Comparison between the correlated-basis-functions method and the density-functional theory for inhomogeneous systems

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As a hypothetical inhomogeneous quantum many-body model, we take a weakly interacting Bose gas made inhomogeneous by the presence of a weak external field. The interaction is assumed to be Fourier transformable and characterized by a strength parameter λ; this is also true for the external field, characterized by a strength parameter ε. The ground-state energy is calculated to order $\varepsilon^2\lambda^2$ using three methods: diagrammatic perturbation theory, correlated basis functions (CBF), and density-functional theory (DFT). The diagrammatic perturbation theoretical calculation is new. It differs from our earlier approach for homogeneous Bose systems which evolved from the Hugenholtz-Pines theory. We are able to reproduce the same results in an efficient manner. For the inhomogeneous system, the results are used to measure CBF against DFT. It is found that in their simplest forms CBF yields results which are better than the renormalized DFT by Ebner and Saam. In particular, CBF is superior to DFT in the local-density approximation, even though the latter was designed to take care of systems with slow and small density variations such as the model considered here.

I. INTRODUCTION

The method of correlated basis functions (CBF) has been applied to treating a wide variety of homogeneous many-body systems,[1–4] including liquid and solid helium, nuclear matter, and Coulomb systems. That the method could be successful for Bose and Fermi systems alike has to do with its apparent ability to sum both ring and ladder diagrams, as demonstrated in an analysis by one of the authors and his collaborators in 1970.[5] In that work, the pair correlation function and ground-state energy for a weakly interacting Bose gas were first calculated exactly in the perturbation theory using the formalism of Hugenholtz and Pines. The same quantities were then obtained using the CBF approach. Results from the two methods were compared order by order in powers of the density and the interaction strength. This helped determine what perturbative diagrams were summed by the CBF. Indeed, from this analysis a systematic scheme was identified that enabled the authors to use the Hugenholtz-Pines theory to suggest optimum three-particle and higher-order factors for correlated wave functions.[6,7] Thus, diagrammatic perturbation theory and CBF became intermingled.

We now have another opportunity to bring together two distinct many-body formalisms—this time for inhomogeneous systems. On the one hand, we have the conventional density-functional theory (DFT), invented and popularized by Kohn and co-workers. On the other, we have again the CBF–a late contender in the field of metal surfaces,[8] but an early leader for inhomogeneous helium systems.[9] An interesting development is that density-functional practitioners are now turning toward employing the CBF for treating metal surfaces.[10]

Once again we return to a weakly interacting Bose gas. The reason is that it is one of the few systems which offer us exact solutions in the perturbation theory against which approximate theories can be compared. We recognize that the conclusions drawn from considering the weakly interacting Bose gas cannot be generalized to liquid-helium or metal surfaces. However, it constitutes a first step and provides us with useful indications and directions for future analyses.

The system under consideration, being weakly interacting, cannot be inhomogeneous in the ground state. The inhomogeneity must be generated and maintained by an external field. We introduce such a weak external field, with a strength parameter ε, to cause a weak inhomogeneity in the system of bosons whose interactions are characterized by a Fourier-transformable potential with a strength λ. As in Ref. 5, we now carry out calculations in powers of ε and λ. The external field is, of course, an added complication. The density is now a function and can no longer serve as an expansion parameter.

The calculation is carried out with three methods, perturbation, CBF, and DFT, rather than two. In the perturbation theory, we use a method somewhat different from that used in Ref. 5. In the CBF, we followed essentially the patterns of Refs. 8 and 9. In the DFT, we use first the local-density function (LDF), which is supposed to work well in the region of mild inhomogeneities; we then take into account the second-order nonlocal density correction using the renormalized DFT by Ebner and Saam.

The results of the three calculations are finally compared.

II. PERTURBATION THEORY

Our system consists of N bosons interacting via a pairwise potential $\lambda v(|\mathbf{r}_i-\mathbf{r}_j|)$, and placed under an external field $\varepsilon U_{\rm ext}(\mathbf{r}_i)$ which has no effect on the normalizing volume Ω. The Hamiltonian of the system is given by

$$H=\sum_{i=1}^{N}-\tfrac{1}{2}\nabla_i^2+\tfrac{1}{2}\sum_{\substack{i=1\\(i\neq j)}}^{N}\lambda v(|\mathbf{r}_i-\mathbf{r}_j|)+\sum_{i=1}^{N}\varepsilon U_{\rm ext}(\mathbf{r}_i)\ , \tag{1}$$

where $\hbar^2/m$ has been set to unity. In the second quantized form, Eq. (1) becomes

$$\hat{H}=-\tfrac{1}{2}\int\Psi^\dagger(\mathbf{r})\nabla^2\Psi(\mathbf{r})d\mathbf{r}+\frac{\lambda}{2}\int\int\Psi^\dagger(\mathbf{r}')\Psi^\dagger(\mathbf{r})v(|\mathbf{r}-\mathbf{r}'|)\Psi(\mathbf{r})\Psi(\mathbf{r}')d\mathbf{r}\,d\mathbf{r}'+\varepsilon\int\Psi^\dagger(\mathbf{r})U_{\rm ext}(\mathbf{r})\Psi(\mathbf{r})d\mathbf{r}\ , \tag{2}$$

where $\Psi^\dagger(\mathbf{r})$ and $\Psi(\mathbf{r})$ are, respectively, the creation and annihilation operators of a boson at point $\mathbf{r}$. Equation (2) can be expressed in the momentum space representation by using the relation

$$\Psi(\mathbf{r})=a_0+\sum_{\mathbf{k}}{}'\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(\Omega)^{1/2}}a_{\mathbf{k}}\ . \tag{3}$$

The prime on the summation indicates that $\mathbf{k}=0$ is excluded.

Since the noninteracting ground state of N bosons is a state of total condensation, i.e., a state in which all N particles are at zero momentum, Wick's theorem, usually used to find the ground state or Green's functions via the perturbation method, does not apply.[11] One way to overcome this difficulty is to replace the zero-momentum operators a_0 and $a_0^\dagger$ by a c-number $(n_0)^{1/2}$, where $n_0=N_0/\Omega$, and N_0 is the true ground-state zero-momentum condensate.[11] The replacement of a_0 and $a_0^\dagger$ by $(n_0)^{1/2}$ in Eq. (3) gives a particle number nonconserving Hamiltonian in Eq. (2). Using the Legendre transformation, the system can be described by the Hermitian operator[12]

$$\hat{K}=\hat{H}-\mu\hat{N}\ , \tag{4}$$

where μ, the Lagrange multiplier, is the chemical potential and $\hat{N}$ the particle number operator

$$\hat{N}=N_0+\sum_{\mathbf{k}}{}'a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\ . \tag{5}$$

Explicitly, Eq. (4) has the form

$$\hat{K}=-\mu N_0+\tfrac{1}{2}\Omega n_0^2\lambda\hat{v}(0)+\sum_{\mathbf{k}}{}'(\tfrac{1}{2}k^2-\mu)a_{\mathbf{k}}^\dagger a_{\mathbf{k}}+\lambda V+\varepsilon U\ , \tag{6}$$

with

$$V=V_1+V_2+V_3+V_4+V_5+V_6\ ,$$

$$U=U_1+U_2+U_3\ ,$$

and

$$V_1=\frac{1}{4\Omega}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}{}'[\hat{v}(\mathbf{k}_1-\mathbf{k}_3)+\hat{v}(\mathbf{k}_1-\mathbf{k}_4)]a_{\mathbf{k}_1}^\dagger a_{\mathbf{k}_2}^\dagger a_{\mathbf{k}_3}a_{\mathbf{k}_4}\times\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\ ,$$

$$V_2=\frac{(N_0)^{1/2}}{2\Omega}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}{}'[\hat{v}(\mathbf{k}_1)+\hat{v}(\mathbf{k}_2)]\times a_{\mathbf{k}_1}^\dagger a_{\mathbf{k}_2}^\dagger a_{\mathbf{k}_3}\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3)\ ,$$

$$V_3=\frac{(N_0)^{1/2}}{2\Omega}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}{}'[\hat{v}(\mathbf{k}_2)+\hat{v}(\mathbf{k}_3)]\times a_{\mathbf{k}_1}^\dagger a_{\mathbf{k}_2}a_{\mathbf{k}_3}\delta(\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3)\ ,$$

$$V_4=\frac{N_0}{2\Omega}\sum_{\mathbf{k}}{}'\hat{v}(\mathbf{k})a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger\ ,$$

$$V_5=\frac{N_0}{2\Omega}\sum_{\mathbf{k}}{}'\hat{v}(\mathbf{k})a_{\mathbf{k}}a_{-\mathbf{k}}\ ,$$

$$V_6=\frac{N_0}{\Omega}\sum_{\mathbf{k}}{}'[\hat{v}(\mathbf{k})+\hat{v}(0)]a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\ ;$$

$$U_1=\frac{(N_0)^{1/2}}{\Omega}\sum_{\mathbf{k}}{}'\hat{U}_{\rm ext}(-\mathbf{k})a_{\mathbf{k}}\ ,$$

$$U_2=\frac{(N_0)^{1/2}}{\Omega}\sum_{\mathbf{k}}{}'\hat{U}_{\rm ext}(\mathbf{k})a_{\mathbf{k}}^\dagger\ ,$$

$$U_3=\frac{1}{\Omega}\sum_{\mathbf{k}\mathbf{q}}{}'\hat{U}_{\rm ext}(\mathbf{q})a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}}\ ;$$

where

$$\hat{v}(\mathbf{k})=\int e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}v(|\mathbf{r}-\mathbf{r}'|)d(\mathbf{r}-\mathbf{r}')$$

and

$$\hat{U}_{\rm ext}(\mathbf{k})=\int e^{-i\mathbf{k}\cdot\mathbf{r}}U_{\rm ext}(\mathbf{r})d\mathbf{r}\ .$$

We have assumed $\hat{U}_{\rm ext}(0)=0$ without losing generality.

