Gaussian time-dependent variational principle for bosons: Contact interaction in one dimension

Arthur K. Kerman
Center for Theoretical Physics, Laboratory for Nuclear Science and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

Paolo Tommasini
Institute for Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138

(Received 11 March 1997; revised manuscript received 15 July 1997)

We investigate the Dirac time-dependent variational method using a Gaussian trial functional for an infinite one-dimensional system of bosons interacting through a repulsive contact interaction. The method produces a set of nonlinear time-dependent equations for the variational parameters. By solving the static equations we have calculated the ground state energy per particle. We have also considered small oscillations about the equilibrium and obtain mode equations which lead us to a gapless dispersion relation. The existence of an exact numerical solution for the ground-state energy and excitations obtained by Lieb allow us to compare with the Gaussian results. We can also, as the system becomes less dilute, see the improvement of the results as compared with the Bogoliubov scheme. [S0163-1829(97)04846-7]

I. INTRODUCTION

Recently Bose-Einstein condensation in atomic traps was achieved[1–3] in a dilute regime ($a^3 n \ll 1$). This is in contrast with the helium 4 regime where a much higher density leads to ($a^3 n \approx 1$). For the high-density regime there is a large ''depletion'' ($\approx 90\%$) (Ref. 4) where as for the dilute regime it is very small ($\approx 1\%$).[5]

Theoretically these experiments have been described very successfully with mean-field theory without quantum fluctuations using the Gross-Pitaevskii equation[6] or the Bogoliubov scheme.[5] The Gaussian self-consistent approximation presented here should be useful in the intermediate regime. Unfortunately due to three-body recombinations there seems to be a limit[7] for increasing the number of particles in the system. Recently it has been pointed out[8] that using a strong magnetic field it would be possible to make the system effectively less dilute by drastically changing the scattering length. This makes the comparison between self-consistent results and dilute theories very important. In this context the one-dimensional δ function case can produce some insight because a contact interaction can be used in the self-consistent theory in contrast with the three-dimensional case.[9,10] The existence of an exact solution for the ground-state energy and for particle and hole excitations makes the comparison very interesting, provide that we understand how the separated particle and hole excitations of the exact solution[20] are connected to the particle-hole excitations given by the approximate methods.

The objective of this paper is to exhibit the most general way of obtaining time-dependent equations of motion in the Gaussian approximation.[11] This will lead to the so-called generalized random-phase approximation (RPA), when one examines infinitesimal oscillations about the equilibrium. The static solution in the uniform case can be obtained using several other methods[12,9] leading to a gap in the quasiboson energy. We show here that the time-dependent RPA equations lead to a gapless mode. In fact this *must* happen because particle number conservation symmetry is broken in the static solution, so the zero gap is exactly the associated Goldstone mode. This discussion can be seen as an alternative to the functional derivative[13,14] method in the Girardeau-Arnowitt[15] approximation.

The Bogoliubov scheme, for a dilute or weak interacting system, can be obtained by a particular truncation of the Gaussian results. So, we can compare the Gaussian variational results, the dilute Bogoliubov scheme, and the exact solution for the particular case under discussion here.

The structure of this paper is as follows. Section II reviews the time-dependent variational principle and the canonical nature of the equations of motion arising from it. In Sec. III we specialize to the one-dimensional uniform case end examine the ground-state energy and the excitations for both the approximate methods and the exact solution. Section IV contains our numerical solutions and conclusions

II. GENERAL FORMALISM

In this section we shall review some of the results of the time-dependent variational principle[11,16] and show how it can be implemented in the nonrelativistic case. First we define an effective action functional for the time-dependent quantum system

$$S=\int L(t)dt=\int dt\langle\Psi,t|(i\partial_t-\hat{H})|\Psi,t\rangle, \tag{1}$$

where $|\Psi,t\rangle$ is the quantum state of the system and $\hat{H}$ is the Hamiltonian of the theory. For a system of nonrelativistic interacting bosons we have [we use the notation: $\int_{\mathbf{x}}=\int d^3x$]

$$\hat{H}=\int_{\mathbf{x},\mathbf{y}}\hat{\psi}(\mathbf{x})^{\dagger}h(\mathbf{x},\mathbf{y})\hat{\psi}(\mathbf{y})+\frac{1}{2}\int_{\mathbf{x},\mathbf{y}}\hat{\psi}(\mathbf{y})^{\dagger}\hat{\psi}(\mathbf{x})^{\dagger}V(\mathbf{x}-\mathbf{y}) \times\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{y}), \tag{2}$$

where the one-body Hamiltonian $h(\mathbf{x},\mathbf{y})$ may include a one-body external potential. The creation and destruction operators $\hat{\psi}^\dagger$ and $\hat{\psi}$ can be written in the form

$$\hat{\psi}(\mathbf{x})=\frac{1}{\sqrt{2}}[\hat{\phi}(\mathbf{x})+i\hat{\pi}(\mathbf{x})], \tag{3}$$

$$\hat{\psi}(\mathbf{x})^\dagger=\frac{1}{\sqrt{2}}[\hat{\phi}(\mathbf{x})-i\hat{\pi}(\mathbf{x})],$$

where $\hat{\phi}(\mathbf{x})$ is the field operator and $\hat{\pi}(\mathbf{x})$ is the canonical field momemtum.

We can obtain the time-dependent Schrödinger equation by requiring that S is stationary, supplemented by appropriate boundary conditions, under the most general variation of $|\Psi,t\rangle$. The variational scheme is implemented by chosing a trial wave functional describing the system. Working in the functional Shrödinger picture we replace the abstract state $|\Psi,t\rangle$ by a wave functional of the field $\phi'(\mathbf{x})$

$$|\Psi,t\rangle\rightarrow\Psi[\phi',t]. \tag{4}$$

The action of the operators $\hat{\phi}(\mathbf{x})$ and the canonical momentum $\hat{\pi}(\mathbf{x})$ are realized, respectively, by

$$\hat{\phi}(\mathbf{x})|\Psi,t\rangle\rightarrow\phi'(\mathbf{x})\Psi[\phi',t], \tag{5}$$

$$\hat{\pi}(\mathbf{x})|\Psi,t\rangle\rightarrow-i\frac{\delta}{\delta\phi'(\mathbf{x})}\Psi[\phi',t].$$

The mean value of any operator is calculated by the functional integral

$$\langle\Psi,t|\mathcal{O}|\Psi,t\rangle=\int(\mathcal{D}\phi')\Psi^*[\phi',t]\mathcal{O}\Psi[\phi',t], \tag{6}$$

where Ψ is normalized to unity. The Gaussian approximation consists of taking a Gaussian trial wave functional in its most general parametrization

$$\Psi[\phi',t]=N\exp\left\{-\int_{\mathbf{x},\mathbf{y}}\delta\phi'(\mathbf{x},t)\left[\frac{G^{-1}(\mathbf{x},\mathbf{y},t)}{4}-i\Sigma(\mathbf{x},\mathbf{y},t)\right]\delta\phi'(\mathbf{y},t)+i\int_{\mathbf{x}}\pi(\mathbf{x},t)\delta\phi'(\mathbf{x},t)\right\}, \tag{7}$$

with $\delta\phi'(\mathbf{x},t)=\phi'(\mathbf{x})-\phi(\mathbf{x},t)$. Due to the fact that the Hamiltonian commutes with the number of particles $\hat{N}=\int_{\mathbf{x}}\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})$, i.e.,

$$[\hat{H},\hat{N}]=0, \tag{8}$$

we can actually define a more general trial functional

$$|\Psi',t\rangle=e^{-i\hat{N}\theta(t)}|\Psi,t\rangle, \tag{9}$$

where $\theta(t)$ is another variational parameter introduced because of this continuous symmetry. Thus our variational parameters are $\phi(\mathbf{x},t)$, $\pi(\mathbf{x},t)$, $\theta(t)$, $G(\mathbf{x},\mathbf{y},t)$, and $\Sigma(\mathbf{x},\mathbf{y},\ t)$, with G and Σ being real symmetric matrices. These quantities are related to the following mean values:

$$\begin{aligned}\langle\Psi',t|\hat{\phi}(\mathbf{x})|\Psi',t\rangle&=\phi(\mathbf{x},t),\\ \langle\Psi',t|\hat{\pi}(\mathbf{x})|\Psi',t\rangle&=\pi(\mathbf{x},t),\end{aligned} \tag{10}$$

$$\langle\Psi',t|\hat{\phi}(\mathbf{x})\hat{\phi}(\mathbf{y})|\Psi',t\rangle=G(\mathbf{x},\mathbf{y},t)+\phi(\mathbf{x},t)\phi(\mathbf{y},t),$$

$$\langle\Psi',t|i\frac{\delta}{\delta t}|\Psi',t\rangle=\int_{\mathbf{x},\mathbf{y}}\Sigma(\mathbf{x},\mathbf{y},t)\dot{G}(\mathbf{y},\mathbf{x},t)+\int_{\mathbf{x}}\pi(\mathbf{x},t)\dot{\phi}(\mathbf{x},t)+\mathcal{N}\dot{\theta}(t)+\text{total time derivatives}. \tag{11}$$

