrt{n_0}\delta_{w_n,0}\delta_{w_p,0}\delta_{w_r,0}\overline{\psi}^1_{m,x} + n_0\sqrt{n_0}\delta_{w_m,0}\delta_{w_p,0}\delta_{w_r,0}\overline{\psi}^1_{n,x} \Big] \\ & + A \sum_{s=0}^{N} \Delta x \Bigg(\sum_{w_n} (iw_n - \mu) \overline{\psi}^1_{n,x} \psi^1_{n,x} \\ & \quad + \sum_{w_n} \frac{-1}{2m\Delta x^2} \left(\overline{\psi}^1_{n,x}\psi^1_{n,x+1} - 2\overline{\psi}^1_{n,x}\psi^1_{n,x} + \overline{\psi}^1_{n,x}\psi^1_{n,x-1} \right) + \frac{U_0}{2\beta} \sum_{w_{n,m,p,r}} \delta_{\substack{w_n+w_m,\\ w_p+w_r}} \\ & \qquad \Big[n_0\delta_{w_n,0}\delta_{w_m,0}\psi^1_{p,x}\psi^1_{r,x} + n_0\delta_{w_n,0}\delta_{w_p,0}\overline{\psi}^1_{m,x}\psi^1_{r,x} + n_0\delta_{w_n,0}\delta_{w_r,0}\overline{\psi}^1_{m,x}\psi^1_{p,x} \end{aligned}$$

$$+ n_0\delta_{w_m,0}\delta_{w_p,0}\overline{\psi}^1_{n,x}\psi^1_{r,x} + n_0\delta_{w_m,0}\delta_{w_r,0}\overline{\psi}^1_{n,x}\psi^1_{p,x} + n_0\delta_{w_p,0}\delta_{w_r,0}\overline{\psi}^1_{m,x}\overline{\psi}^1_{n,x}\Big]\Big)\Big). \tag{6.35}$$

After doing a few line simplifications Action looks like the following

$$\begin{aligned} S =& A\sum_{s=0}^{N}\Delta x\Bigg(\frac{-n_0^2U_0\beta}{2}A\sum_{s=0}^{N}\Delta x\Big[-\mu\sqrt{n_0}(\psi^1_{0,x}+\overline{\psi}^1_{0,x}) \\ &+\frac{-1}{2m\Delta x^2}n_0\big(\psi^1_{0,x+1}-2\psi^1_{0,x}+\psi^1_{0,x-1}\big)+\frac{U_0}{\beta}n_0\sqrt{n_0}(\psi^1_{0,x}+\overline{\psi}^1_{0,x})\Big] \\ &A\sum_{s=0}^{N}\Delta x\Big[\sum_{w_n}(iw_n-\mu)\overline{\psi}^1_{n,x}\psi^1_{n,x}-\frac{\overline{\psi}^1_{n,x}\psi^1_{n,x+1}-2\overline{\psi}^1_{n,x}\psi^1_{n,x}+\overline{\psi}^1_{n,x}\psi^1_{n,x-1}}{2m\Delta x^2} \\ &+\frac{U_0n_0}{2\beta}\big[\sum_{w_p}\psi^1_{p,x}\psi^1_{-p,x}\big]+2\sum_{w_m}\psi^1_{m,x}\psi^1_{m,x}+2\sum_{w_n}\psi^1_{n,x}\psi^1_{n,x}+\sum_{w_m}\psi^1_{-m,x}\psi^1_{m,x}\Big]\Bigg) \end{aligned} \tag{6.36}$$

S_0 gives the known first order energy, S_1 is zero. S_2 is

$$\begin{aligned} S^n_{u,2} =& A\sum_{x=1}^{N}\Delta x\,\big[\overline{\psi}^1_{n,x}(iw_n-\mu+\frac{1}{m\Delta x^2}+\frac{4U_0n_0}{2\beta})\psi^1_{n,x}+\psi^1_{n,x}(\frac{U_0n_0}{2\beta})\psi^1_{-n,x} \\ &\qquad+\overline{\psi}^1_{n,x}(\frac{U_0n_0}{2\beta})\overline{\psi}^1_{-n,x}+\overline{\psi}^1_{n,x}(\frac{-1}{2m\Delta x^2})\psi^1_{n,x+1} \\ &\qquad+\overline{\psi}^1_{n,x}(\frac{-1}{2m\Delta x^2})\psi^1_{n,x-1}\big] \\ =& A\sum_{\substack{x=1\\y=1}}^{N}\Delta x\,\big[\overline{\psi}^1_{n,x}L^n_1\psi^1_{n,y}+\psi^1_{n,x}L^n_2\psi^1_{-n,y}\overline{\psi}^1_{n,x}L^n_3\overline{\psi}^1_{-n,y}+\psi^1_{n,x}L^n_4\overline{\psi}^1_{n,y}\big] \end{aligned} \tag{6.37}$$