Since $U_{\rm ext}(\mathbf{r})$ is real, we have

$$\hat{U}_{\rm ext}(\mathbf{k})=\hat{U}^*_{\rm ext}(-\mathbf{k})\ .$$

The quantities $\{V_i\}$ and $\{U_i\}$ can be represented by diagrams as shown in Fig. 1.

The normalized ground state of $\hat{K}$ in Eq. (6), $|\psi_0(\mu,N_0)\rangle$, can be obtained by using the Gell-Mann and Low theorem. The condensate N_0 is determined at the value which minimizes the thermodynamic potential at zero temperature,

$$K_0=\langle\psi_0(\mu,N_0)|\hat{K}|\psi_0(\mu,N_0)\rangle\ .$$

This condition gives

$$\left.\frac{\partial K_0(T=0,\,\Omega,\,\mu,\,N_0)}{\partial N_0}\right|_{\Omega,\mu}=0\ . \tag{7}$$

For any given mean particle density $\bar{n}=N/\Omega$, the ground state of the original system, Eq. (2), can be obtained by the following procedure.

(i) K_0 is obtained, using Goldstone's theorem, from

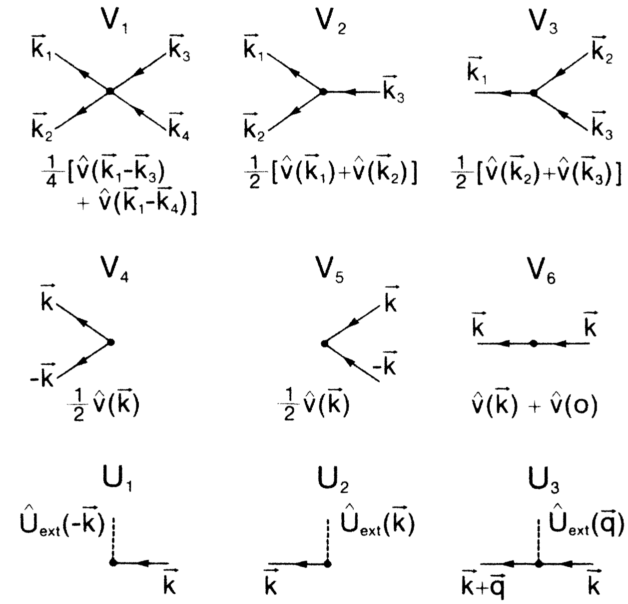

FIG. 1. Diagrams for vertices V and U.

Eq. (6):

$$K_0=-\mu N_0+\frac{\Omega}{2}n_0^2\lambda\hat{v}(0)+\Delta K_0(\mu,N_0)\ , \tag{8}$$

with

$$\Delta K_0=\left\langle 0\left|(\lambda V+\varepsilon U)\sum_{m=0}^{\infty}\left[\frac{-1}{\sum_{\mathbf{k}}'\left[\frac{k^2}{2}-\mu\right]a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}}\times(\lambda V+\varepsilon U)\right]^m\right|0\right\rangle_c$$

$$\equiv\sum_{m=0}^{\infty}I_m\varepsilon^m\ , \tag{9}$$

where $|0\rangle$ denotes the noninteracting ground state ($\lambda=0,\varepsilon=0$). Only connected diagrams are taken on the right-hand side of Eq. (9). We expand ΔK_0 in order of the external-field strength ε.

(ii) Equations (7) and (8) give

$$\mu=n_0\lambda\hat{v}(0)+\left.\frac{\partial\Delta K_0(\mu,N_0)}{\partial N_0}\right|_{\mu}\ . \tag{10}$$

(iii) From Eq. (5) we have

$$N\equiv\langle\psi_0(\mu,N_0)\,|\,\hat{N}\,|\,\psi_0(\mu,N_0)\rangle$$
$$=N_0+\sum_{\mathbf{k}}'\langle\psi_0(\mu,N_0)\,|\,a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\,|\,\psi_0(\mu,N_0)\rangle\ . \tag{11}$$

(iv) Using Eqs. (4) and (8) the ground-state energy E is obtained:

$$E=K_0+\mu N=\mu(N-N_0)+\frac{\Omega}{2}n_0^2\lambda\hat{v}(0)+\Delta K_0(\mu,N_0)\ . \tag{12}$$

From Eqs. (10) and (11), we are able to express μ and N_0 functions only of N, i.e., $\mu(\bar{n})$, $n_0(\bar{n})$. Substituting these functions into Eq. (12) we finally obtain the energy density E/Ω as a function only of the mean density $\bar{n}$.

The method used here to calculate E/Ω and μ differs from the method used by Sim *et al.*[5] The latter called upon the following relations for E/Ω and μ in the homogeneous interacting case ($\varepsilon=0$),

$$\frac{E_0}{\Omega}=\tfrac{1}{2}\bar{n}\mu_0+\frac{i}{(2\pi)^4}\int d\mathbf{k}\int_C d\epsilon_0\,\tfrac{1}{2}(\epsilon_0+\tfrac{1}{2}k^2)G(\mathbf{k},\epsilon_0)\ , \tag{13}$$

and

$$\mu_0=\Sigma_{11}(0,0)-\Sigma_{02}(0,0)\ , \tag{14}$$

where $G(\mathbf{k},\epsilon_0)$ is the time Fourier transform of the time-ordered Green's function

$$G(\mathbf{k};t,t')$$
$$=-i\langle\psi_0(\mu,N_0)\,|\,T[a_{\mathbf{k}}(t)a_{\mathbf{k}}^{\dagger}(t')]\,|\,\psi_0(\mu,N_0)\rangle\ , \tag{15}$$

and the operator $a_{\mathbf{k}}(t)$ is shown in the Heisenberg representation. The contour C in Eq. (13) closes in the upper half-plane. $\Sigma_{11}(0,0)$ and $\Sigma_{02}(0,0)$ are the self-energies at zero energy and momentum arguments.[5,11,12]

In the presence of an external field ($\varepsilon\neq0$), it can be shown that an additional term

$$(\varepsilon/2)\langle\psi_0(\mu,N_0)\,|\,U\,|\,\psi_0(\mu,N_0)\rangle$$

has to appear on the right-hand side of Eq. (13). Equation (14) remains valid, except that Σ_{11} and Σ_{02} now include additional diagrams which contain U vertices. The method used here, Eqs. (8)–(12), is much simpler. It recovers the results of Sim *et al.*[5] to $O(\lambda^4)$ when applied to the homogeneous case, as will be seen below.

A. Homogeneous case

Consider $\varepsilon=0$. The nonvanishing connected diagrams which contribute to I_0 in Eq. (9) are given in Fig. 2 for $m=0$, 1, 2, and 3. These diagrams are evaluated using the $\{V,U\}$ defined in Eq. (6) and Fig. 1. The following results are obtained:

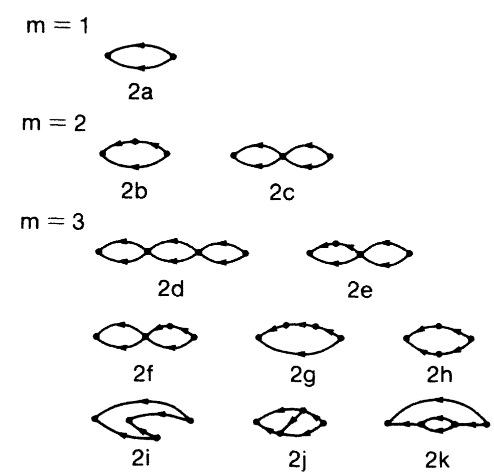

FIG. 2. Nonvanishing connected diagrams for the homogeneous system.

$$\frac{I_0}{\Omega}=\frac{-\lambda^2 n_0^2}{2(2\pi)^3}\int d\mathbf{k}\frac{\hat{v}^2(\mathbf{k})}{k^2-2\mu}+\frac{\lambda^3 n_0^3}{(2\pi)^3}\int d\mathbf{k}\frac{[\hat{v}(\mathbf{k})+\hat{v}(0)]v^2(\mathbf{k})}{(k^2-2\mu)^2}$$

(2a) (2b)

$$+\frac{\lambda^3 n_0^2}{2(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}(\mathbf{k})\hat{v}(\mathbf{p})\hat{v}(\mathbf{k}+\mathbf{p})}{(k^2-2\mu)(p^2-2\mu)}-\frac{\lambda^4 n_0^2}{2(2\pi)^9}\int d\mathbf{k}\int d\mathbf{p}\int d\mathbf{q}\frac{\hat{v}(\mathbf{k})\hat{v}(\mathbf{q})\hat{v}(\mathbf{k}+\mathbf{p})\hat{v}(\mathbf{q}+\mathbf{p})}{(k^2-2\mu)(p^2-2\mu)(q^2-2\mu)}$$

(2c) (2d)

$$-\frac{2\lambda^4 n_0^3}{(2\pi)^6}\int d\mathbf{p}\int d\mathbf{k}\frac{\hat{v}(\mathbf{p})[\hat{v}(\mathbf{p})+\hat{v}(0)]\hat{v}(\mathbf{p}+\mathbf{k})\hat{v}(\mathbf{k})}{(k^2-2\mu)(p^2-2\mu)^2}$$

(2e),(2f)

$$-\frac{2\lambda^4 n_0^4}{(2\pi)^3}\int d\mathbf{k}\frac{[\hat{v}(\mathbf{k})+\hat{v}(0)]^2 v^2(\mathbf{k})}{(k^2-2\mu)^3}-\frac{\lambda^4 n_0^4}{2(2\pi)^3}\int d\mathbf{k}\frac{\hat{v}^4(\mathbf{k})}{(k^2-2\mu)^3}$$