We may ignore the total time derivatives because they do not contribute to the equations of motion. If now we write the action we will get

$$S=\int dt\left(\int_{\mathbf{x}}\pi(\mathbf{x},t)\dot{\phi}(\mathbf{x},t)+\int_{\mathbf{x},\mathbf{y}}\Sigma(\mathbf{x},\mathbf{y},t)\dot{G}(\mathbf{y},\mathbf{x},t)+\mathcal{N}\dot{\theta}(t)-\mathcal{H}\right), \tag{12}$$

where

$$\mathcal{H}=\langle\Psi',t|\hat{H}|\Psi',t\rangle \tag{13}$$

and

$$\mathcal{N}=\langle\Psi',t|\hat{N}|\Psi',t\rangle. \tag{14}$$

From Eq. (12) we see that $(\mathcal{N},\theta)$, (π,ϕ), and (Σ,G) are canonical pairs. Because of the symmetry $\mathcal{H}$ has no dependence on θ and it follows that $\dot{N}=0$ and $\dot{\theta}(t)=\text{const}\equiv\mu$. We can now write the remaining Hamilton equations,

$$\begin{aligned}\dot{\phi}(\mathbf{x},t)&=\frac{\delta(\mathcal{H}-\mu\mathcal{N})}{\delta\pi(\mathbf{x},t)},\\ \dot{\pi}(\mathbf{x},t)&=-\frac{\delta(\mathcal{H}-\mu\mathcal{N})}{\delta\phi(\mathbf{x},t)},\\ \dot{G}(\mathbf{x},\mathbf{y},t)&=\frac{\delta(\mathcal{H}-\mu\mathcal{N})}{\delta\Sigma(\mathbf{x},\mathbf{y},t)},\\ \dot{\Sigma}(\mathbf{x},\mathbf{y},t)&=-\frac{\delta(\mathcal{H}-\mu\mathcal{N})}{\delta G(\mathbf{x},\mathbf{y},t)}.\end{aligned} \tag{15}$$

For convenience we introduce

$$\psi(\mathbf{x},t)\equiv\langle\hat{\psi}(\mathbf{x})\rangle=\frac{\phi(\mathbf{x},t)+i\pi(\mathbf{x},t)}{\sqrt{2}}, \tag{16}$$

so that the equations for ϕ and π become

$$\imath\dot{\psi}(\mathbf{x},t)=\frac{\delta(\mathcal{H}-\mu\mathcal{N})}{\delta\psi^*(\mathbf{x},t)}. \tag{17}$$

To obtain $\mathcal{H}-\mu\mathcal{N}$ we have to compute

$$\mathcal{H}-\mu\mathcal{N}=\int(\mathcal{D}\phi')\Psi^*[\phi',t][\hat{H}-\mu\hat{N}]\Psi[\phi',t]. \tag{18}$$

Using Eqs. (3) and (5) we have

$$\mathcal{H}-\mu\mathcal{N}=\int(\mathcal{D}\phi')\Psi^*[\phi',t]\left(\phi'(\mathbf{x})-\frac{\delta}{\delta\phi'(\mathbf{x})}\right)h(\mathbf{x},\mathbf{y})\left(\phi'(\mathbf{y})+\frac{\delta}{\delta\phi'(\mathbf{y})}\right)\Psi[\phi']+\int_{\mathbf{x},\mathbf{y}}(\mathcal{D}\phi')\Psi^*[\phi']\left(\phi'(\mathbf{x})-\frac{\delta}{\delta\phi'(\mathbf{x})}\right)$$
$$\times\left(\phi'(\mathbf{y})-\frac{\delta}{\delta\phi'(\mathbf{y})}\right)V(\mathbf{x}-\mathbf{y})\left(\phi'(\mathbf{x})+\frac{\delta}{\delta\phi'(\mathbf{x})}\right)\left(\phi'(\mathbf{y})+\frac{\delta}{\delta\phi'(\mathbf{y})}\right)\Psi[\phi']. \tag{19}$$

All the functional integrals can be easily computed using an additional source term (Appendix A) leading to

$$\mathcal{H}-\mu\mathcal{N}=\int_{\mathbf{x},\mathbf{y}}\left\{[h(\mathbf{x},\mathbf{y})-\mu\delta(\mathbf{x}-\mathbf{y})]\rho(\mathbf{x},\mathbf{y},t)+\frac{1}{2}V(\mathbf{x}-\mathbf{y})|\psi(\mathbf{x},t)|^2|\psi(\mathbf{y},t)|^2\right\}+\frac{1}{2}\int_{\mathbf{x},\mathbf{y}}V(\mathbf{x}-\mathbf{y})[R(\mathbf{y},\mathbf{x},t)R(\mathbf{x},\mathbf{y},t)$$
$$+R(\mathbf{x},\mathbf{x},t)R(\mathbf{y},\mathbf{y},t)+D^*(\mathbf{x},\mathbf{y},t)D(\mathbf{x},\mathbf{y},t)]+\int_{\mathbf{x},\mathbf{y}}V(\mathbf{x}-\mathbf{y})\left[\frac{1}{2}\psi^*(\mathbf{x},t)\psi(\mathbf{y},t)R(\mathbf{x},\mathbf{y},t)+\frac{1}{2}\psi^*(\mathbf{y},t)\psi(\mathbf{x},t)R(\mathbf{y},\mathbf{x},t)\right.$$
$$\left.+|\psi(\mathbf{x},t)|^2R(\mathbf{y},\mathbf{y},t)\right]-\frac{1}{2}\int_{\mathbf{x},\mathbf{y}}V(\mathbf{x}-\mathbf{y})[\psi(\mathbf{x},t)\psi(\mathbf{y},t)D^*(\mathbf{x},\mathbf{y},t)+\psi^*(\mathbf{x},t)\psi^*(\mathbf{y},t)D(\mathbf{x},\mathbf{y},t)] \tag{20}$$

and

$$\rho(\mathbf{x},\mathbf{y},t)=\langle\psi^\dagger(\mathbf{x})\psi(\mathbf{y})\rangle=\psi^*(\mathbf{x},t)\psi(\mathbf{y},t)+R(\mathbf{x},\mathbf{y},t), \tag{21}$$
$$\Delta(\mathbf{x},\mathbf{y},t)=-\langle\psi(\mathbf{x})\psi(\mathbf{y})\rangle=-\psi(\mathbf{x},t)\psi(\mathbf{y},t)+D(\mathbf{x},\mathbf{y},t),$$

with

$$R(\mathbf{x},\mathbf{y},t)=\frac{1}{2}\left[\frac{G^{-1}(\mathbf{x},\mathbf{y},t)}{4}+G(\mathbf{x},\mathbf{y},t)-\delta(\mathbf{x}-\mathbf{y})\right]+2\int_{\mathbf{w},\mathbf{z}}\Sigma(\mathbf{x},\mathbf{w},t)G(\mathbf{w},\mathbf{z},t)\Sigma(\mathbf{z},\mathbf{y},t)$$
$$+i\int_{\mathbf{z}}[G(\mathbf{x},\mathbf{z},t)\Sigma(\mathbf{z},\mathbf{y},t)-\Sigma(\mathbf{x},\mathbf{z},t)G(\mathbf{z},\mathbf{y},t)], \tag{22}$$

$$D(\mathbf{x},\mathbf{y},t)=\frac{1}{2}\left[\frac{G^{-1}(\mathbf{x},\mathbf{y},t)}{4}-G(\mathbf{x},\mathbf{y},t)\right]+2\int_{\mathbf{w},\mathbf{z}}\Sigma(\mathbf{x},\mathbf{w},t)G(\mathbf{w},\mathbf{z},t)\Sigma(\mathbf{z},\mathbf{y},t)-i\int_{\mathbf{z}}[\Sigma(\mathbf{x},\mathbf{z},t)G(\mathbf{z},\mathbf{y},t)+G(\mathbf{x},\mathbf{z},t)\Sigma(\mathbf{z},\mathbf{y},t)],$$

because of Eq. (10). It is easy to check that in terms of R and D the mean value $\mathcal{H}-\mu\mathcal{N}$ corresponds to the standard mean-field factorization.[9,12] We note that the density gets contributions from the condensate field ψ as well as from the fluctuations (G,Σ). The contribution from $\psi^*\psi$ is the condensate density. So that the term with four ψ's can be interpreted as the condensate self-interaction. The interaction of particles not in the condensate with the condensate is taken into account by the terms with two ψ's. Finally the self-interaction of the particles not in the condensate comes from the terms with no ψ (RR and DD).