where L_1^n, L_2^n,L_3^n, and L_4^n are the matrices respectively given by

$$L_1^n = \begin{bmatrix} f(n) & c & 0 & \dots & 0 \\ c & f(n) & \cdots & \dots & 0 \\ 0 & c & f(n) & c & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & c & f(n) \end{bmatrix} \tag{6.38}$$

$$L_2^n = \begin{bmatrix} U_0n_0/2\beta & 0 & 0 & \dots & 0 \\ 0 & U_0n_0/2\beta & 0 & \dots & 0 \\ 0 & 0 & U_0n_0/2\beta & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \vdots & 0 & U_0n_0/2\beta \end{bmatrix} \tag{6.39}$$

$$L_3^n = L_2^n \tag{6.40}$$

$$L_4^n = L_1^n \tag{6.41}$$

where

$$f(n) = \frac{1}{2}\Big(iw_n - \mu - \frac{1}{m\Delta x^2} + \frac{4U_0n_0}{2\beta}\Big) \qquad \text{and} \qquad c = \frac{-1}{2m\Delta x^2}. \tag{6.42}$$

We define Φ

$$\Phi_{n,us} = \begin{bmatrix} \psi^1_{n,us} \\ \overline{\psi^1}_{n,us} \end{bmatrix}, \tag{6.43}$$

and write partition function as

$$\begin{aligned} Z &= \exp\{-S_{0,bs}\} \prod_n \Bigg[\int \frac{1}{N} d\psi d\overline{\psi} \exp\Bigg\{ -A \sum_{x=1,y=1}^{2N} \Delta x \bar{\Phi}^1 \mathbb{L}^n_{xy} \Phi^1 \Bigg\} \Bigg] \\ &= \exp\{-S_{0,bs}\} \prod_n \frac{1}{\det \mathbb{L}^n}, \end{aligned} \tag{6.44}$$

where

$$\mathbb{L}^n = \begin{bmatrix} L_1^n & L_2^n \\ L_3^n & L_4^n \end{bmatrix}. \tag{6.45}$$

The corresponding initial value problem for the uniform solution case is $\mathbb{L}^n_{us}\Phi_{n,us} = 0$ where $\Phi_{n,us}(0) = 0$ and $\Phi'_{n,us}(0) = 1$:

$$\mathbb{L}^n \Phi_{n,us} = 0; \qquad \mathbb{L}^n_{us} \begin{bmatrix} \psi^1_{n,us} \\ \overline{\psi^1}_{n,us} \end{bmatrix} = 0; \qquad \begin{bmatrix} L_1^n & L_2^n \\ L_3^n & L_4^n \end{bmatrix} \begin{bmatrix} \psi^1_{n,us} \\ \overline{\psi^1}_{n,us} \end{bmatrix} = 0 \tag{6.46}$$

$$L_1^n \psi_{n,us}^1 + L_2^n \overline{\psi^1}_{n,us} = 0 \tag{6.47}$$
$$L_3^n \psi_{n,us}^1 + L_4^n \overline{\psi^1}_{n,us} = 0 \tag{6.48}$$

We rewrite the matrices

$$L_1^n = L_4^n = A\mathbb{1}\Big(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{(iw_n - \mu)}{2} + \frac{U_0 n_0}{\beta}\Big) \tag{6.49}$$
$$L_2^n = L_3^n = A\mathbb{1}\frac{U_0 n_0}{2\beta}. \tag{6.50}$$