(2g),(2h) (2i)

$$-\frac{2\lambda^4 n_0^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}(\mathbf{k}+\mathbf{p})\hat{v}(\mathbf{k})[\hat{v}(\mathbf{p})+\hat{v}(\mathbf{k})][\hat{v}(\mathbf{p})+\hat{v}(\mathbf{p}+\mathbf{k})]}{(k^2-2\mu)(|\mathbf{p}+\mathbf{k}|^2-2\mu)[k^2+p^2+|\mathbf{k}+\mathbf{p}|^2-6\mu]}$$

(2j)

$$-\frac{\lambda^4 n_0^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}^2(\mathbf{k})[\hat{v}(\mathbf{p})+\hat{v}(\mathbf{k}+\mathbf{p})]^2}{(k^2-2\mu)^2[k^2+p^2+|\mathbf{k}+\mathbf{p}|^2-6\mu]}$$

(2k)

$$+O(\lambda^5)\ . \tag{16}$$

Using Eqs. (10) and (16), we have

$$\mu_0=n_0\lambda\hat{v}(0)-\frac{\lambda^2 n_0}{(2\pi)^3}\int d\mathbf{k}\frac{\hat{v}^2(\mathbf{k})}{k^2-2\mu}+\frac{3\lambda^3 n_0^3}{(2\pi)^3}\int d\mathbf{k}\frac{[\hat{v}(\mathbf{k})+\hat{v}(0)]\hat{v}^2(\mathbf{k})}{(k^2-2\mu)^2}+\frac{\lambda^3 n_0}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}(\mathbf{k})\hat{v}(\mathbf{p})\hat{v}(\mathbf{k}+\mathbf{p})}{(k^2-2\mu)(p^2-2\mu)}$$
$$-\frac{\lambda^4 n_0}{(2\pi)^9}\int d\mathbf{k}\int d\mathbf{p}\int d\mathbf{q}\frac{\hat{v}(\mathbf{k})\hat{v}(\mathbf{q})\hat{v}(\mathbf{k}+\mathbf{p})\hat{v}(\mathbf{q}+\mathbf{p})}{(k^2-2\mu)(p^2-2\mu)(q^2-2\mu)}-\frac{6\lambda^4 n_0^2}{(2\pi)^6}\int d\mathbf{p}\int d\mathbf{k}\frac{\hat{v}(\mathbf{p})[\hat{v}(\mathbf{p})+\hat{v}(0)]\hat{v}(\mathbf{p}+\mathbf{k})\hat{v}(\mathbf{k})}{(k^2-2\mu)(p^2-2\mu)^2}$$
$$-\frac{8\lambda^4 n_0^3}{(2\pi)^3}\int d\mathbf{k}\frac{[\hat{v}(\mathbf{k})+\hat{v}(0)]^2\hat{v}^2(\mathbf{k})}{(k^2-2\mu)^3}-\frac{2\lambda^4 n_0^3}{(2\pi)^3}\int d\mathbf{k}\frac{\hat{v}^4(\mathbf{k})}{(k^2-2\mu)^3}$$
$$-\frac{6\lambda^4 n_0^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}(\mathbf{k}+\mathbf{p})\hat{v}(\mathbf{k})[\hat{v}(\mathbf{p})+\hat{v}(\mathbf{k})][\hat{v}(\mathbf{p})+\hat{v}(\mathbf{p}+\mathbf{k})]}{(k^2-2\mu)(|\mathbf{p}+\mathbf{k}|^2-2\mu)[k^2+p^2+|\mathbf{k}+\mathbf{p}|^2-6\mu]}$$
$$+\frac{3\lambda^4 n_0^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}^2(\mathbf{k})[\hat{v}(\mathbf{p})+\hat{v}(\mathbf{k}+\mathbf{p})]^2}{(k^2-2\mu)^2[k^2+p^2+|\mathbf{k}+\mathbf{p}|^2-6\mu]}+O(\lambda^5)\ . \tag{17}$$

Now, using the Green's function expression Eq. (15), Eq. (11) can be written as

$$\bar{n}=n_0+\frac{i}{(2\pi)^4}\int d\mathbf{k}\int_C d\epsilon_0\, G(\mathbf{k},\epsilon_0)\ . \tag{18}$$

To third order in λ, from Ref. 5 for $\varepsilon=0$ we find

$$\Delta n_0\equiv\bar{n}-n_0=\frac{\lambda^2 n_0^2}{(2\pi)^3}\int d\mathbf{k}\frac{\hat{v}^2(\mathbf{k})}{(k^2-2\mu)^2}-\frac{4\lambda^3 n_0^3}{(2\pi)^3}\int d\mathbf{k}\frac{\hat{v}^2(\mathbf{k})[\hat{v}(\mathbf{k})+\hat{v}(0)]}{(k^2-2\mu)^3}-\frac{2\lambda^3 n_0^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}(\mathbf{p})\hat{v}(\mathbf{k})\hat{v}(\mathbf{k}+\mathbf{p})}{(k^2-2\mu)(p^2-2\mu)^2}\ . \tag{19}$$

Now we expand $\mu_0\equiv\mu(\varepsilon=0)$,

$$\mu_0 = \sum_{m=0}^{\infty} \mu_0^{(m)} \lambda^m \,, \tag{20}$$

and write

$$n_0 = \bar{n} f_0 \equiv \bar{n} \sum_{m=0}^{\infty} f_0^{(m)} \lambda^m \,. \tag{21}$$

Substituting Eqs. (20) and (21) into Eqs. (17) and (18), comparing order by order, we find

$$\begin{aligned}
&f_0^{(0)} = 1 \,, \\
&f_0^{(1)} = 0 \,, \\
&f_0^{(2)} = \frac{-\bar{n}}{(2\pi)^3} \int d\mathbf{k} \frac{\hat{v}^2(\mathbf{k})}{k^4} \,, \\
&f_0^{(3)} = \frac{4\bar{n}^2}{(2\pi)^3} \int d\mathbf{k} \frac{\hat{v}^3(\mathbf{k})}{k^6} + \frac{2\bar{n}}{(2\pi)^6} \int d\mathbf{k} \int d\mathbf{p} \frac{\hat{v}(\mathbf{k})\hat{v}(\mathbf{p})\hat{v}(\mathbf{k}+\mathbf{p})}{k^2 p^4} \,, \\
&\vdots
\end{aligned} \tag{22}$$

$$\begin{aligned}
&\mu_0^{(0)} = 0 \,, \\
&\mu_0^{(1)} = \bar{n}\,\hat{v}(0) \,, \\
&\mu_0^{(2)} = \frac{-\bar{n}}{(2\pi)^3} \int d\mathbf{k} \frac{\hat{v}^2(\mathbf{k})}{k^2} \,, \\
&\mu_0^{(3)} = \frac{3\bar{n}^2}{(2\pi)^3} \int d\mathbf{k} \frac{\hat{v}^3(\mathbf{k})}{k^4} + \frac{\bar{n}}{(2\pi)^6} \int d\mathbf{k} \int d\mathbf{p} \frac{\hat{v}(\mathbf{k})\hat{v}(\mathbf{p})\hat{v}(\mathbf{k}+\mathbf{p})}{k^2 p^2} \,, \\
&\mu_0^{(4)} = \frac{3\bar{n}^2}{(2\pi)^6} \int d\mathbf{k} \int d\mathbf{p} \frac{\hat{v}^2(\mathbf{k})\hat{v}^2(\mathbf{p})}{k^2 p^4} - \frac{\bar{n}}{(2\pi)^9} \int d\mathbf{k} \int d\mathbf{p} \int d\mathbf{q} \frac{\hat{v}(\mathbf{k})\hat{v}(\mathbf{q})\hat{v}(\mathbf{k}+\mathbf{p})\hat{v}(\mathbf{q}+\mathbf{p})}{k^2 p^2 q^2} \\
&\qquad - \frac{6\bar{n}^2}{(2\pi)^6} \int d\mathbf{p} \int d\mathbf{k} \frac{\hat{v}^2(\mathbf{p})\hat{v}(\mathbf{k})\hat{v}(\mathbf{p}+\mathbf{k})}{k^2 p^4} - \frac{10\bar{n}^3}{(2\pi)^3} \int d\mathbf{k} \frac{\hat{v}^4(\mathbf{k})}{k^6} \\
&\qquad - \frac{6\bar{n}^2}{(2\pi)^6} \int d\mathbf{k} \int d\mathbf{p} \frac{\hat{v}(\mathbf{k}+\mathbf{p})\hat{v}(\mathbf{k})[\hat{v}(\mathbf{p})+\hat{v}(\mathbf{k})][\hat{v}(\mathbf{p})+\hat{v}(\mathbf{p}+\mathbf{k})]}{k^2 |\mathbf{p}+\mathbf{k}|^2 (k^2+p^2+|\mathbf{k}+\mathbf{p}|^2)} \\
&\qquad - \frac{3\bar{n}^2}{(2\pi)^6} \int d\mathbf{k} \int d\mathbf{p} \frac{\hat{v}^2(\mathbf{k})[\hat{v}(\mathbf{p})+\hat{v}(\mathbf{k}+\mathbf{p})]^2}{k^4 (k^2+p^2+|\mathbf{k}+\mathbf{p}|^2)} \\
&\vdots
\end{aligned} \tag{23}$$