We introduce the generalized potentials

$$\mathcal{U}_d(\mathbf{x},\mathbf{y},t)=\delta(\mathbf{x}-\mathbf{y})\int_{\mathbf{z}}\rho(\mathbf{z},\mathbf{z},t)V(\mathbf{x}-\mathbf{z}),$$
$$\mathcal{U}_e(\mathbf{x},\mathbf{y},t)=\rho(\mathbf{x},\mathbf{y},t)V(\mathbf{x}-\mathbf{y})\equiv\mathcal{U}_e^r+i\mathcal{U}_e^i, \tag{23}$$
$$\mathcal{U}_p(\mathbf{x},\mathbf{y},t)=\Delta(\mathbf{x},\mathbf{y},t)V(\mathbf{x}-\mathbf{y})\equiv\mathcal{U}_p^r+i\mathcal{U}_p^i,$$

where the notation emphasizes real and imaginary parts of $\mathcal{U}_p$. We also define the matrices

$$A(\mathbf{x},\mathbf{y},t)=h(\mathbf{x},\mathbf{y})-\mu+\mathcal{U}_p^r(\mathbf{x},\mathbf{y},t)+\mathcal{U}_e^r(\mathbf{x},\mathbf{y},t)+\mathcal{U}_d(\mathbf{x},\mathbf{y},t),$$
$$B(\mathbf{x},\mathbf{y},t)=h(\mathbf{x},\mathbf{y})-\mu-\mathcal{U}_p^r(\mathbf{x},\mathbf{y},t)+\mathcal{U}_e^r(\mathbf{x},\mathbf{y},t)+\mathcal{U}_d(\mathbf{x},\mathbf{y},t), \tag{24}$$
$$C(\mathbf{x},\mathbf{y},t)=h(\mathbf{x},\mathbf{y})-\mu+\mathcal{U}_e(\mathbf{x},\mathbf{y},t)+\mathcal{U}_d(\mathbf{x},\mathbf{y},t).$$

From Eqs. (15) and (17) we obtain an abstract matrix form of the equations of motion

$$\dot{\Sigma}=\frac{1}{8}G^{-1}AG^{-1}-2\Sigma A\Sigma-\frac{B}{2}+\{\mathcal{U}_p^i,\Sigma\}-[\mathcal{U}_e,\Sigma],$$
$$\dot{G}=\{A,\{G,\Sigma\}\}-\{\mathcal{U}_p^i,G\}-[\mathcal{U}_e,G], \tag{25}$$
$$\imath\dot{\psi}=C\psi-\mathcal{U}_p\psi^*,$$

where $\Sigma,G,\mathcal{U}_e,\mathcal{U}_p^i,\mathcal{U}_p^i$ are now Hermitian matrices. These equations (25) are the nonlinear field equations for an arbitrary interaction V between the particles and contain any external potential through h. As an example the matrix product $G^{-1}AG^{-1}$ can be written in coordinate representation as

$$\int_{\mathbf{z},\mathbf{w}}G^{-1}(\mathbf{x},\mathbf{z},t)A(\mathbf{z},\mathbf{w})G^{-1}(\mathbf{w},\mathbf{y},t). \tag{26}$$

The static equations can be obtained by setting the canonical momenta to zero, that is, $\Sigma(\mathbf{x},\mathbf{t},t)=\pi(\mathbf{x},t)=0$, $\dot{G}(\mathbf{x},\mathbf{y},t)=\dot{\phi}(\mathbf{x},t)=0$. From Eqs. (16) and (22) we then have

$$R(\mathbf{x},\mathbf{y},0)\equiv R(\mathbf{x},\mathbf{y})=\frac{1}{2}\left[\frac{G^{-1}(\mathbf{x},\mathbf{y})}{4}+G(\mathbf{x},\mathbf{y})-\delta(\mathbf{x}-\mathbf{y})\right],$$

$$D(\mathbf{x},\mathbf{y},0)\equiv D(\mathbf{x},\mathbf{y})=\frac{1}{2}\left[\frac{G^{-1}(\mathbf{x},\mathbf{y})}{4}-G(\mathbf{x},\mathbf{y})\right], \tag{27}$$

$$\psi(\mathbf{x},0)\equiv\psi(\mathbf{x})=\frac{\phi(\mathbf{x})}{\sqrt{2}}.$$

So that for the static case we have to self-consistently solve

$$\frac{1}{4}\int_{\mathbf{z},\mathbf{w}}G^{-1}(\mathbf{x},\mathbf{z})A(\mathbf{z},\mathbf{w})G^{-1}(\mathbf{w},\mathbf{y})-B(\mathbf{x},\mathbf{y})=0,$$

$$\int_{\mathbf{z}}[B(\mathbf{x},\mathbf{z})\psi(\mathbf{z})-2\psi(\mathbf{x})\psi^2(\mathbf{z})V(\mathbf{x}-\mathbf{z})]=0. \tag{28}$$

using Eqs. (21)–(24). We note that if we constrain $G=1/2$ for the static solution this leads to $R=D=0$ and $A=B$ so that Eq. (44) is to the usual nonlinear equation for the single quantity ψ (Ref. 6) obtained from a many-body product wave function (permanent) for bosons. However the time-dependent Eqs. (25) are more general, because our trial Gaussian is actually a coherent state with an indefinite number of particles.

III. CONTACT INTERACTION IN THE ONE-DIMENSIONAL UNIFORM CASE

A. Gaussian approximation

We will specialize the results of the previous section for the one-dimensional case and for a contact interaction so that

$$V(x-y)=\lambda\,\delta(x-y). \tag{29}$$

Because of the existence of exact numerical solutions we will treat the uniform case so that the momentum representation is the natural choice where the quantities A, B, and G can simultaneously be diagonalized and $\phi(k)=\phi\,\delta(k)$. The static equations (28) become [we use the notation : $\int_k=(1/2\pi)\int_{-\infty}^{\infty}dk$],

$$\frac{1}{4}G^{-2}(k)A(k)-B(k)=0, \tag{30}$$

$$\phi[B(0)-\lambda\phi^2]=0. \tag{31}$$

The static version of A and B from Eq. (24) can be written as

$$A(\mathbf{k})=e(\mathbf{k})-\mu+\mathcal{U}_p+2\mathcal{U}+\lambda\frac{\phi^2}{2},$$

$$B(\mathbf{k})=e(\mathbf{k})-\mu-\mathcal{U}_p+2\mathcal{U}+\frac{3}{2}\lambda\phi^2, \tag{32}$$

where $e(k)=\hbar^2k^2/2m$ and the generalized potentials become

$$\mathcal{U}\equiv\mathcal{U}_d=\mathcal{U}_e=\lambda\int_{k'}R(k'),$$

$$\mathcal{U}_p=\lambda\int_{k'}D(k'). \tag{33}$$

So, we can write the solution for Eq. (30) as

$$G(k)=\frac{1}{2}\sqrt{\frac{A(k)}{B(k)}} \tag{34}$$

and for Eq. (31) we have

$$\phi=0, \tag{35}$$

or

$$B(0)=\lambda\phi^2. \tag{36}$$

Using Eq. (34) with Eq. (27) we can express D and R as functions of A,B

$$D(k)=\frac{1}{2}\left[\frac{G^{-1}(k)}{4}-G(k)\right]=\frac{1}{4}\frac{B(k)-A(k)}{\sqrt{A(k)B(k)}}, \tag{37}$$

$$R(k)=\frac{1}{2}\left[\frac{G^{-1}(k)}{4}+G(k)-1\right]=\frac{1}{2}\left\{\frac{B(k)+A(k)}{2\sqrt{A(k)B(k)}}-1\right\}.$$