The coupled initial value problems becomes

$$A \cdot -\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi + A\Big[\frac{iw_n - \mu}{2} + \frac{U_0 n_0}{\beta}\Big]\psi + A \cdot \frac{U_0 n_0}{2\beta}\overline{\psi} = 0 \tag{6.51}$$
$$A \cdot \frac{U_0 n_0}{2\beta}\psi + A \cdot -\frac{1}{2}\frac{\partial^2}{\partial x^2}\overline{\psi} + A\Big[\frac{iw_n - \mu}{2} + \frac{U_0 n_0}{\beta}\Big]\overline{\psi} = 0 \tag{6.52}$$

can be simplified to

$$\psi'' = \big(iw_n - \mu + \frac{2U_0 n_0}{\beta}\big)\psi + \frac{U_0 n_0}{\beta}\overline{\psi} \tag{6.53}$$
$$\overline{\psi}'' = \big(iw_n - \mu + \frac{2U_0 n_0}{\beta}\big)\overline{\psi} + \frac{U_0 n_0}{\beta}\psi \tag{6.54}$$

and then to

$$\psi'' = a\psi + b\overline{\psi} \tag{6.55}$$
$$\overline{\psi}'' = a\overline{\psi} + b\psi \tag{6.56}$$

where $a = (iw_n - \mu + 2U_0 n_0/\beta)$ and $b = U_0 n_0/\beta$. The subscripts and superscripts of ψ are dropped till the end of this calculation.

We seek for the solutions of the form

$$\psi = \hat{\psi}\cos(kx - \alpha) \qquad \overline{\psi} = \hat{\overline{\psi}}\cos(kx - \alpha) \tag{6.57}$$

After plugging them into the above coupled differential equations, we get

$$-k^2\hat{\psi}\cos(kx - \alpha) = a\hat{\psi}\cos(kx - \alpha) + b\hat{\overline{\psi}}\cos(kx - \alpha) \tag{6.58}$$
$$-k^2\hat{\overline{\psi}}\cos(kx - \alpha) = a\hat{\overline{\psi}}\cos(kx - \alpha) + b\hat{\psi}\cos(kx - \alpha). \tag{6.59}$$

These two gives

$$\hat{\psi}\left(\frac{-(a+k^2)^2+b^2}{b}\right)=0 \tag{6.60}$$

where $k_1 = \sqrt{b-a}$ and $k_2 = \sqrt{-b-a}$ are the wavenumbers since $\hat{\psi} = \hat{\overline{\psi}} = 0$ is the trivial solution that we are not looking for. Here we neglect $-k_1$ and $-k_2$ since cosine is an even function. k_1 and k_2 corresponds to the normal modes of the system and the most general motion of such a system is a linear combination of the two normal modes:

$$\boxed{k=\sqrt{b-a}} \Rightarrow \hat{\overline{\psi}} = -\hat{\psi}$$
$$\psi = \hat{\psi}_1 \cos(k_1 x - \alpha_1) \overline{\psi} = -\hat{\overline{\psi}}_1 \cos(k_1 x - \alpha_1) \tag{6.61}$$

and

$$\boxed{k=\sqrt{-b-a}} \Rightarrow \hat{\overline{\psi}} = \hat{\psi}$$
$$\psi = \hat{\psi}_2 \cos(k_2 x - \alpha_2) \overline{\psi} = \hat{\overline{\psi}}_2 \cos(k_2 x - \alpha_2) \tag{6.62}$$

as

$$\psi = \hat{\psi}_1 \cos\Big(\sqrt{b-a}x - \alpha_1\Big) + \hat{\psi}_2 \cos\Big(\sqrt{-b-a}x - \alpha_2\Big) \tag{6.63}$$
$$\overline{\psi} = -\hat{\psi}_1 \cos\Big(\sqrt{b-a}x - \alpha_1\Big) + \hat{\psi}_2 \cos\Big(\sqrt{-b-a}x - \alpha_2\Big). \tag{6.64}$$

The unknown coefficients $\hat{\psi}_1$, $\hat{\psi}_2$, α_1 and α_2 are to be determined from the initial conditions

$$\Phi(0) = 0 \quad \text{and} \quad \Phi'(0) = 1. \tag{6.65}$$

But these are not enough, we need four. Therefore we add two more initial conditions, namely the complex conjugates of the original two:

$$\overline{\Phi}(0) = 0 \quad \text{and} \quad \overline{\Phi}'(0) = 1. \tag{6.66}$$

The relation between $\Phi(x)$ and $\psi(x)$ via the corresponding matrix is

$$\Phi(x) = \psi(x) \quad \text{if} \quad x \leq L, \qquad \Phi(x) = \overline{\psi}(x-L) \quad \text{if} \quad x \geq L, \tag{6.67}$$

which gives $\Phi(0) = \psi(0)$, $\Phi'(0) = \psi'(0)$ and $\Phi(2L) = \overline{\psi}(L)$.