Equations (22) and (23) are identical to Eqs. (16) and (17) of Ref. 5. Substituting Eqs. (21), (22), and (23) into Eq. (12), using Eq. (16), we find for

$$\begin{aligned}
&\frac{E_0}{\Omega} = \sum_{m=0}^{\infty} \frac{E_0^{(m)}}{\Omega} \lambda^m \,, \\
&\frac{E_0^{(0)}}{\Omega} = 0 \,, \\
&\frac{E_0^{(1)}}{\Omega} = \tfrac{1}{2} \bar{n}^2 \hat{v}(0) \,, \\
&\frac{E_0^{(2)}}{\Omega} = \frac{-\bar{n}^2}{2(2\pi)^3} \int d\mathbf{k} \frac{\hat{v}^2(\mathbf{k})}{k^2} \,, \\
&\frac{E_0^{(3)}}{\Omega} = \frac{\bar{n}^3}{(2\pi)^3} \int d\mathbf{k} \frac{\hat{v}^3(\mathbf{k})}{k^4} + \frac{\bar{n}^2}{2(2\pi)^6} \int d\mathbf{k} \int d\mathbf{p} \frac{\hat{v}(\mathbf{k})\hat{v}(\mathbf{p})\hat{v}(\mathbf{k}+\mathbf{p})}{k^2 p^2} \,,
\end{aligned}$$

and

$$\frac{E_0^{(4)}}{\Omega}=\frac{\bar{n}^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}^2(\mathbf{k})\hat{v}^2(\mathbf{p})}{k^2p^4}-\frac{\bar{n}^2}{2(2\pi)^9}\int d\mathbf{k}\int d\mathbf{p}\int d\mathbf{q}\frac{\hat{v}(\mathbf{k})\hat{v}(\mathbf{q})\hat{v}(\mathbf{k}+\mathbf{p})\hat{v}(\mathbf{q}+\mathbf{p})}{k^2p^2q^2}$$
$$-\frac{2\bar{n}^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}^2(\mathbf{p})\hat{v}(\mathbf{k})\hat{v}(\mathbf{p}+\mathbf{k})}{k^2p^4}-\frac{5\bar{n}^4}{2(2\pi)^3}\int d\mathbf{k}\frac{\hat{v}^4(\mathbf{k})}{k^6}$$
$$-\frac{2\bar{n}^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}(\mathbf{k}+\mathbf{p})\hat{v}(\mathbf{k})[\hat{v}(\mathbf{p})+\hat{v}(\mathbf{k})][\hat{v}(\mathbf{p})+\hat{v}(\mathbf{p}+\mathbf{k})]}{k^2|\mathbf{p}+\mathbf{k}|^2(k^2+p^2+|\mathbf{k}+\mathbf{p}|^2)}$$
$$-\frac{\bar{n}^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}^2(\mathbf{k})[\hat{v}(\mathbf{p})+\hat{v}(\mathbf{k}+\mathbf{p})]^2}{k^4(k^2+p^2+|\mathbf{k}+\mathbf{p}|^2)}\ . \qquad (24)$$

By using the identities

$$-\frac{2\bar{n}^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}(\mathbf{k}+\mathbf{p})\hat{v}(\mathbf{k})[\hat{v}(\mathbf{p})+\hat{v}(\mathbf{k})][\hat{v}(\mathbf{p})+\hat{v}(\mathbf{p}+\mathbf{k})]}{k^2|\mathbf{p}+\mathbf{k}|^2(k^2+p^2+|\mathbf{k}+\mathbf{p}|^2)}$$
$$=\frac{-2\bar{n}^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}(\mathbf{p})\hat{v}(\mathbf{p}+\mathbf{k})\hat{v}^2(\mathbf{k})}{k^2p^2|\mathbf{k}+\mathbf{p}|^2}-\frac{2\bar{n}^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}^2(\mathbf{k})\hat{v}^2(\mathbf{p}+\mathbf{k})}{k^2|\mathbf{p}+\mathbf{k}|^2(k^2+p^2+|\mathbf{k}+\mathbf{p}|^2)}$$

and

$$-\frac{\bar{n}^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}^2(\mathbf{k})[\hat{v}(\mathbf{p})+\hat{v}(\mathbf{k}+\mathbf{p})]^2}{k^4(k^2+p^2+|\mathbf{k}+\mathbf{p}|^2)}$$
$$=\frac{-2\bar{n}^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}^2(\mathbf{k})v^2(\mathbf{p}+\mathbf{k})}{k^4(k^2+p^2+|\mathbf{k}+\mathbf{p}|^2)}-\frac{2\bar{n}^3}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{p}\frac{\hat{v}^2(\mathbf{k})\hat{v}(\mathbf{p})\hat{v}(\mathbf{p}+\mathbf{k})}{k^4(k^2+p^2+|\mathbf{k}+\mathbf{p}|^2)}\ ,$$

we find Eq. (24) identical to Eq. (19) of Ref. 5.

B. Inhomogeneous case

Now we are ready to consider the inhomogeneous case—$\varepsilon\neq 0$. We will consider only the diagrams in Eq. (9) with interactions up to order $\varepsilon^2\lambda^2$. Using conservation of momentum, it is easy to see that $I_1=0$ to all orders of λ. The nonvanishing diagrams which contribute to I_2 are shown in Fig. 3 to order λ^2.

These diagrams are now evaluated using V and U as defined in Eq. (6). We find the following results:

$$I_2=\underbrace{\frac{-2n_0}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2}{k^2-2\mu}}_{(3a)}+\underbrace{\frac{4n_0^2\lambda}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2[\hat{v}(\mathbf{k})+\hat{v}(0)]}{(k^2-2\mu)^2}}_{(3b)}$$
$$+\underbrace{\frac{4n_0^2\lambda}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(\mathbf{k})}{(k^2-2\mu)^2}}_{(3c),(3d)}-\underbrace{\frac{8n_0^3\lambda^2}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|\hat{v}^2(\mathbf{k})}{(k^2-2\mu)^3}}_{(3e),(3f),(3q),(3r),(3t)}$$
$$-\underbrace{\frac{2n_0^2\lambda^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{q})|^2\hat{v}^2(\mathbf{k})}{(k^2-2\mu)^2(k^2+|\mathbf{k}+\mathbf{q}|^2-4\mu)}}_{(3g)}$$
$$-\underbrace{\frac{2n_0^2\lambda^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{q})|^2\hat{v}(\mathbf{k})\hat{v}(\mathbf{k}+\mathbf{q})}{(k^2-2\mu)(|\mathbf{k}+\mathbf{q}|^2-2\mu)(k^2+|\mathbf{k}+\mathbf{q}|^2-4\mu)}}_{(3h)}$$
$$-\underbrace{\frac{16n_0^3\lambda^2}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(\mathbf{k})[\hat{v}(\mathbf{k})+\hat{v}(0)]}{(k^2-2\mu)^3}}_{(3i),(3j),(3m),(3n)}-\underbrace{\frac{4n_0^2\lambda^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(\mathbf{k}+\mathbf{q})\hat{v}(\mathbf{q})}{(k^2-2\mu)^2(|\mathbf{k}+\mathbf{q}|^2-2\mu)}}_{(3k),(3l)}$$
$$-\underbrace{\frac{8n_0^2\lambda^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(\mathbf{q})[\hat{v}(\mathbf{q})+\hat{v}(\mathbf{k}+\mathbf{q})]}{(k^2-2\mu)(q^2-2\mu)(q^2+|\mathbf{k}+\mathbf{q}|^2-4\mu)}}_{(3o),(3p)}$$
$$-\underbrace{\frac{8n_0^3\lambda^2}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2[\hat{v}(\mathbf{k})+\hat{v}(0)]^2}{(k^2-2\mu)^3}}_{(3s)}$$
$$-\underbrace{\frac{4n_0^2\lambda^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2[\hat{v}(\mathbf{q})+\hat{v}(\mathbf{k}+\mathbf{q})]^2}{(k^2-2\mu)^2(q^2+|\mathbf{q}+\mathbf{k}|^2-4\mu)}}_{(3u)}+O(\lambda^3)\ . \qquad (25)$$

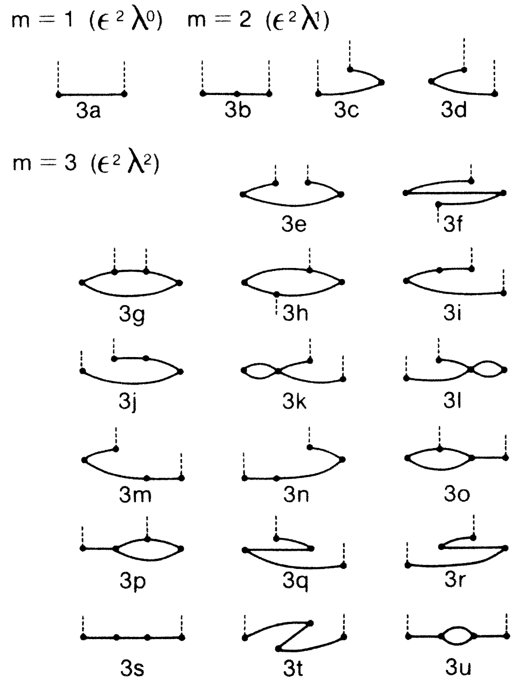

FIG. 3. Nonvanishing connected diagrams for the inhomogeneous system.

From Eq. (10), up to the second order in ε, we have

$$\mu = n_0\lambda\hat{v}(0) + \frac{\partial}{\partial n_0}\left[\frac{1}{\Omega}I_0(\mu,n_0)+\frac{\varepsilon^2}{\Omega}I_2(\mu,n_0)\right]\bigg|_{\mu} + O(\varepsilon^3) , \tag{26}$$

where I_0 and I_2 are given by Eqs. (16) and (25). We can also write μ as

$$\mu = \mu_0+\mu_1\varepsilon+\mu_2\varepsilon^2+\cdots ,$$

with (27)

$$\mu_i = \sum_{m=0}^{\infty} \mu_i^{(m)}\lambda^m .$$

μ_0 has already been obtained for the homogeneous case in Eq. (23) to $O(\lambda^4)$. Here we proceed to determine μ_1 and μ_2 to $O(\varepsilon^2\lambda^2)$.