From Eqs. (32), (33), and (34) we see that $A(0)$ and $B(0)$ must be positive so that if $\lambda<0$, Eq. (36) demands that $B(0)<0$ which is inconsistent with the previous statement. So the only possible solution in this case is $\phi=0$. For $\lambda>0$ the symmetry-breaking solution $\phi\neq0$, using Eq. (36), gives us

$$\mu=\lambda\int_{k'}[2R(k')-D(k')]+\frac{\lambda}{2}\phi^2. \tag{38}$$

Having solved for μ we can rewrite A and B in (32) and (33) as

$$A(k)=e(k)+2\lambda\int_{k'}D_{k'}\equiv e(k)+2\lambda a, \tag{39}$$

$$B(k)=e(k)+\lambda\phi^2\equiv e(k)+2\lambda b.$$

On the other hand, using Eqs. (37) and (39) we can write a pair of nonlinear equations for a and b

$$a=\frac{\lambda}{2}\int_{k'}\frac{[b-a]}{\sqrt{[e(k')+2\lambda a][e(k')+2\lambda b]}},$$

$$b=\rho-\frac{1}{2}\int_{k'}\left\{\frac{e(k)+\lambda[b+a]}{\sqrt{[e(k')+2\lambda a][e(k')+2\lambda b]}}-1\right\}, \tag{40}$$

where we have used the total density constraint

$$\rho=\frac{\phi^2}{2}+\int_{k'}R(k'), \tag{41}$$

which actually becomes our scale. This nonlinear set of equations can be solved for a given ρ, given a and b. Once we have calculated a and b we can compute the chemical potential through

$$\mu=\lambda[2\rho-a-b]. \tag{42}$$

In the same fashion the ground-state energy density $(E/L=(\mathcal{H})/L)$ can be computed obtaining

$$E/L=\frac{\lambda}{2}a^2-\frac{\lambda}{2}b^2-\lambda ab+\lambda\rho^2+K, \tag{43}$$

where K, the contribution from the kinetic energy can also be computed in terms of a and b as

$$K=\frac{1}{2}\int_{k'}e(k')\left\{\frac{e(k')+\lambda[a+b]}{\sqrt{[e(k')+2\lambda a][e(k')+2\lambda b]}}-1\right\}. \tag{44}$$

As an aside we remark that for a dilute system we can approximate the self-consistent equations for a and b by truncating them at a second iteration. A first iteration on Eq. (40) takes $a\approx 0$, $b\approx\rho$ which implies zero depletion and $\mathcal{U}_p=0$. This leads us to a nonpairing theory (Gross-Pitaevskii equation[6]). Then the next iteration leads to

$$\begin{aligned} a&\approx\frac{\lambda\rho}{2}\int_{k'}\frac{1}{\sqrt{e(k')^2+2\lambda\rho e(k')}},\\ b&\approx\rho-\frac{1}{2}\int_{k'}\left\{\frac{e(k')+\lambda\rho}{\sqrt{e(k')^2+2\lambda\rho e(k')}}-1\right\}. \end{aligned} \tag{45}$$

Then we can calculate R and D truncating the self-consistency and giving the same results as the Bogoliubov scheme. Physically this means neglecting the effect of the terms that take into account the self-intercation of the particles not in the condensate (DD and RR). This approximation is usually valid for dilute systems where these terms are not important. With this truncation the ground-state energy can be easily computed giving

$$\frac{E}{N}=\frac{\lambda}{2}\rho\left[1-\frac{4}{3\pi}\sqrt{\gamma}\right], \tag{46}$$

where the dimensionless parameter γ is

$$\gamma=\frac{\lambda m}{\rho\hbar^2}. \tag{47}$$

Returning to our discussion we determine the excitations through the RPA equations which can be found by expanding all quantities around their equilibrium value.[17] Thus we write

$$\begin{aligned} G(k,k',t)&=G(k)\delta(k-k')+\delta G(k,k',t),\\ \Sigma(k,k',t)&\to\delta\Sigma(k,k',t),\\ \phi(k,t)&=\phi\delta(k)+\delta\phi(k,t),\\ \pi(k,t)&\to\delta\pi(k,t). \end{aligned} \tag{48}$$

Thus we have written G and Σ in the basis where the equilibrium G is diagonal and kept terms up to first order in small quantities, of course the diagonal basis is plane waves.

It will be useful to introduce new momentum coordinates so that

$$P=k-k', \tag{49}$$

$$q=\frac{k+k'}{2}, \tag{50}$$

and

$$\delta G(k,k')\to\delta G(P,q). \tag{51}$$

We will see that P and q can be interpreted as total and relative momenta, respectively , of a pair of quasibosons. We can then write the RPA equations in a form where P is diagonal and can be considered as a dummy variable

$$\begin{aligned} \delta\dot{G}(q,P,t)&=s_K(q,P)\delta\Sigma(q,P,t)+c_K(q,P)\delta\pi(P,t)\\ &\quad+\int_{q'}S_K(q,q',P)\delta\Sigma(q',P,t),\\ -\delta\dot{\Sigma}(q,P,t)&=s_M(q,P)\delta G(q,P,t)+c_M(q,P)\delta\phi(P,t)\\ &\quad+\int_{q'}S_M(q,q',P)\delta G(q',P,t),\\ \delta\dot{\phi}(P,t)&=\delta\pi(P,t)A(P)+\int_{q'}c_K(q',P)\delta\Sigma(q',P,t),\\ -\delta\dot{\pi}(P,t)&=\delta\phi(P,t)B(P)+\int_{q'}c_M(q',P)\delta G(q',P,t). \end{aligned} \tag{52}$$

We note that for a given value of P the (π,ϕ) degree of freedom is coupled to the much more numerous degrees of freedom (Σ,G) which are labeled by q. Different q values among (Σ,G) are also coupled. Introducing the notation $f(q'+P/2)=f'_+$ and $f(q-P/2)=f_-$, we find nondiagonal matrices in (q,q')

$$\begin{aligned} S_K(\mathbf{q},\mathbf{q}',\mathbf{P})&=\lambda[G_++G_-][G'_++G'_-]+\lambda[G_+-G_-]\\ &\quad\times[G'_+-G'_-], \end{aligned} \tag{53}$$

$$\begin{aligned} S_M(\mathbf{q},\mathbf{q}',\mathbf{P})&=\frac{\lambda}{2}+\frac{\lambda}{4}\left[1-\frac{G_+^{-1}G_-^{-1}}{4}\right]\left[1-\frac{G_+'^{-1}G_1'^{-1}}{4}\right]\\ &\quad+\left[\frac{G_+^{-1}G_-^{-1}}{4}\right]\left[\frac{G_+'^{-1}G_-'^{-1}}{4}\right], \end{aligned}$$

and diagonal elements

$$s_K(\mathbf{q},\mathbf{P})=2[A_+G_-+A_-G_+], \tag{54}$$

$$s_M(\mathbf{q},\mathbf{P})=\frac{G_+^{-2}G_-^{-1}A_++G_-^{-2}G_+^{-1}A_-}{8}.$$

Finally we see the coupling elements between (π,ϕ) and (Σ,G)

$$c_K(\mathbf{q},\mathbf{P})=\lambda\phi[G_++G_-], \tag{55}$$

$$c_M(\mathbf{q},\mathbf{P})=\frac{\lambda}{2}\phi\left[3-\frac{G_+^{-1}G_-^{-1}}{4}\right],$$

which vanish when the symmetry in ϕ is conserved ($\phi=0$). As pointed out above the equations are diagonal in $\mathbf{P}$ so we can interpret it as the total momentum of a pair of quasibosons. Because δG, $\delta\Sigma$, and $\delta\phi$, $\delta\pi$ are canonical variables we may invert the definitions of momentum and coordinate. For convenience, we define column vectors

$$\Theta(q,P,t)=\begin{pmatrix}\delta\Sigma(q,P,t)\\ \delta\pi(P,t)\end{pmatrix},\quad \Pi(q,P,t)=-\begin{pmatrix}\delta G(q,P,t)\\ \delta\phi(P,t)\end{pmatrix}. \tag{56}$$

Then we can write a coupled oscillator Hamiltonian that corresponds to the RPA equations of motion in a suggestive matrix element form

$$H_{\rm RPA}=\frac{1}{2}\tilde{\Pi}M^{-1}\Pi+\frac{1}{2}\tilde{\Theta}K\Theta, \tag{57}$$

where the matrices M^{-1} and K are the generalizations of oscillator mass and spring constant

$$K=\begin{pmatrix}S_K+s_K & c_K\\ c_K & A\end{pmatrix},\quad M^{-1}=\begin{pmatrix}S_M+s_M & c_M\\ c_M & B\end{pmatrix}. \tag{58}$$

We may separate the diagonal part of $H_{\rm RPA}$ so that

$$H_{\rm RPA}=H_0+H_{\rm int}, \tag{59}$$

where

$$H_0=\frac{1}{2}(\delta\Sigma^* \quad \delta\pi^*)\begin{pmatrix}s_K & 0\\ 0 & A\end{pmatrix}\begin{pmatrix}\delta\Sigma\\ \delta\pi\end{pmatrix}+\frac{1}{2}(\delta G^* \quad \delta\phi^*)\times\begin{pmatrix}s_M & 0\\ 0 & B\end{pmatrix}\begin{pmatrix}\delta G\\ \delta\phi\end{pmatrix}, \tag{60}$$

$$H_{\rm int}=\frac{1}{2}(\delta\Sigma^* \quad \delta\pi^*)\begin{pmatrix}S_K & c_M\\ c_M & 0\end{pmatrix}\begin{pmatrix}\delta\Sigma\\ \delta\pi\end{pmatrix}+\frac{1}{2}(\delta G^* \quad \delta\phi^*)\times\begin{pmatrix}S_M & c_M\\ c_M & 0\end{pmatrix}\begin{pmatrix}\delta G\\ \delta\phi\end{pmatrix}.$$