We rewrite the initial conditions

$$\begin{aligned}
\Phi(0) = \psi(0) = 0, \qquad & \Phi'(0) = \psi'(0) = 1 \\
\overline{\Phi}(0) = \overline{\psi}(0) = 0, \qquad & \overline{\Phi}'(0) = \overline{\psi}'(0) = 1
\end{aligned} \tag{6.68}$$

and apply them to the general solutions

$$\hat{\psi}_1 \cos(\alpha_1) + \hat{\psi}_2 \cos(\alpha_2) = 0 \tag{6.69}$$

$$-k_1\hat{\psi}_1 \sin(-\alpha_1) - k_2\hat{\psi}_2 sin(-\alpha_2) = 1 \tag{6.70}$$

$$-\hat{\psi}_1 \cos(\alpha_1) + \hat{\psi}_2 \cos(\alpha_2) = 0 \tag{6.71}$$

$$k_1\hat{\psi}_1 \sin(-\alpha_1) - k_2\hat{\psi}_2 sin(-\alpha_2) = 1. \tag{6.72}$$

Adding the first and the third gives

$$2\hat{\psi}_2 \cos(\alpha_2) = 0, \qquad \alpha_2 = (n_2 + \frac{1}{2})\pi, \tag{6.73}$$

and subtracting them gives

$$2\hat{\psi}_1 \cos(\alpha_1) = 0, \qquad \alpha_1 = (n_1 + \frac{1}{2})\pi. \tag{6.74}$$

$\sin(\alpha_1)$ and $\sin(\alpha_2)$ can be written as $(-1)^{n_1+1}$ and $(-1)^{n_2+1}$ respectively. After a few line of calculations

$$\hat{\psi}_1 = \frac{1 - k_2\hat{\psi}_2(-1)^{n_2}}{k_1(-1)^{n_1}} \tag{6.75}$$

are

$$k_1^* \frac{1 - k_2\hat{\psi}_2(-1)^{n_2}}{k_1(-1)^{n_1}} (-1)^{n_1+1} + k_2^*\hat{\psi}_2(-1)^{n_2} = 1 \tag{6.76}$$

are obtained. From these, $\hat{\psi}_1$ and $\hat{\psi}_2$ are found as

$$\boxed{\begin{aligned}
\hat{\psi}_1 &= (-1)^{n_1} \frac{k_2^* - k_2}{k_1^* k_2 + k_1 k_2^*} \qquad \alpha_1 = (n_1 + \frac{1}{2})\pi \quad (6.77a) \\
\hat{\psi}_2 &= (-1)^{n_2} \frac{k_1^* + k_1}{k_1^* k_2 + k_1 k_2^*} \qquad \alpha_2 = (n_2 + \frac{1}{2})\pi \quad (6.77b)
\end{aligned}}$$

We need $\Phi_{us}(2L)$. It is obtained as

$$\begin{aligned}\Phi_{us}(2L) = \overline{\psi}(L) &= -\hat{\psi}_1 \cos(k_1 L - \alpha_1) + \hat{\psi}_2 \cos(k_2 L - \alpha_2) \\ &= \frac{(-1)^{n_1+1}(k_2^* - k_2)}{k_1^* k_2 + k_1 k_2^*} \cos(k_1 L - \alpha_1) \\ &+ \frac{(-1)^{n_2}(k_1^* + k_1)}{k_1^* k_2 + k_1 k_2^*} \cos(k_2 L - \alpha_2) \\ &= \frac{k_2^* - k_2}{k_1^* k_2 + k_1 k_2^*} \sin(k_1 L) + \frac{k_1^* + k_1}{k_1^* k_2 + k_1 k_2^*} \sin(k_2 L) \end{aligned} \tag{6.78}$$

where k_1 and k_2 are

$$k_1 = \sqrt{b-a} = \sqrt{\frac{U_0 n_0}{\beta} - \left(iw_n - \mu + \frac{2U_0 n_0}{\beta}\right)} = \sqrt{\mu - iw_n - \frac{U_0 n_0}{\beta}} \tag{6.79}$$

$$k_2 = \sqrt{-b-a} = \sqrt{-\frac{U_0 n_0}{\beta} - \left(iw_n - \mu + \frac{2U_0 n_0}{\beta}\right)} = \sqrt{\mu - iw_n - \frac{3U_0 n_0}{\beta}}. \tag{6.80}$$