To find the relation between n_0 and n, we again use Eq. (18). Expanding Δn in orders of the number of external-field vertices in $G(\mathbf{k},\epsilon_0)$, we write

$$\Delta n = \bar{n} - n_0 = \Delta n_0 + \Delta n_1\varepsilon + \Delta n_2\varepsilon^2 + \cdots . \tag{28}$$

Δn_0 has already been given by Eq. (19). From the conservation of momentum it is easily see that $\Delta n_1 \equiv 0$ to all orders in λ. The lowest-order diagrams in λ which have nonvanishing contributions to Δn_2 are of order λ^2.

We now write n_0 in the "true" expansions of ε and λ,

$$n_0 = \bar{n}f = \bar{n}(f_0+f_1\varepsilon+f_2\varepsilon^2+\cdots) ,$$
$$f_i = \sum_{m=0}^{\infty} f_i^{(m)}\lambda^m . \tag{29}$$

The expression for f_0 has been given in Eq. (22). We will next determine f_1 and f_2 up to $O(\varepsilon^2\lambda)$.

To find the first-order terms μ_1 and f_1, we substitute Eqs. (27) and (29) into Eq. (26). To first order in ε we have

$$\mu_1 = \bar{n}\lambda\hat{v}(0)f_1 + \frac{\partial A(\mu,n_0)}{\partial n_0}\bigg|_{\substack{n_0=\bar{n}f_0,\\ \mu=\mu_0}} \bar{n}f_1 + \frac{\partial A(\mu,n_0)}{\partial \mu}\bigg|_{\substack{\mu=\mu_0,\\ n_0=\bar{n}f_0}} \mu_1 , \tag{30}$$

where

$$A \equiv \frac{\partial}{\partial n_0}\left[\frac{I_0}{\Omega}\right] .$$

Similarly, substituting Eqs. (27) and (29) into Eq. (28) using the fact that $\Delta n_1 \equiv 0$, we find to first order in ε,

$$\bar{n}f_1 = \frac{\partial \Delta n_0(\mu,n_0)}{\partial n_0}\bigg|_{\substack{n_0=\bar{n}f_0,\\ \mu=\mu_0}} \bar{n}f_1 + \frac{\partial \Delta n_0(\mu,n_0)}{\partial \mu}\bigg|_{\substack{\mu=\mu_0,\\ n_0=\bar{n}f_0}} \mu_1 . \tag{31}$$

From Eqs. (30) and (31), expanding in λ order by order, one can prove that the only solution is the trivial solution $f_1^{(m)} \equiv 0$ and $\mu_1^{(m)} \equiv 0$ for all m. This is because Δn_0 and A have different structures in the integrand to all orders of λ.

In order to find E/Ω up to $O(\varepsilon^2\lambda^2)$, we still need to know $\mu_2^{(0)}$, $\mu_2^{(1)}$, $f_2^{(0)}$, and $f_2^{(1)}$. Since the lowest-order terms in λ for both Δn_0 and Δn_2 are of $O(\lambda^2)$, we find from Eqs. (28) and (29) $f_2^{(0)} = f_2^{(1)} = 0$.

To find $\mu_2^{(0)}$, $\mu_2^{(1)}$, and $\mu_2^{(2)}$, we substitute Eqs. (27) and (29) into both sides of Eq. (26) and make order-by-order comparisons. In the limit $\Omega \rightarrow \infty$,

$$\Omega\mu_2^{(0)} = \frac{-2}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2}{k^2} ,$$

$$\Omega\mu_2^{(1)} = \frac{16\bar{n}}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2 v(\mathbf{k})}{k^4} + \frac{4\bar{n}\,\hat{v}(0)}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2}{k^4} ,$$

and

$$\Omega\mu_2^{(2)}=\frac{-32\bar{n}^{\,2}\hat{v}(0)}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(\mathbf{k})}{k^6}+\frac{4\bar{n}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}^{\,2}(\mathbf{q})}{k^2q^4}$$
$$+\frac{4\bar{n}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}^{\,2}(\mathbf{q})}{k^4q^2}-\frac{96\bar{n}^{\,2}}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}^{\,2}(\mathbf{k})}{k^6}$$
$$-\frac{4\bar{n}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{q})|^2\hat{v}^{\,2}(\mathbf{k})}{k^4(k^2+|\mathbf{k}+\mathbf{q}|^2)}-\frac{4\bar{n}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{q})|^2\hat{v}(\mathbf{k})\hat{v}(\mathbf{k}+\mathbf{q})}{k^2|\mathbf{k}+\mathbf{q}|^2(k^2+|\mathbf{k}+\mathbf{q}|^2)}$$
$$-\frac{8\bar{n}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(\mathbf{k}+\mathbf{q})\hat{v}(\mathbf{q})}{k^4|\mathbf{k}+\mathbf{q}|^2}-\frac{16\bar{n}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(\mathbf{q})[\hat{v}(\mathbf{q})+\hat{v}(\mathbf{k}+\mathbf{q})]}{k^2q^2(q^2+|\mathbf{k}+\mathbf{q}|^2)}$$
$$-\frac{8\bar{n}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2[\hat{v}(\mathbf{q})+\hat{v}(\mathbf{k}+\mathbf{q})]}{k^4(q^2+|\mathbf{q}+\mathbf{k}|^2)}\;. \tag{32}$$

Finally, from Eq. (12), the ground-state energy can be written as

$$E=\Omega\frac{n_0^2}{2}\lambda\hat{v}(0)+\mu N(1-f)+I_0(\mu,n_0)+\varepsilon^2 I_2(\mu,n_0)+O(\varepsilon^3)\;, \tag{33}$$

where f_1, I_0, and I_2 are given by Eqs. (29), (16), and (25) respectively. Expand E as

$$E=E_0+E_1\varepsilon+E_2\varepsilon^2+\cdots\;,$$

with

$$E_i=\sum_{m=0}^{\infty}E_i^{(m)}\lambda^m\;.$$

E_0/Ω is given by Eq. (24). Using the known results $f_1\equiv\mu_1\equiv 0$, we find from Eq. (33) that $E_1=0$. Substituting the results obtained for $\mu_0^{(0)}$, $\mu_0^{(1)}$, $\mu_0^{(2)}$, $\mu_2^{(0)}$, $\mu_2^{(1)}$, $f_0^{(2)}$, $f_2^{(0)}$, and $f_2^{(1)}$ into the right-hand side of Eq. (33), we find

$$E_2^{(0)}=\frac{-2\bar{n}}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2}{k^2}\;,$$

$$E_2^{(1)}=\frac{8\bar{n}}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2v(\mathbf{k})}{k^4}\;,$$

and

$$E_2^2=\frac{4\bar{n}^{\,2}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}^{\,2}(\mathbf{q})}{k^4q^2}-\frac{32\bar{n}^{\,3}}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}^{\,2}(\mathbf{k})}{k^6}$$
$$-\frac{2\bar{n}^{\,2}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{q})|^2\hat{v}^{\,2}(\mathbf{k})}{k^4(k^2+|\mathbf{k}+\mathbf{q}|^2)}-\frac{2\bar{n}^{\,2}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{q})|^2\hat{v}(\mathbf{k})\hat{v}(\mathbf{k}+\mathbf{q})}{k^2|\mathbf{k}+\mathbf{q}|^2(k^2+|\mathbf{k}+\mathbf{q}|^2)}$$
$$-\frac{4\bar{n}^{\,2}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(\mathbf{k}+\mathbf{q})\hat{v}(\mathbf{q})}{k^4|\mathbf{k}+\mathbf{q}|^2}-\frac{8\bar{n}^{\,2}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(\mathbf{q})[\hat{v}(\mathbf{q})+\hat{v}(\mathbf{k}+\mathbf{q})]}{k^2q^2(q^2+|\mathbf{k}+\mathbf{q}|^2)}$$
$$-\frac{4\bar{n}^{\,2}}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2[\hat{v}(\mathbf{q})+\hat{v}(\mathbf{k}+\mathbf{q})]^2}{k^4(q^2+|\mathbf{q}+\mathbf{k}|^2)}\;. \tag{34}$$

III. CBF THEORY

For a system of N bosons governed by the Hamiltonian of Eq. (1), a simple choice of the CBF variational ground-state wave function is

$$\Psi_{\rm CBF}=\prod_{i=1}^{N}\varphi(\mathbf{r}_i)\prod_{j<k}^{N}e^{u(\mathbf{r}_j,\mathbf{r}_k)/2}\;, \tag{35}$$

where $\varphi(\mathbf{r}_i)$ is to account for the presence of the external field $U_{\rm ext}(\mathbf{r})$, and only two-body correlating factors $u(\mathbf{r}_j,\mathbf{r}_k)$ are included. [We neglect higher-order correlating factors such as $u_3(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k)$, $u_4(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k,\mathbf{r}_l),\ldots$.] Note that $u(\mathbf{r}_j,\mathbf{r}_k)$ need not be a function only of $|\mathbf{r}_j-\mathbf{r}_k|$ as in the homogeneous case. Our task now is to determine the $\varphi(\mathbf{r}_i)$ and $u(\mathbf{r}_j,\mathbf{r}_k)$ which minimize the ground-state energy.