Introducing the trivial canonical transformation

$$\delta\Sigma\to\sqrt{s_M}\,\delta\Sigma,\quad \delta G\to\frac{\delta G}{\sqrt{s_M}},$$
$$\delta\pi\to\sqrt{B}\,\delta\pi,\quad \delta\phi\to\frac{\delta\phi}{\sqrt{B}}, \tag{61}$$

we obtain a simpler form for the diagonal part

$$H_0=\frac{1}{2}(\delta\Sigma^* \quad \delta\pi^*)\begin{pmatrix}s_Ms_K & 0\\ 0 & AB\end{pmatrix}\begin{pmatrix}\delta\Sigma\\ \delta\pi\end{pmatrix}+\frac{1}{2}(\delta G^* \quad \delta\phi^*)\times\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\delta G\\ \delta\phi\end{pmatrix}. \tag{62}$$

If we define Ω_1 and Ω_2

$$\Omega_1(\mathbf{P})=\sqrt{A(P)B(P)}, \tag{63}$$

$$\Omega_2(q,P)=\sqrt{s_K(q,P)s_M(q,P)}, \tag{64}$$

and use the definitions of s_K and s_M from Eq. (54) we get, after some algebra, the remarkable result

$$\Omega_2(q,P)=\sqrt{A_+B_+}+\sqrt{A_-B_-}=\Omega_1(k)+\Omega_1(k'), \tag{65}$$

so that $\Omega_1(P)$ and $\Omega_2(q,P)$ can be interpreted as the one and two free quasiboson energies. We note that $\Omega_2(0,P)=2\Omega_1(P/2)$, which means that at zero relative momentum $\Omega_2(P,0)$ corresponds to two quasibosons with momentum $P/2$. Thus the oscillations of the $\delta\phi$, $\delta\pi$ pair can be interpreted as a quasiboson mode, while the oscillations of δG, $\delta\Sigma$ can be interpreted as an interacting pair of these same quasibosons. When $\phi=0$, we get $c_K=c_M=0$ and the one and two quasibosons systems are calculated independently. When $\phi\neq 0$ we must rediagonalize so that our final modes will be mixtures of one and two quasibosons. The variable q represents the internal motion of the quasiboson pair with interaction given by the quantities S. In general this is a scattering problem and we must search for the scattering amplitude at a given energy and P, where the asymptotic conditions are determined by Eq. (64). In addition the coupling of one and two quasibosons will always lead to a bound state which is a particular mixture of the one quasiboson mode with a bound component of the two quasibosons.

As we did for the static results it is straightforward to see that the truncation that gives the Bogoliubov results implies neglecting the coupling ($H_{\rm int}=0$) and will lead to the usual result

$$\Omega_1^b(P)=\sqrt{e^2(P)+2\lambda\rho e(P)}. \tag{66}$$

We can see that the Bogoliubov excitations consider no interaction between the quasibosons. Note that because the Bogoliubov does not take into account the self-interaction of the particles not in the condensate, we have $k'=0$ which means $P=k$.

Returning to the dispersion relation for the bound mode one can finally eliminate the two quasiboson components. To see this we try oscillatory solutions for Eq. (52) such as

$$\Theta(t)=\Theta e^{i\Omega t},$$
$$\Pi(t)=\Pi e^{i\Omega t}, \tag{67}$$

and Eqs. (52) can be written in a compact form

$$\mathcal{M}\cdot\mathcal{X}=\mathcal{Y}, \tag{68}$$

that is,

$$\begin{pmatrix}-\Omega & -s_K & 0 & -\lambda x\phi\\ s_M & \Omega & \lambda v\phi & 0\\ 0 & 0 & -\Omega & -A\\ 0 & 0 & B & \Omega\end{pmatrix}\cdot\begin{pmatrix}\delta G\\ \delta\Sigma\\ \delta\phi\\ \delta\pi\end{pmatrix}$$

$$= \begin{pmatrix} \lambda(xX+rR) \\ -\lambda yY - 2\lambda zZ \\ \lambda\phi X \\ -\lambda\phi(Y+2Z) \end{pmatrix}, \tag{69}$$

where for simplicity we have used

$$r(q,P) = G_+ - G_-,$$

$$x(q,P) = G_+ + G_-,$$

$$y(q,P) = \frac{1}{2}\left[1 + \frac{G_+^{-1}G_-^{-1}}{4}\right], \tag{70}$$

$$z(q,P) = \frac{1}{2}\left[1 - \frac{G_+^{-1}G_-^{-1}}{4}\right],$$

$$v(q,P) = y(q,P) + 2z(q,P),$$

and also

$$R(P) = \int_{q'} r(q',P)\,\delta\Sigma(q',P), \tag{71}$$

$$X(P) = \int_{q'} x(q',P)\,\delta\Sigma(q',P),$$

$$Y(P) = \int_{q'} y(q',P)\,\delta G(q',P),$$

$$Z(P) = \int_{q'} z(q',P)\,\delta G(q',P).$$

Note that the condition $\det\mathcal{M}=0$ from the homogeneous equation ($\mathcal{Y}=0$) gives us back Ω_1 and Ω_2 discussed above.

In the discussion which follows we look for the bound state referred to above by holding $\Omega<\Omega_1<\Omega_2$ so that it is not necessary here to include the usual scattering $i\epsilon$ in the denominators. We can invert $\mathcal{M}$ obtaining

$$\delta G = -\frac{\lambda\Omega rR}{(\Omega^2-\Omega_2^2)} - \left[\frac{x}{(\Omega^2-\Omega_2^2)} + \lambda\phi^2\frac{s_K v + Bx}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)}\right]\lambda\Omega X + \lambda^2\phi^2\frac{As_K v + x\Omega^2}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)}(Y+2Z) + \lambda s_K\frac{yY+2zZ}{(\Omega^2-\Omega_2^2)},$$

$$\delta\Sigma = \frac{\lambda s_K rR}{(\Omega^2-\Omega_2^2)} + \left[\frac{s_M x}{\Omega^2-\Omega_2^2} + \lambda\phi^2\frac{Bs_M x + v\Omega^2}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)}\right]\lambda X - \lambda^2\phi^2\Omega\frac{Av + s_M x}{(\Omega^2-\Omega_2^2)(\Omega^2-\Omega_1^2)}(Y+2Z) - \lambda\Omega\frac{yY+2zZ}{\Omega^2-\Omega_2^2},$$

$$\delta\phi = -\lambda\phi\frac{\Omega X - A(Y+2Z)}{(\Omega^2-\Omega_1^2)},$$

$$\delta\pi = -\lambda\phi\frac{\Omega(Y+2Z) - BX}{(\Omega^2-\Omega_1^2)}. \tag{72}$$

Now we substitute Eq. (72) in the definitions of the quantities R, X, Y, and Z, Eq. (71). Because $r(q,P)$ is an odd function, i.e., $r(-q,P)=-r(q,P)$ it is easy to check and we end up with a linear and homogeneous system for X, Y, and Z, that looks like

$$W(P,\Omega)\cdot F = 0, \tag{73}$$

where, omitting the P dependence we have

$$W = \begin{pmatrix} W_{1,1} & W_{1,2} & W_{1,3} \\ W_{2,1} & W_{2,2} & W_{2,3} \\ W_{3,1} & W_{3,2} & W_{3,3} \end{pmatrix}, \quad F = \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}. \tag{74}$$

The elements of W are given in Appendix B. The system (73) will have a nontrivial solution if

$$\det W(P,\Omega(P)) = 0, \tag{75}$$

so that we have for each P the corresponding energy $\Omega(P)$. Numerically the problem reduces to calculating determinants of a 3×3 matrix.

A very general property[18] of the dispersion relation $\Omega(P)$ can be proven for the particular case where $P=0$. In this case the first line of the matrix (74) using Eqs. (40) and (64) is

$$W_{1,1} = 1 - \lambda\frac{A(0)-B(0)}{A(0)}\int_q \frac{x^2(q,0)}{s_K(q,0)}, \quad W_{1,2}=0, \quad W_{1,3}=0 \tag{76}$$

and now using Eqs. (39)–(40) we have that

$$\lambda\int_{\mathbf{q}}\frac{x^2(q,0)}{s_K(q,0)} = \frac{\lambda}{2}\int_q\frac{1}{\sqrt{A(q)B(q)}} = \frac{A(0)}{A(0)-B(0)}. \tag{77}$$

So that the first line of the matrix is zero, making the determinant vanish, showing that we will always have a gapless dispersion relation independently of the value of λ,

$$\Omega(0) = 0. \tag{78}$$

This zero mode of the RPA equations is the standard Goldstone mode as its structure is associated with the symmetry breaking (indefinite particle number) by the trial wave functional.[18]

We note that the dispersion relation that comes from the RPA depends on the total momentum defined in Eq. (49) which means that Ω is a function of $(k-k')$, so that it takes into account that to obtain an excitation we remove a particle with momentum k' and create a particle with momentum k. This result is very different from the Bogoliubov excitation where k' is taken to be zero. In other words the Gaussian approximation takes into account the effect of the depletion on the excitations.