6.3.2 Partition function of black soliton

We also need $\Phi_{bs}(2L)$. The corresponding initial value problem for black soliton is $\mathbb{K}^n_{us}\Phi_{n,bs} = 0$ where $\Phi_{n,bs}(0) = 0$ and $\Phi'_{n,bs}(0) = 1$:

$$\mathbb{K}^n \Phi_{n,bs} = 0; \qquad \mathbb{K}^n_{bs} \begin{bmatrix} \psi^1_{n,bs} \\ \overline{\psi^1}_{n,bs} \end{bmatrix} = 0; \qquad \begin{bmatrix} K^n_1 & K^n_2 \\ K^n_3 & K^n_4 \end{bmatrix} \begin{bmatrix} \psi^1_{n,bs} \\ \overline{\psi^1}_{n,bs} \end{bmatrix} = 0 \tag{6.81}$$

$$K^n_1 \psi^1_{n,bs} + K^n_2 \overline{\psi^1}_{n,bs} = 0 \tag{6.82}$$

$$K^n_3 \psi^1_{n,bs} + K^n_4 \overline{\psi^1}_{n,bs} = 0 \tag{6.83}$$

The matrices are found in Chapter 5 as

$$K^n_1 = K^n_4 = \frac{1}{2} A \mathbb{1} \big(- \frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{(iw_n - \mu)}{2} + U_0 |\psi_0|^2 \tanh^2\left(\frac{x}{\sqrt{2}\xi}\right)\big) \tag{6.84}$$

$$K^n_2 = K^n_3 = A\mathbb{1}\left(\frac{U_0}{2}|\psi_0|^2 \tanh^2\left(\frac{x}{\sqrt{2}\xi}\right)\right). \tag{6.85}$$

The coupled initial value problems becomes

$$
\begin{aligned}
&A \cdot -\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi + A[\frac{iw_n - \mu}{2} + U_0|\psi_0|^2 \tanh^2\left(\frac{x}{\sqrt{2}\xi}\right)]\psi \\
&\qquad + A \cdot \left(\frac{U_0}{2}|\psi_0|^2 \tanh^2\left(\frac{x}{\sqrt{2}\xi}\right)\right)\overline{\psi} = 0 && (6.86) \\
&A \cdot \left(\frac{U_0}{2}|\psi_0|^2 \tanh^2\left(\frac{x}{\sqrt{2}\xi}\right)\right)\psi + A \cdot -\frac{1}{2}\frac{\partial^2}{\partial x^2}\overline{\psi} \\
&\qquad + A[\frac{iw_n - \mu}{2} + U_0|\psi_0|^2 \tanh^2\left(\frac{x}{\sqrt{2}\xi}\right)]\overline{\psi} = 0. && (6.87)
\end{aligned}
$$

It is hard to solve these equations analytically. So, we solve them numerically by using 4th order Runge Kutta method.

6.3.2.1 4^{th} order Runge Kutta method for coupled differential equations

4^{th} order Runge Kutta method is used to solve differential equations numerically. Consider a differential equation

$$\frac{dy}{dt} = f(y,t) \tag{6.88}$$

. k_1, k_2, k_3, and k_4 are defined in intermediate steps as

$$
\begin{aligned}
k_1 &= dt \cdot f(y_N, t_N) \\
k_2 &= dt \cdot f(y_N + \frac{k_1}{2}, t_N + \frac{\Delta t}{2}) \\
k_3 &= dt \cdot f(y_N + \frac{k_2}{2}, t_N + \frac{\Delta t}{2}) \\
k_4 &= dt \cdot f(y_N + k_3, t_N + \Delta t)
\end{aligned} \tag{6.89}
$$

.