The l-particle distribution function $n(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_l)$ and correlation function $g(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_l)$ for the chosen variational wave function are defined by

$$n(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_l)=\frac{N!}{(N-l)!}\frac{\int\Psi_{\rm CBF}^2 d\mathbf{r}_{l+1}d\mathbf{r}_{l+2}\cdots d\mathbf{r}_N}{\int\Psi_{\rm CBF}^2 d\mathbf{r}_1 d\mathbf{r}_2\cdots d\mathbf{r}_N} \tag{36}$$

$$=n(\mathbf{r}_1)n(\mathbf{r}_2)\cdots n(\mathbf{r}_l)g(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_l)\;, \tag{37}$$

where $n(\mathbf{r})$ is the single-particle density distribution.

Take the gradients of both sides of Eq. (36): For $l=1$ and 2, we obtain the generalized Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) equations

$$\nabla_1 n(\mathbf{r}_1)=2n(\mathbf{r}_1)\nabla_1 \ln\varphi(\mathbf{r}_1) + \int d\mathbf{r}_2\, n(\mathbf{r}_1)n(\mathbf{r}_2)g(\mathbf{r}_1,\mathbf{r}_2)\nabla_1 u(\mathbf{r}_1,\mathbf{r}_2)\ , \tag{38}$$

and

$$\nabla_1 g(\mathbf{r}_1,\mathbf{r}_2)=g(\mathbf{r}_1,\mathbf{r}_2)\nabla_1 u(\mathbf{r}_1,\mathbf{r}_2) + \int d\mathbf{r}_3\, n(\mathbf{r}_3)[g(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) - g(\mathbf{r}_1,\mathbf{r}_2)g(\mathbf{r}_1,\mathbf{r}_3)] \times \nabla_1 u(\mathbf{r}_1,\mathbf{r}_3)\ . \tag{39}$$

Equation (38) has been used to obtain Eq. (39). Using Eq. (38), the variational ground-state energy

$$E_{\mathrm{CBF}}=\frac{\langle \Psi_{\mathrm{CBF}} | H | \Psi_{\mathrm{CBF}} \rangle}{\langle \Psi_{\mathrm{CBF}} | \Psi_{\mathrm{CBF}} \rangle}$$

can be expressed as

$$\begin{aligned} E_{\mathrm{CBF}}=&\tfrac{1}{2}\int d\mathbf{r}[\nabla\sqrt{n(\mathbf{r})}]^2+\varepsilon\int d\mathbf{r}\, U_{\mathrm{ext}}(\mathbf{r})n(\mathbf{r})+\frac{\lambda}{2}\int d\mathbf{r}_1\int d\mathbf{r}_2\, n(\mathbf{r}_1)n(\mathbf{r}_2)g(\mathbf{r}_1,\mathbf{r}_2)v(|\mathbf{r}_1-\mathbf{r}_2|)\\ &+\tfrac{1}{8}\int d\mathbf{r}_1\int d\mathbf{r}_2\, n(\mathbf{r}_1)n(\mathbf{r}_2)g(\mathbf{r}_1,\mathbf{r}_2)[\nabla_1 u(\mathbf{r}_1,\mathbf{r}_2)]^2\\ &-\tfrac{1}{8}\int d\mathbf{r}_1\, n(\mathbf{r}_1)\left[\int d\mathbf{r}_2\, n(\mathbf{r}_2)[\nabla_1 u(\mathbf{r}_1,\mathbf{r}_2)]g(\mathbf{r}_1,\mathbf{r}_2)\right]^2\\ &+\tfrac{1}{8}\int d\mathbf{r}_1\int d\mathbf{r}_2\int d\mathbf{r}_3\, n(\mathbf{r}_1)n(\mathbf{r}_2)n(\mathbf{r}_3)[\nabla_1 u(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u(\mathbf{r}_1,\mathbf{r}_3)]g(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\ . \end{aligned} \tag{40}$$

Using Eqs. (39), Eq. (40) can be written as

$$\begin{aligned} E_{\mathrm{CBF}}=&\tfrac{1}{2}\int d\mathbf{r}[\nabla\sqrt{n(\mathbf{r})}]^2+\varepsilon\int d\mathbf{r}\, U_{\mathrm{ext}}(\mathbf{r})n(\mathbf{r})+\frac{\lambda}{2}\int d\mathbf{r}_1\int d\mathbf{r}_2\, n(\mathbf{r}_1)n(\mathbf{r}_2)g(\mathbf{r}_1,\mathbf{r}_2)v(|\mathbf{r}_1-\mathbf{r}_2|)\\ &+\tfrac{1}{8}\int d\mathbf{r}_1\int d\mathbf{r}_2\, n(\mathbf{r}_1)n(\mathbf{r}_2)\nabla_1 g(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u(\mathbf{r}_1,\mathbf{r}_2)\ . \end{aligned} \tag{41}$$

Now we expand $n(\mathbf{r})$, $g(\mathbf{r}_1,\mathbf{r}_2)$, and $u(\mathbf{r}_1,\mathbf{r}_2)$ in orders of ε and λ:

$$n(\mathbf{r})=\sum_{\alpha=0}^{\infty} n_\alpha(\mathbf{r})\varepsilon^\alpha,\quad n_\alpha(\mathbf{r})=\sum_{m=0}^{\infty} n_\alpha^{(m)}(\mathbf{r})\lambda^m\ , \tag{42}$$

$$g(\mathbf{r}_1,\mathbf{r}_2)=\sum_{\alpha=0}^{\infty} g_\alpha(\mathbf{r}_1,\mathbf{r}_2)\varepsilon^\alpha,\quad g_\alpha(\mathbf{r}_1,\mathbf{r}_2)=\sum_{m=0}^{\infty} g_\alpha^{(m)}(\mathbf{r}_1,\mathbf{r}_2)\lambda^m\ , \tag{43}$$

$$u(\mathbf{r}_1,\mathbf{r}_2)=\sum_{\alpha=0}^{\infty} u_\alpha(\mathbf{r}_1,\mathbf{r}_2)\varepsilon^\alpha,\quad u_\alpha(\mathbf{r}_1,\mathbf{r}_2)=\sum_{m=0}^{\infty} u_\alpha^{(m)}(\mathbf{r}_1,\mathbf{r}_2)\lambda^m\ . \tag{44}$$

The following properties are known for n_α, g_α, and u_α.

(i) In the homogeneous case we have

$$n_0(\mathbf{r})=\bar{n}\equiv N/\Omega\ ,$$

and

$$g_0(\mathbf{r}_1,\mathbf{r}_2)=g_0(|\mathbf{r}_1-\mathbf{r}_2|),\quad u_0(\mathbf{r}_1,\mathbf{r}_2)=u_0(|\mathbf{r}_1-\mathbf{r}_2|)\ . \tag{45}$$

(ii) Since

$$N=\bar{n}\Omega=\int n(\mathbf{r})d\mathbf{r}=\sum_{\alpha=0}^{\infty}\varepsilon^\alpha\int n_\alpha(\mathbf{r})d\mathbf{r}=\bar{n}\Omega+\sum_{\alpha=1}^{\infty}\varepsilon^\alpha\int n_\alpha(\mathbf{r})d\mathbf{r}\ ,$$

we have

$$\hat{n}_\alpha(0)\equiv\int n_\alpha(\mathbf{r})d\mathbf{r}=0,\quad \alpha=1,2,\ldots,\infty\ . \tag{46}$$

(iii) For $\alpha\geq 1$, we still have the following symmetry properties:

$$g_\alpha(\mathbf{r}_1,\mathbf{r}_2)=g_\alpha(\mathbf{r}_2,\mathbf{r}_1)\ ,$$

and

$$u_\alpha(\mathbf{r}_1,\mathbf{r}_2)=u_\alpha(\mathbf{r}_2,\mathbf{r}_1)\ . \tag{47}$$

(iv) When there is no interaction between the particles, i.e., $\lambda=0$, we should have

$$g(\mathbf{r}_1,\mathbf{r}_2)=1 ,$$

and

$$u(\mathbf{r}_1,\mathbf{r}_2)=0 .$$

Since $g_0^{(0)}(\mathbf{r}_1,\mathbf{r}_2)=1$, Eqs. (43) and (44) then lead to

$$g_\alpha^{(0)}(\mathbf{r}_1,\mathbf{r}_2)=0, \quad \alpha=1,2,\ldots,\infty$$

and

$$u_\alpha^{(0)}(\mathbf{r}_1,\mathbf{r}_2)=0, \quad \alpha=0,1,2,\ldots,\infty . \tag{48}$$

Using the expansion formulas (42)–(44) and the properties given above in Eqs. (45)–(47), Eq. (41) can be rewritten as

$$E_{\mathrm{CBF}}=E_0+\varepsilon E_1+\varepsilon^2 E_2+\cdots , \tag{49}$$

with

$$E_0=\frac{\Omega}{2}\bar{n}^2\lambda\int g_0(r)v(r)d\mathbf{r}+\frac{\Omega}{8}\bar{n}^2\int \nabla g_0(r)\cdot\nabla u_0(r)d\mathbf{r} , \tag{50}$$

$$E_1=\frac{\bar{n}^2\lambda}{2}\int\int g_1(\mathbf{r}_1,\mathbf{r}_2)v(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2+\frac{\bar{n}^2}{8}\int\int \nabla_1 g_1(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_0(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 + \frac{\bar{n}^2}{8}\int\int \nabla_1 g_0(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_1(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 , \tag{51}$$

and

$$\begin{aligned}E_2=&\frac{1}{8\bar{n}}\int[\nabla n_1(\mathbf{r})]^2 d\mathbf{r}+\int U_{\mathrm{ext}}(\mathbf{r})n_1(\mathbf{r})d\mathbf{r}+\frac{\lambda}{2}\int\int n_1(\mathbf{r}_1)n_1(\mathbf{r}_2)g_0(\mathbf{r}_1,\mathbf{r}_2)v(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2\\
&+\bar{n}\lambda\int\int n_1(\mathbf{r}_1)g_1(\mathbf{r}_1,\mathbf{r}_2)v(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2+\frac{\bar{n}^2\lambda}{2}\int\int g_2(\mathbf{r}_1,\mathbf{r}_2)v(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2\\
&+\tfrac{1}{8}\int\int n_1(\mathbf{r}_1)n_1(\mathbf{r}_2)\nabla_1 g_0(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_0(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2\\
&+\frac{\bar{n}}{8}\int\int n_1(\mathbf{r}_1)\nabla_1 g_0(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_1(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2+\frac{\bar{n}}{8}\int\int n_1(\mathbf{r}_2)\nabla_1 g_0(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_1(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2\\
&+\frac{\bar{n}}{8}\int\int n_1(\mathbf{r}_1)\nabla_1 g_1(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_0(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2+\frac{\bar{n}}{8}\int\int n_1(\mathbf{r}_2)\nabla_1 g_1(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_0(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2\\
&+\frac{\bar{n}^2}{8}\int\int \nabla_1 g_0(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_2(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2+\frac{\bar{n}^2}{8}\int\int \nabla_1 g_1(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_1(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2\\
&+\frac{\bar{n}^2}{8}\int\int \nabla_1 g_2(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_0(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 ,\end{aligned} \tag{52}$$

where we have once again assumed $\hat{U}_{\mathrm{ext}}(\mathbf{k}=0)=0$ in Eq. (51) without loss of generality.