B. The exact solution

All the results summarized in this section were obtained by Lieb and Lininger[19,20] who calculated the exact ground-state energy and also the excitations in terms of independent particle and hole excitations. Our purpose is to make a connection with this work which showed that interacting bosons in one dimension can be analogous to a Fermi gas. We will show how our modes correspond to Lieb's particle-hole excitations.

First of all when $\lambda\to\infty$ it is possible to recover the well-known result[21] that for an infinite coupling constant interacting bosons behave like a system of free fermions, so that the ground-state energy can be easily computed by

$$\frac{E}{N}=\frac{1}{\rho}\frac{1}{2\pi}\int_{-K_f}^{K_f}e(k)dk, \tag{79}$$

where K_f is the Fermi momentum. In this case it is trivial to calculate

$$\rho=\frac{1}{2\pi}\int_{-K_f}^{K_f}dk, \tag{80}$$

which gives $K_f=\pi\rho$. So, in this particular limit

$$\frac{E}{N}=\frac{\hbar^2}{2m}\frac{\pi^2\rho^2}{3}. \tag{81}$$

We can divide the particle-hole excitations of the free Fermi gas into two parts. The particular hole excitations that correspond to removing a particle from an occupied state to just above the Fermi level (K_f)

$$\epsilon_{\rm h}(k')=\frac{\hbar^2\pi^2\rho^2}{2m}-\frac{\hbar^2k'^2}{2m}, \tag{82}$$

where $K_f<k'<K_f$, and the particle excitations where we remove a particle from the Fermi level to an unoccupied state

$$\epsilon_p(k)=\frac{\hbar^2k^2}{2m}-\frac{\hbar^2\pi^2\rho^2}{2m}, \tag{83}$$

where $k>K_f$ or $k<-K_f$. To produce a particle-hole excitation we must add these excitations giving us

$$\epsilon_p(k,k')=\frac{\hbar^2k^2}{2m}-\frac{\hbar^2k'^2}{2m}. \tag{84}$$

Using ϵ_h and ϵ_p one can look at $E(k',k)$ as a function of the total and relative momentum $P=k-k'$ and $q=(k+k')/2$. Because the hole excitations are limited to $(-K<k'<K)$ we need to separate two cases, for $P>0$ we have

$$\text{if}\quad P<2K_f\rightarrow\begin{cases}k=K_f\\ k'=K_f-P,\end{cases} \tag{85}$$

$$\text{if}\quad P>2K_f\rightarrow\begin{cases}k=P-K_f\\ k'=-K_f.\end{cases}$$

The first case means fixing the momentum of the particle and moving the momentum of the hole, while in the second one we fix the momentum of the hole at it lowest possible value and move the momentum of the particle. So that once we know ϵ_h and ϵ_p the threshold curve defined by the lowest value of $E(k',k)$ for a given P will be given by

$$E(P)=\begin{cases}\epsilon_h(K_f-P)+\epsilon_p(K_f) & \text{for}\quad P<2K_f\\ \epsilon_h(-K_f)+\epsilon_p(P-K_f) & \text{for}\quad P>2K_f,\end{cases} \tag{86}$$

which gives us

$$E(P)=\begin{cases}2\pi\rho P-P^2 & \text{for}\quad P<2K_f\\ P^2+2\pi\rho P & \text{for}\quad P>2K_f.\end{cases} \tag{87}$$

Note that the $E(P)$ curve contain two parts. Finite range part $P<2K_f$ where the contribution comes basically from the hole excitations. Infinite range part $P>2K_f$ from the particle excitations. The more dilute the system the less the finite range part in $E(P)$.

The generalization for bosons interacting with a finite λ was carried out by Lieb and Lininger.[19,20] They showed the ground state can be calculated as

$$\frac{E}{N}=\frac{1}{\rho}\int_{-K}^{K}f(k)e(k)dk, \tag{88}$$

where $f(k)$ is the solution of

$$2\gamma\rho\int_{-K}^{K}\frac{f(p)}{\rho^2\gamma^2+(p-k)^2}dp=2\pi f(k)-1 \tag{89}$$

with γ given in Eq. (47). The condition

$$\int_{-K}^{K}f(k)dk=\rho \tag{90}$$

determines K. For the excitations Lieb defined two different basic interactions which he called ''particle'' and ''hole'' excitations. To determine these excitations

Lieb showed that it was sufficient to solve new integral equations. For the particle energy

$$\epsilon_p(k)=\frac{\hbar^2k^2}{2m}-\mu+\frac{\hbar^2}{m}\int_{-K}^{K}pJ_p(p)dp, \tag{91}$$

where $J_p(p)$ could be obtained by solving

$$2\pi J_p(p)=2\gamma\rho\int_{-K}^{K}\frac{J_p(r)}{\rho^2\gamma^2+(p-r)^2}dr-\pi+2\tan^{-1}\left[\frac{k-p}{\gamma\rho}\right], \tag{92}$$

and for the hole energy $\epsilon_h(P,\lambda)$ he had

$$\epsilon_h(k')=\mu-\frac{\hbar^2k'^2}{2m}+\frac{\hbar^2}{m}\int_{-K}^{K}pJ_h(p)dp, \tag{93}$$

where $J_h(p)$ was obtained from

$$2\pi J_h(p)=2\gamma\rho\int_{-K}^{K}\frac{J_h(r)}{\rho^2\gamma^2+(p-r)^2}dr+\pi -2\tan^{-1}\left[\frac{k'-p}{\gamma\rho}\right]. \tag{94}$$

In the limit $\lambda\rightarrow\infty$ we can see that $J(p)\rightarrow 0$ and $\mu\rightarrow(\hbar^2K^2)/(2m)=(\hbar^2\pi^2\rho)/(2m)$ recovering the free fermion results. Looking at the expressions for the ground-state energy and the excitations for a given λ, Lieb interpreted them as those of a quasi-Fermi gas where K is an interaction-dependent Fermi momentum and the distributions factors $f(k)$ and $J(k)$ give a special weight for each k. Using this analogy is very reasonable, since it is correct in both the $\lambda=0$ and $\lambda=\infty$. To obtain the threshold curve $E(P)$ we can use Eq. (86). The difference is that now ϵ_p and ϵ_h will have different curvatures depending on the interaction. Note that in his original work Lieb compared the Bogoliubov scheme with particle and holes excitations separately and got very good agreement with the particle excitations. This is interesting, as we pointed out earlier, and just tells us that the Bogoliubov scheme does not contain hole excitations. In general as γ increases the contribution of the holes for the particle-hole excitation energy becomes more and more important and this effect is in part described by the Gaussian theory.

IV. NUMERICAL RESULTS AND CONCLUSIONS

For the numerical computations we follow Lieb and use the dimensionless coupling constant γ and scale all lengths by ρ and all energies by $(\hbar^2\rho^2)/(2m)$. In these units we can write the ground-state energy per particle as

$$\frac{E}{N}=g(\gamma). \tag{95}$$

For the Gaussian static results we solve the nonlinear system (40)–(44) and determine a and b for $0<\gamma<10$. After computing K defined in (44) one can get $g(\gamma)$ using (43). In the Bogoliubov scheme, Eq. (46) leads to

$$g_B(\gamma)=\gamma\left[1-\frac{4}{3\pi}\sqrt{\gamma}\right]. \tag{96}$$

Finally the exact result for $g(\gamma)$ was obtained by Lieb solving Eqs. (88)–(90). The results as a function of γ can be seen in Fig. 1, where one can basically see the very good agreement of both Gaussian and Bogoliubov for low γ ($\gamma\leqslant 1$) with the difference that by construction the Gaussian result is always an upper bound and the Bogoliubov energy is below the exact result. For higher values of γ the Bogoliubov result, as expected, collapses ($\gamma\sim 5$) while the Gaussian theory still gives a result. In the hard-core limit ($\gamma\rightarrow\infty$) the Gaussian approximation fails to go to the finite free Fermi energy of the exact solution.

To obtain the ''exact'' excitation energies we used Lieb's results for ϵ_h and ϵ_p obtained by solving Eqs. (91)–(94). Using Eq. (86) we obtain the excitation curves $E(P)$ as a function of P as shown in Fig. 2 for $\gamma=0$, 0.787, 4.527, and ∞. Note that for $P<2$ K the contribution from the hole excitations produce quite interesting dispersion curves.