The method gives y_{N+1} in terms of y_N as

$$y_{N+1} = y_N + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6}. \tag{6.90}$$

We have two coupled second order differential equations. They can be written as four first order differential equations,

$$\begin{aligned}
\frac{dy_1}{dt} &= g(y_2, t) &&= y_2 \\
\frac{d\overline{y}_1}{dt} &= g(\overline{y}_2, t) &&= \overline{y}_2 \\
\frac{dy_2}{dt} &= f(y_1, \overline{y}_1, t) &&= h(x)y_1 + s(x)\overline{y}_1 \\
\frac{d\overline{y}_2}{dt} &= f(\overline{y}_1, y_1, t) &&= h(x)\overline{y}_1 + s(x)y_1
\end{aligned} \tag{6.91}$$

where

$$\begin{aligned}
y_1 &= \psi \\
\overline{y}_1 &= \overline{\psi}
\end{aligned} \tag{6.92}$$

and where

$$\begin{aligned}
h(x) &= 2\Big[\frac{iw_n - \mu}{2} + U_0|\psi_0|^2 \tanh^2\left(\frac{x}{\sqrt{2}\xi}\right)\Big] \\
s(x) &= 2\left(\frac{U_0}{2}|\psi_0|^2 \tanh^2\left(\frac{x}{\sqrt{2}\xi}\right)\right)
\end{aligned} \tag{6.93}$$

.

We modify the intermediate steps for coupled differential equations by following the original trace in the method,

$$\begin{aligned}
k_{11} &= dt \cdot g(y_{2,N}, t_N) \\
k_{21} &= dt \cdot g(\overline{y}_{2,N}, t_N) \\
k_{31} &= dt \cdot f(y_{1,N}, \overline{y}_{1,N}, t_N) \\
k_{41} &= dt \cdot f(\overline{y}_{1,N}, y_{1,N}, t_N)
\end{aligned} \tag{6.94}$$

$$\begin{aligned}
k_{12} &= dt \cdot g(y_{2,N} + \frac{k_{31}}{2}, t_N + \frac{\Delta t}{2}) \\
k_{22} &= dt \cdot g(\overline{y}_{2,N} + \frac{k_{41}}{2}, t_N + \frac{\Delta t}{2})
\end{aligned}$$

$$k_{32} = dt \cdot f(y_{1,N} + \frac{k_{11}}{2}, \overline{y}_{1,N} + \frac{k_{21}}{2}, t_N + \frac{\Delta t}{2})$$
$$k_{42} = dt \cdot f(\overline{y}_{1,N} + \frac{k_{21}}{2}, y_{1,N} + \frac{k_{11}}{2}, t_N + \frac{\Delta t}{2}) \tag{6.95}$$

$$k_{13} = dt \cdot g(y_{2,N} + \frac{k_{32}}{2}, t_N + \frac{\Delta t}{2})$$
$$k_{23} = dt \cdot g(\overline{y}_{2,N} + \frac{k_{42}}{2}, t_N + \frac{\Delta t}{2})$$
$$k_{33} = dt \cdot f(y_{1,N} + \frac{k_{12}}{2}, \overline{y}_{1,N} + \frac{k_{22}}{2}, t_N + \frac{\Delta t}{2})$$
$$k_{43} = dt \cdot f(\overline{y}_{1,N} + \frac{k_{22}}{2}, y_{1,N} + \frac{k_{12}}{2}, t_N + \frac{\Delta t}{2}) \tag{6.96}$$

$$k_{14} = dt \cdot g(y_{2,N} + k_{33}, t_N + \Delta t)$$
$$k_{24} = dt \cdot g(\overline{y}_{2,N} + k_{43}, t_N + \Delta t)$$
$$k_{34} = dt \cdot f(y_{1,N} + k_{13}, \overline{y}_{1,N} + k_{23}, t_N + \Delta t)$$
$$k_{44} = dt \cdot f(\overline{y}_{1,N} + k_{23}, y_{1,N} + +k_{13}, t_N + \Delta t). \tag{6.97}$$

At each step, increments are given as

$$y_{1,N+1} = y_{1,N} + \frac{k_{11}}{6} + \frac{k_{12}}{3} + \frac{k_{13}}{3} + \frac{k_{14}}{6}$$
$$\overline{y}_{1,N+1} = \overline{y}_{1,N} + \frac{k_{21}}{6} + \frac{k_{22}}{3} + \frac{k_{23}}{3} + \frac{k_{24}}{6}$$
$$y_{2,N+1} = y_{2,N} + \frac{k_{31}}{6} + \frac{k_{32}}{3} + \frac{k_{33}}{3} + \frac{k_{34}}{6}$$
$$\overline{y}_{2,N+1} = \overline{y}_{2,N} + \frac{k_{41}}{6} + \frac{k_{42}}{3} + \frac{k_{43}}{3} + \frac{k_{44}}{6} \tag{6.98}$$

.