The homogeneous case, $\varepsilon=0$, has been discussed thoroughly in Ref. 5. In the Appendix, we shall derive some of its variational properties.

We now consider the first-order terms in ε. Expand E_1 of Eq. (51) in orders of λ, and write it in the momentum representation, we have

$$E_1=\sum_{m=0}^{\infty}E_1^{(m)}\lambda^m , \tag{53}$$

with

$$E_1^{(0)}=0 , \tag{54}$$

$$E_1^{(1)}=0 , \tag{55}$$

$$E_1^{(2)}=\frac{\bar{n}^2}{2(2\pi)^3}\int \hat{g}_1^{(1)}(\mathbf{k},\mathbf{k})\left[\hat{v}(k)+\frac{k^2}{4}\hat{u}_0^{(1)}(k)\right]d\mathbf{k}+\frac{\bar{n}^2}{8(2\pi)^3}\int k^2\hat{g}_0^{(1)}(k)\hat{u}_1^{(1)}(\mathbf{k},\mathbf{k})d\mathbf{k} , \tag{56}$$

and

$$E_1^{(3)}=\frac{\bar{n}^2}{2(2\pi)^3}\int \hat{g}_1^{(2)}(\mathbf{k},\mathbf{k})\hat{v}(k)d\mathbf{k}+\frac{\bar{n}^2}{8(2\pi)^3}\int k^2\hat{g}_1^{(2)}(\mathbf{k},\mathbf{k})\hat{u}_0^{(1)}(k)d\mathbf{k}+\frac{\bar{n}^2}{8(2\pi)^3}\int k^2\hat{g}_1^{(1)}(\mathbf{k},\mathbf{k})\hat{u}_0^{(2)}(k)d\mathbf{k}$$
$$+\frac{\bar{n}^2}{8(2\pi)^3}\int k^2\hat{g}_0^{(1)}(k)\hat{u}_1^{(2)}(\mathbf{k},\mathbf{k})d\mathbf{k}+\frac{\bar{n}^2}{8(2\pi)^3}\int k^2\hat{g}_0^2(k)\hat{u}_1^{(1)}(\mathbf{k},\mathbf{k})d\mathbf{k}\ . \tag{57}$$

The properties (i) and (iv), Eqs. (45) and (48), have been used in obtaining Eqs. (56) and (57). The Fourier transform of any function $F(\mathbf{r}_1,\mathbf{r}_2)$ is defined by

$$\hat{F}(\mathbf{k}_1,\mathbf{k}_2)=\int F(\mathbf{r}_1,\mathbf{r}_2)e^{-i(\mathbf{k}_1\cdot\mathbf{r}_1-\mathbf{k}_2\cdot\mathbf{r}_2)}d\mathbf{r}_1d\mathbf{r}_2\ . \tag{58}$$

In order to determine the relationship between $g_1^{(m)}$ and $u_1^{(m)}$, as for the homogeneous case shown in the Appendix, we call on the use of the BBGKY equation (39) in conjunction with the Kirkwood superposition approximation,

$$g(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\approx g(\mathbf{r}_1,\mathbf{r}_2)g(\mathbf{r}_2,\mathbf{r}_3)g(\mathbf{r}_3,\mathbf{r}_1)\ .$$

To first order in ε, expanding both sides of Eq. (39) in powers of λ, we find with the assistance of the properties (i)–(iv) in Eqs. (45)–(48)

$$\hat{g}_1^{(1)}(\mathbf{k}_1,\mathbf{k}_2)=\hat{u}_1^{(1)}(\mathbf{k}_1,\mathbf{k}_2) \tag{59}$$

and

$$\hat{g}_1^{(2)}(\mathbf{k}_1,\mathbf{k}_2)=\hat{u}_1^{(2)}(\mathbf{k}_1,\mathbf{k}_2)+\bar{n}\,\hat{u}_1^{(1)}(\mathbf{k}_1,\mathbf{k}_2)\hat{u}_0^{(1)}(k_1)+\bar{n}\,\hat{u}_1^{(1)}(\mathbf{k}_1,\mathbf{k}_2)\hat{u}_0^{(1)}(k_2)+\hat{n}_1^{(0)}(\mathbf{k}_1-\mathbf{k}_2)\hat{g}_0^{(1)}(k_1)\hat{u}_0^{(1)}(k_2)$$
$$+\frac{1}{(2\pi)^3}\int \hat{u}_1^{(1)}(\mathbf{k}_1-\mathbf{q},\mathbf{k}_2-\mathbf{q})\hat{u}_0^{(1)}(q)d\mathbf{q}\ . \tag{60}$$

Equation (59), together with the relations given for the homogeneous case in Eqs. (A6) and (A10), immediately gives rise to

$$E_1^{(2)}=0\ . \tag{61}$$

Using Eqs. (60), (59), (A6), and (A10), and noting that $\hat{n}_1^{(0)}(0)=0$, Eq. (57) for $E_1^{(3)}$ can be rewritten in the form

$$E_1^{(3)}=\frac{\bar{n}^2}{8(2\pi)^3}\int d\mathbf{k}\,k^2\hat{g}_1^{(1)}(\mathbf{k},\mathbf{k})\left[2\hat{g}_0^{(2)}(k)-\Delta\hat{g}_0^{(2)}(k)-2\bar{n}[\hat{g}_0^{(1)}(k)]^2-\frac{1}{(2\pi)^3}\int\frac{q^2}{k^2}\hat{g}_0^{(1)}(q)\hat{g}_0^{(1)}(|\mathbf{q}-\mathbf{k}|)d\mathbf{q}\right]\ , \tag{62}$$

where $\Delta\hat{g}_0^{(2)}(k)$ is as defined in Eq. (A8). It has been shown in Eq. (A16) of the Appendix that the expression in large parentheses in Eq. (62) vanishes identically. Consequently,

$$E_1^{(3)}=0\ . \tag{63}$$

While these results could have been obtained as a consequence of directly minimizing the energy expression with respect to $\varphi(\mathbf{r}_i)$ and $u(\mathbf{r}_j,\mathbf{r}_k)$, we have carried out term-by-term evaluation to illustrate how higher-order terms will be treated.

Next we consider ε^2 terms. Expanding E_2 of Eq. (52) in orders of λ using expansion formulas (42)–(44) and properties (45)–(48), we find to order $\varepsilon^2\lambda^2$

$$E_2=\sum_{m=0}^{\infty}E_2^{(m)}\lambda^m\ , \tag{64}$$

$$E_2^{(0)}=\frac{1}{8\bar{n}}\int[\nabla n_1^{(0)}(\mathbf{r})]^2d\mathbf{r}+\int U_{\rm ext}(\mathbf{r})n_1^{(0)}(\mathbf{r})d\mathbf{r}$$
$$=\frac{1}{8\bar{n}(2\pi)^3}\int k^2\hat{n}_1^{(0)}(\mathbf{k})\hat{n}_1^{(0)}(-\mathbf{k})d\mathbf{k}+\frac{1}{(2\pi)^3}\int\hat{U}_{\rm ext}(\mathbf{k})\hat{n}_1^{(0)}(-\mathbf{k})d\mathbf{k}\ , \tag{65}$$

$$E_2^{(1)}=\frac{1}{4\bar{n}}\int\nabla n_1^{(0)}(\mathbf{r})\cdot\nabla n_1^{(1)}(\mathbf{r})d\mathbf{r}+\int U_{\rm ext}(\mathbf{r})n_1^{(1)}(\mathbf{r})d\mathbf{r}+\tfrac{1}{2}\int\int n_1^{(0)}(\mathbf{r}_1)n_1^{(0)}(\mathbf{r}_2)v(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1d\mathbf{r}_2$$
$$=\frac{1}{4\bar{n}(2\pi)^3}\int k^2\hat{n}_1^{(0)}(\mathbf{k})n_1^{(1)}(-\mathbf{k})d\mathbf{k}+\frac{1}{(2\pi)^3}\int\hat{U}_{\rm ext}(\mathbf{k})\hat{n}_1^{(1)}(-\mathbf{k})d\mathbf{k}$$
$$+\frac{1}{2(2\pi)^3}\int\hat{n}_1^0(\mathbf{k})\hat{n}_1^{(0)}(-\mathbf{k})\hat{v}(\mathbf{k})d\mathbf{k}\ , \tag{66}$$