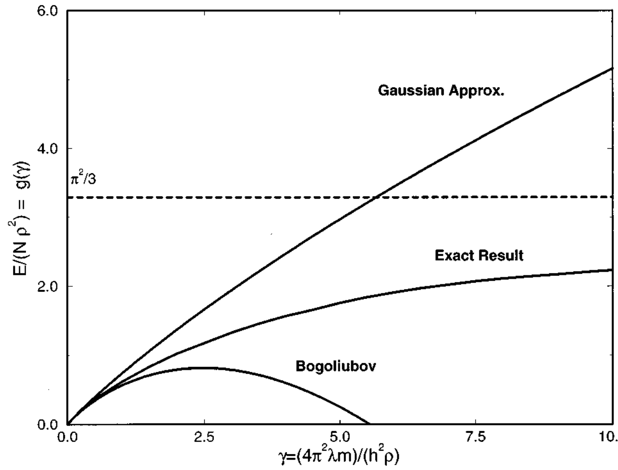

FIG. 1. The ground-state energy per particle can be written as $E/N=\rho^2 g(\gamma)$. The curves give $g(\gamma)$ as a function of γ for the Gaussian, the Bogoliubov, and the exact result.

To illustrate the RPA results we plot in Fig. 3, Ω_1, Ω_2, and Ω as a function of P for $\gamma=7.551$. The relative momentum variable q will gives us a continuum that corresponds to a scattering region and one can see clearly how Ω_1 gets pushed down by the interaction producing the gapless Ω. We compare the bound-state dispersion relation Ω with the Bogoliubov one and with the exact results for $\gamma=0.787$ (Fig. 4) and $\gamma=4.527$ (Fig. 5). We note that the improvement of the RPA compared to the Bogoliubov result increases with γ. When γ goes to infinity both the RPA and the Bogoliubov schemes fail.

The results of this paper can be summarized in three points:

(1) We have seen that the Gaussian variational method takes into account the self-interactions of the particles out of the condensate. This fact starts improving the ground-state energy results when compared with Bogoliubov theory once γ increases ($\gamma>2$). It is very difficult however for the Gaussian variational results to get close to exact for high γ

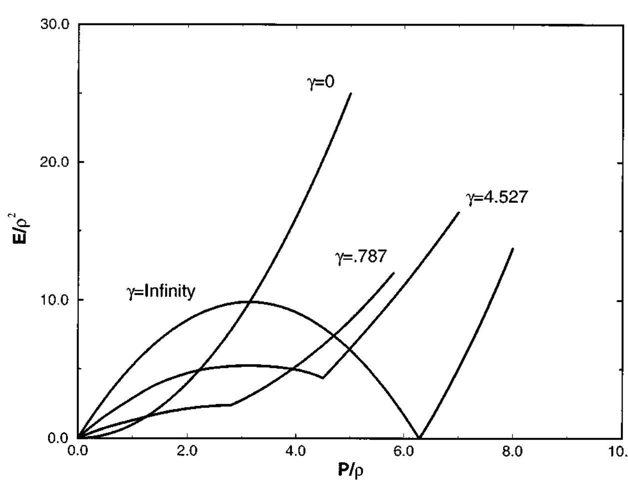

FIG. 2. The exact threshold curves for the particle-hole excitation as a function of the total particle-hole momentum $P=k-k'$ as obtained using Eq. (86).

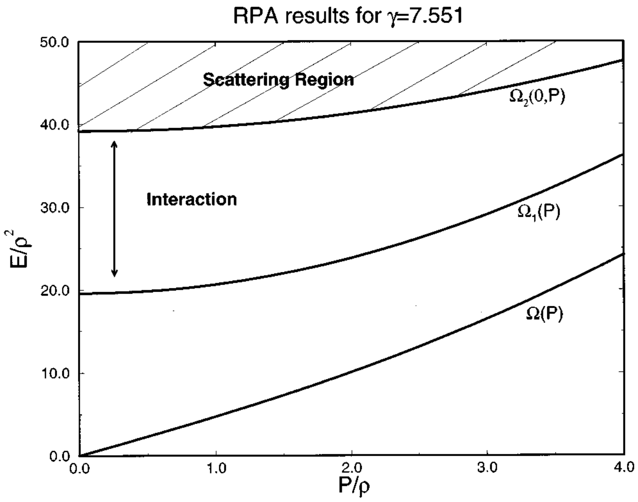

FIG. 3. The free quasiboson energy $\Omega_1(P)$ given by Eq. (63). The two free quasiboson energies $\Omega_2(P,q)$ given by Eq. (64) and the new gapless $\Omega(P)$ mode energy obtained with the RPA calculation by solving Eq. (75). Note that, as expected, the gapless property of $\Omega(P)$ comes from the Goldstone mode associated with the symmetry breaking.

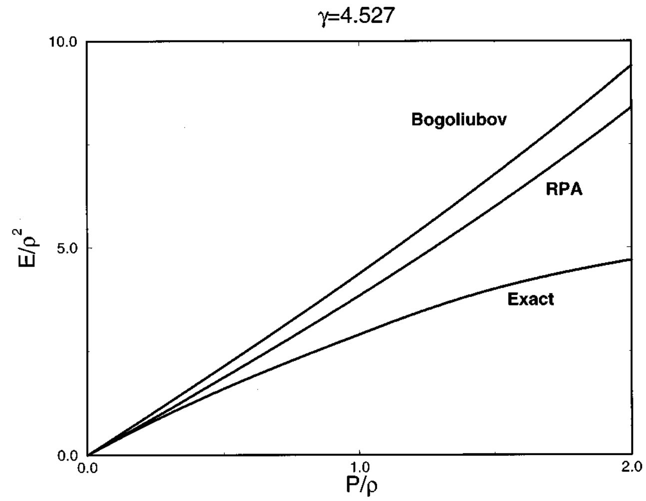

FIG. 5. Comparison between the three particle-hole excitations curves: $\Omega_1^b(P)$ given by Eq. (66), $\Omega(P)$ by solving Eq. (75) and the exact using Eq. (86) as a function of the total particle-hole momentum P for $\gamma=5.527$.

values. In the one-dimensional case when $\gamma\to\infty$ the Gaussian ground-state energy diverges while the exact goes to the finite Fermi energy.

(2) For the particle-hole excitations the Gaussian results take into account that when we remove a particle from an occupied state in order to make an excitation, this particle can be out of the condensate which does not happen in the Bogoliubov scheme. Again this seems an improved description for intermediate values of γ. As γ increases the depletion starts to grow and in this particular case goes to a Fermi sea when $\lambda\to\infty$, which cannot be described by our methods since they do not deal with very short-range correlations.

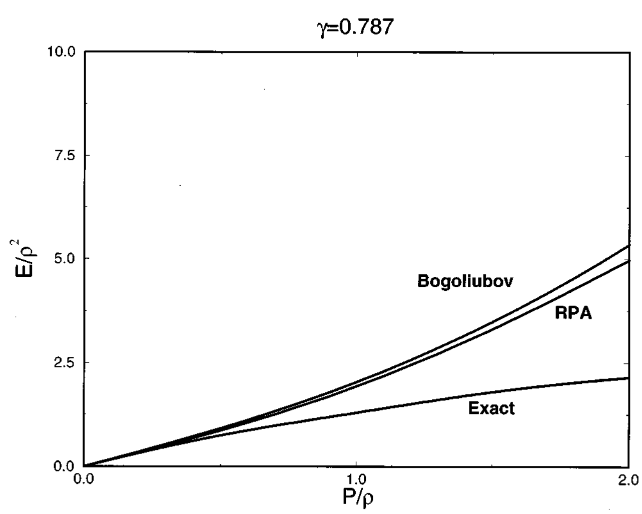

FIG. 4. Comparison between the three different particle-hole excitations curves: Bogoliubov $\Omega_1^b(P)$ given by Eq. (66), the RPA $\Omega(P)$ by solving Eq. (75) and the exact using Eq. (86). These are given as a function of the total particle-hole momentum P for $\gamma=0.787$.

(3) Another important point that is somehow related to item 2 is that to solve the RPA equation we had decoupled harmonic oscillators which, in the quasiboson picture means that the RPA takes into account the interaction between the quasibosons generating modes that are mixtures of one $(\delta\phi,\delta\pi)$ and two quasibosons $(\delta G,\delta\Sigma)$. In the Bogoliubov scheme we always have free quasibosons when their interaction starts to be relevant as γ increases.

We can conclude that the Gaussian variational method can describe systems where the depletions cannot be neglected (when dilute theories break down) but because of the absence of short-range correlation will require corrections for highly depleted systems (like helium 4).