By using this code we get $\Phi_{bs}(2L)$. The corrected ground state energy up to the Bogoliubov level of order is

$$E_{bs} - E_{us} = \lim_{T\to 0} A_{bs} - A_{us} = \lim_{T\to 0} \left\{ \frac{4\hbar}{3\sqrt{m}U_0}\mu^{3/2} - \frac{1}{\beta}\sum_n \ln\left(\frac{\Phi^n_{us}(2L)}{\Phi^n_{bs}(2L)}\right) \right\}$$
$$= \lim_{T\to 0} \left\{ \frac{4\hbar}{3\sqrt{m}U_0}\mu^{3/2} - \frac{1}{\beta}\ln\prod_n \left(\frac{\Phi^n_{us}(2L)}{\Phi^n_{bs}(2L)}\right) \right\}. \tag{6.99}$$

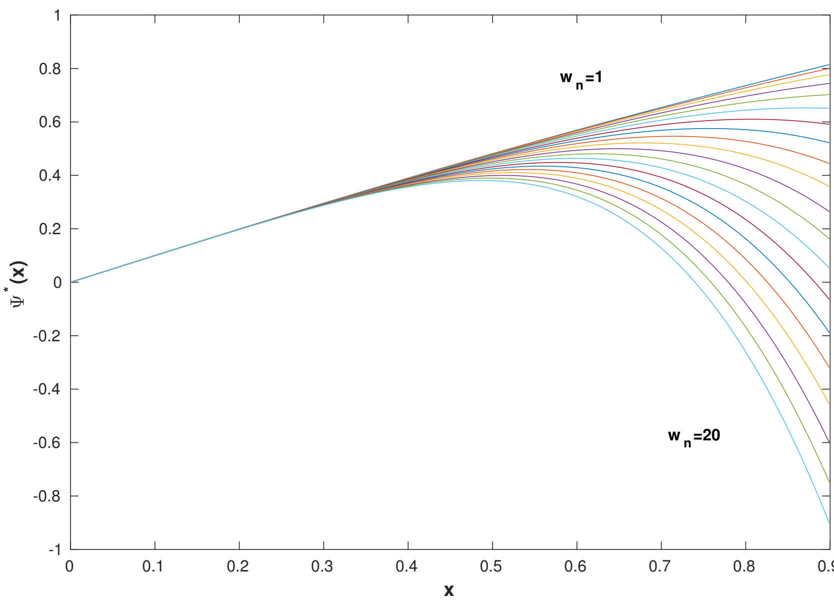

Figure 6.3: $\overline{\psi}(x)$ for first 20 modes

In the figure, the divergence of the higher modes are seen. We should perform a renormalization like in the case of uniform solution.

6.4 Conclusion

Corrections to the ground state energy of a Bose gas which calculated via mean field Hamiltonian can be added by considering the contributions of quantum fluctuations. Bogoliubov de Gennes equaitons possesses information of these fluctuations. In the case of uniform gas, BdG equations can be solved analytically and the dispersion relation of all modes can be obtained. By performing a renormalization, the ground state energy of uniform gas is calculated.

In the case of a Bose gas with a single stationary dark soliton, BdG equations become complicated and can not be solved analytically for all modes. Numerically, the contributions of only a few modes can be calculated. In this thesis, we formulate the usage of Gelfand Yaglom method to calculate ground state energy up to the Bogoliubov order from quantum partition function. We solve two coupled initial value equations numerically but the rest part of the calculation is analytic. We should perform a renormalization like in the case of uniform gas in the next step.

We calculate the corrected ground state energies for a Bose gas with zero external potential. As further studies, we will generalize our calculation for trapped Bose gas to compare the result with empirical values since experiments are done for trapped gas in harmonic oscillator potentials.

Moreover, we will implement this usage of Gelfand Yaglom method in the calculation of ground state energies of collective excitations for Fermionic condensates.

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