ACKNOWLEDGMENTS

P.T. thanks Eddy Timmermans for useful discussions. This work was supported in part by funds provided by the U.S. Department of Energy under cooperative agreement No. DE-FC-94ER 40818. P.T. was supported by Conselho Nacional de Desenvolvimento Cientifico e Tecnologico (CNPq), Brazil.

APPENDIX A

If we carefully examine expression (19) we see that the functional integral that must be computed involves moments of a Gaussian. Namely,

$$\int (\mathcal{D}\phi')\Psi^*[\phi',t]\phi'(\mathbf{x}_1)\cdots\phi'(\mathbf{x}_4)\Psi[\phi',t], \quad \text{(A1)}$$

where $\Psi[\phi']$ is our normalized trial wave functional given by Eq. (7). This functional integral can be computed easily if we include a source term[22] in the normalization integral, i.e.,

$$\int (\mathcal{D}\phi')\Psi^*[\phi',t]e^{\int_{\mathbf{x}}J(\mathbf{x})\delta\phi'(\mathbf{x})}\Psi[\phi',t]. \tag{A2}$$

Using the expression for $\Psi[\phi',t]$ we complete the squares in the exponential getting

$$\int (\mathcal{D}\phi')\Psi^*[\phi',t]e^{\int_{\mathbf{x}}J(\mathbf{x})\delta\phi'(\mathbf{x},t)}\Psi[\phi',t] = e^{(1/2)\int_{\mathbf{x}}J(\mathbf{x})G(\mathbf{x},\mathbf{y},t)J(\mathbf{y})}. \tag{A3}$$

The source term allows us to compute the functional integral of any moment of the Gaussian

$$\int (\mathcal{D}\phi')\delta\phi'(\mathbf{x}_1)\cdots\delta\phi'(\mathbf{x}_n)e^{-\int_{\mathbf{x},\mathbf{y}}\delta\phi'(\mathbf{x},t)[G^{-1}(\mathbf{x},\mathbf{y},t)/2]\delta\phi'(\mathbf{y},t)} = \frac{\delta}{\delta J(\mathbf{x}_1)}\cdots\frac{\delta}{\delta J(\mathbf{x}_n)}e^{(1/2)\int_{\mathbf{x}}J(\mathbf{x})G(\mathbf{x},\mathbf{y},t)J(\mathbf{y})}\Big|_{J=0}. \tag{A4}$$

For instance, we can calculate

$$\int (\mathcal{D}\phi')\Psi^*[\phi',t]\phi'(\mathbf{x})\phi'(\mathbf{y})V(\mathbf{x}-\mathbf{y})\phi'(\mathbf{x})\phi'(\mathbf{y})\Psi[\phi',t] = 4\phi(\mathbf{x},t)\phi(\mathbf{y},t)V(\mathbf{x}-\mathbf{y})G(\mathbf{x},\mathbf{y},t) + \phi^2(\mathbf{x},t)V(\mathbf{x}-\mathbf{y})G(\mathbf{y},\mathbf{y},t) + \phi^2(\mathbf{y},t)V(\mathbf{x}-\mathbf{y})G(\mathbf{x},\mathbf{x},t)2G(\mathbf{x},\mathbf{y},t)V(\mathbf{x}-\mathbf{y})G(\mathbf{x},\mathbf{y},t) + G(\mathbf{x},\mathbf{x},t)V(\mathbf{x}-\mathbf{y})G(\mathbf{y},\mathbf{y},t). \tag{A5}$$

Note that the last two terms of Eq. (A5) show, as expected, the mean-field factorization.

APPENDIX B

After some algebra one gets the elements of the matrix W which appears in Eq. (75). For calculating the dispersion relation, Ω will be below the lowest pole appearing in Eqs. (B1)–(B9).

$$W_{1,1} = 1-\lambda\int_q\frac{s_M x^2}{(\Omega^2-\Omega_2^2)} - \lambda^2\phi^2\int_q\frac{Bs_M x^2+vx\Omega^2}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)}, \tag{B1}$$

$$W_{1,2} = \lambda^2\Omega\phi^2\int_q\frac{Avx+s_M x^2}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)} + \lambda\Omega\int_q\frac{xy}{(\Omega^2-\Omega_1^2)}, \tag{B2}$$

$$W_{1,3} = 2\lambda^2\phi^2\Omega\int_q\frac{Avx+s_M x^2}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)} + 2\lambda\Omega\int_q\frac{xz}{(\Omega^2-\Omega_2^2)}, \tag{B3}$$

$$W_{2,1} = \lambda\Omega\int_q\frac{xy}{(\Omega^2-\Omega_2^2)} + \lambda^2\phi^2\Omega\int_q\frac{s_K vy+Bxy}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)}, \tag{B4}$$

$$W_{2,2} = 1-\lambda^2\phi^2\int_q\frac{As_K vy+xy\Omega^2}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)} - \lambda\int_q\frac{s_K y^2}{(\Omega^2-\Omega_1^2)}, \tag{B5}$$

$$W_{2,3} = -2\lambda^2\phi^2\int_q\frac{As_K vy+xy\Omega^2}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)} - 2\lambda\int_q\frac{s_K yz}{(\Omega^2-\Omega_2^2)}, \tag{B6}$$

$$W_{3,1} = \lambda\Omega\int_q\frac{xz}{(\Omega^2-\Omega_2^2)} + \lambda^2\phi^2\Omega\int_q\frac{s_K vz+Bxz}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)}, \tag{B7}$$

$$W_{3,2} = -\lambda^2\phi^2\int_q\frac{As_K vz+xz\Omega^2}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)} - \lambda\int_q\frac{s_K yz}{(\Omega^2-\Omega_2^2)}, \tag{B8}$$

$$W_{3,3} = 1-2\lambda^2\phi^2\int_q\frac{As_K vz+xz\Omega^2}{(\Omega^2-\Omega_1^2)(\Omega^2-\Omega_2^2)} - 2\lambda\int_q\frac{s_K z^2}{(\Omega^2-\Omega_2^2)}. \tag{B9}$$

[1] M.H. Anderson, J.R. Ensher, M.R. Mathews, C.E. Wieman, and E.A. Cornell, Science **269**, 198 (1995).
[2] K.B. Davis, M.O. Mewes, M.R. Andrews, N.J. van Druten, D.D. Durfee, D.M. Kum, and W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995).
[3] M.R. Andrews, C.G. Townsend, H.-J. Miesner, D.S. Durfee, D.M. Kurn, and W. Ketterle, Science **275**, 637 (1996).
[4] O. Penrose and L. Osnager, Phys. Rev. **104**, 576 (1956); W.L. McMillan, *ibid.* **138**, 442 (1965).
[5] E. Timmermans, P. Tommasini, and K. Huang, Phys. Rev. A **55**, 3645 (1997).
[6] L.P. Pitaevskii, Zh. Éksp. Teor. Fiz. **40**, 646 (1961) [Sov. Phys.

JETP **13**, 451 (1961)]; E.P. Goss, Nuovo Cimento **20**, 454 (1961); E.P. Gross, J. Math. Phys. **4**, 195 (1963).
[7] A.J. Moerdijk, H.M.J.M. Boesten, and B.J. Verhaar, Phys. Rev. A **53**, 916 (1996).
[8] E. Tiesinga, B.J. Verhaar, and H.T.C. Stoof, Phys. Rev. A **47**, 4114 (1993).
[9] Kerson Huang and Paolo Tommasini, J. Res. Natl. Inst. Stand. Technol. **101**, 435 (1996).
[10] Paolo Tommasini and A.F.R. de Toledo Piza, Ann. Phys. (N.Y.) **253**, 198 (1997).
[11] A.K. Kerman and S.E. Koonin, Ann. Phys. (N.Y.) **100**, 742 (1976).
[12] A. Griffin, Phys. Rev. B **53**, 9341 (1996).
[13] P.C. Hohenberg and P.C. Martin, Ann. Phys. (N.Y.) **34**, 291 (1965).
[14] Stig Stenholm, Ann. Phys. (N.Y.) **254**, 41 (1997).
[15] M. Girardeau and R. Arnowitt, Phys. Rev. **113**, 755 (1959).
[16] A.K. Kerman and Chi-Young Lin, Ann. Phys. (N.Y.) **241**, 185 (1995), and part II for the repulsive ϕ^4 case in preparation.
[17] In Eqs. (48) for the G equation, the first δ is a Dirac delta and the second means an infinitesimal change.
[18] A.K. Kerman and Paolo Tommasini, Ann. Phys. (N.Y.) (to be published).
[19] Elliott H. Lieb and W. Lininger, Phys. Rev. **130**, 1605 (1963).
[20] Elliott H. Lieb, Phys. Rev. **130**, 1616 (1963).
[21] M. Girardeau, J. Math. Phys. **1**, 516 (1960).
[22] Brian Hatfield, *Quantum Field Theory of Point Particles and Strings* (Addison-Wesley, Reading, MA, 1992).