and

$$
\begin{aligned}
E_2^{(2)} = & \frac{1}{8\bar{n}} \int [2\nabla n_1^{(0)}(\mathbf{r})\cdot\nabla n_1^{(2)}(\mathbf{r}) + \nabla n_1^{(1)}(\mathbf{r})\cdot\nabla n_1^{(1)}(\mathbf{r})]d\mathbf{r} \\
& + \int\int U_{\text{ext}}(\mathbf{r}) n_1^{(2)}(\mathbf{r})d\mathbf{r} + \tfrac{1}{2}\int n_1^{(0)}(\mathbf{r}_1) n_1^{(0)}(\mathbf{r}_2) g_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)v(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2 \\
& + \int\int n_1^{(0)}(\mathbf{r}_1) n_1^{(1)}(\mathbf{r}_2) v(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2 + \frac{\bar{n}^2}{2}\int g_2^{(1)}(\mathbf{r}_1,\mathbf{r}_2)v(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2 \\
& + \bar{n}\int\int n_1^{(0)}(\mathbf{r}_2) g_1^{(1)}(\mathbf{r}_1,\mathbf{r}_2) v(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2 \\
& + \tfrac{1}{8}\int\int n_1^{(0)}(\mathbf{r}_1) n_1^{0}(\mathbf{r}_2)\nabla_1 g_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)\cdot\nabla_1 u_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2 \\
& + \frac{\bar{n}}{8}\int\int n_1^{(0)}(\mathbf{r}_1)\nabla_1 g_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)\cdot\nabla_1 u_1^{(1)}(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 \\
& + \frac{\bar{n}}{8}\int\int n_1^{(0)}(\mathbf{r}_2)\nabla_1 g_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)\cdot\nabla_1 u_1^{(1)}(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 \\
& + \frac{\bar{n}}{8}\int\int n_1^{(0)}(\mathbf{r}_1)\nabla_1 g_1^{(1)}(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2 \\
& + \frac{\bar{n}}{8}\int\int n_1^{(0)}(\mathbf{r}_2)\nabla_1 g_1^{(1)}(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2 \\
& + \frac{\bar{n}^2}{8}\int\int \nabla_1 g_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)\cdot\nabla_1 u_2^{(1)}(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 \\
& + \frac{\bar{n}^2}{8}\int\int \nabla_1 g_1^{(1)}(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_1^{(1)}(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 + \frac{\bar{n}^2}{8}\int\int \nabla_1 g_2^{(1)}(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1 u_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)d\mathbf{r}_1 d\mathbf{r}_2 \\
= & \frac{1}{8\bar{n}(2\pi)^3}\int [2k^2\hat{n}_1^{(0)}(\mathbf{k})\hat{n}_1^{2}(\mathbf{k}) + k^2\hat{n}_1^{(1)}(\mathbf{k})\hat{n}_1^{(1)}(-\mathbf{k})]d\mathbf{k} + \frac{1}{(2\pi)^3}\int \hat{U}_{\text{ext}}(\mathbf{k})\hat{n}_1^{(2)}(-\mathbf{k})d\mathbf{k} \\
& + \frac{1}{2(2\pi)^3}\int\int \hat{n}_1^{(0)}(\mathbf{k}_1-\mathbf{k}_2)\hat{n}_1^{(0)}(\mathbf{k}_2-\mathbf{k}_1)\hat{g}_0^{(1)}(k_2)\hat{v}(k_1)d\mathbf{k}_1 d\mathbf{k}_2 \\
& + \frac{1}{(2\pi)^3}\int\int \hat{n}_1^{(0)}(\mathbf{k})\hat{n}_1^{(1)}(-\mathbf{k})\hat{v}(k)d\mathbf{k} + \frac{\bar{n}^2}{2(2\pi)^3}\int \hat{g}_2^{(1)}(\mathbf{k},\mathbf{k})\hat{v}(k)d\mathbf{k} \\
& + \frac{\bar{n}}{(2\pi)^3}\int\int \hat{n}_1^{(0)}(\mathbf{k}_1-\mathbf{k}_2)\hat{g}_1^{(1)}(-\mathbf{k}_1,-\mathbf{k}_2)\hat{v}(k_1)d\mathbf{k}_1 d\mathbf{k}_2 \\
& + \frac{1}{8(2\pi)^3}\int\int \hat{n}_1^{(0)}(\mathbf{k}_1-\mathbf{k}_2)\hat{n}_1^{(0)}(\mathbf{k}_2-\mathbf{k}_1)(\mathbf{k}_1\cdot\mathbf{k}_2)\hat{g}_0^{(1)}(k_2)\hat{u}_0^{(1)}(k_1)d\mathbf{k}_1 d\mathbf{k}_2 \\
& + \frac{\bar{n}}{8(2\pi)^3}\int\int \hat{n}_1^{(0)}(\mathbf{k}_2-\mathbf{k}_1)(\mathbf{k}_1\cdot\mathbf{k}_2)\hat{g}_0^{(1)}(k_2)\hat{u}_1^{(1)}(\mathbf{k}_1,\mathbf{k}_2)d\mathbf{k}_1 d\mathbf{k}_2 \\
& + \frac{\bar{n}}{8(2\pi)^3}\int\int \hat{n}_1^{(0)}(\mathbf{k}_1-\mathbf{k}_2)k_1^2\hat{g}_0^{(1)}(k_1)\hat{u}_1^{(1)}(\mathbf{k}_1,\mathbf{k}_2)d\mathbf{k}_1 d\mathbf{k}_2 \\
& + \frac{\bar{n}}{8(2\pi)^3}\int\int \hat{n}_1^{(0)}(\mathbf{k}_2-\mathbf{k}_1)(\mathbf{k}_1\cdot\mathbf{k}_2)\hat{g}_1^{(1)}(\mathbf{k}_1,\mathbf{k}_2)\hat{u}_0^{(1)}(k_2)d\mathbf{k}_1 d\mathbf{k}_2 \\
& + \frac{\bar{n}}{8(2\pi)^3}\int\int \hat{n}_1^{(0)}(\mathbf{k}_1-\mathbf{k}_2)k_1^2\hat{g}_1^{(1)}(\mathbf{k}_1,\mathbf{k}_2)\hat{u}_0^{(1)}(k_1)d\mathbf{k}_1 d\mathbf{k}_2 \\
& + \frac{\bar{n}^2}{8(2\pi)^3}\int\int k^2\hat{g}_0^{(1)}(k)\hat{u}_2^{(1)}(\mathbf{k},\mathbf{k})d\mathbf{k} + \frac{\bar{n}^2}{8(2\pi)^3}\int\int k_1^2\hat{g}_1^{(1)}(\mathbf{k}_1,\mathbf{k}_2)\hat{u}_1^{(1)}(-\mathbf{k}_1,-\mathbf{k}_2)d\mathbf{k}_1 d\mathbf{k}_2 \\
& + \frac{\bar{n}^2}{8(2\pi)^3}\int k^2\hat{g}_2^{(1)}(\mathbf{k},\mathbf{k})\hat{u}_0^{(1)}(k)d\mathbf{k}\ . \qquad (67)
\end{aligned}
$$

Before we consider the variation of $E_2^{(0)}$, $E_2^{(1)}$, and $E_2^{(2)}$, we should point out some useful relations that exist for $n_\alpha^{(m)}$, $g_\alpha^{(m)}$, U_{ext}, and $u_\alpha^{(m)}$. Since $n_\alpha^{(m)}(\mathbf{r})$, $g_\alpha^{(m)}(\mathbf{r}_1,\mathbf{r}_2)$, $U_{\text{ext}}(\mathbf{r})$, and $u_\alpha^{(m)}(\mathbf{r}_1,\mathbf{r}_2)$ are real, we have

$$\hat{n}_\alpha^{(m)}(\mathbf{k})=[\hat{n}_\alpha^{(m)}(-\mathbf{k})]^*,\quad \hat{g}_\alpha^{(m)}(\mathbf{k}_1,\mathbf{k}_2)=[\hat{g}_\alpha^{(m)}(-\mathbf{k}_1,-\mathbf{k}_2)]^* ,$$
$$\hat{U}_{\text{ext}}(\mathbf{k})=[\hat{U}_{\text{ext}}(-\mathbf{k})]^*,\quad \hat{u}_\alpha^{(m)}(\mathbf{k}_1,\mathbf{k}_2)=[\hat{u}_\alpha^{(m)}(-\mathbf{k}_1,-\mathbf{k}_2)]^* . \tag{68}$$

Also, the symmetry property of $g_\alpha^{(m)}(\mathbf{r}_1,\mathbf{r}_2)$ and $u_\alpha^{(m)}(\mathbf{r}_1,\mathbf{r}_2)$, Eq. (47), gives

$$\hat{g}_\alpha^{(m)}(\mathbf{k}_1,\mathbf{k}_2)=\hat{g}_\alpha^{(m)}(-\mathbf{k}_2,-\mathbf{k}_1),\quad \hat{u}_\alpha^{(m)}(\mathbf{k}_1,\mathbf{k}_2)=\hat{u}_\alpha^{(m)}(-\mathbf{k}_2,-\mathbf{k}_1) . \tag{69}$$

As in the derivation of Eq. (59), the BBGKY Eq. (39) in conjunction with the Kirkwood superposition approximation yields

$$\hat{g}_2^{(1)}(\mathbf{k}_1,\mathbf{k}_2)=\hat{u}_2^{(1)}(\mathbf{k}_1,\mathbf{k}_2) . \tag{70}$$

By Eqs. (70), (A6), and (A10), $\hat{u}_2^{(1)}$ and $\hat{g}_2^{(1)}$ disappear from $E_2^{(2)}$. We are finally ready to apply the variational principle by minimizing $E_2^{(0)}$, $E_2^{(1)}$, and $E_2^{(2)}$ with respect to $\hat{n}_1^{(0)}$, $\hat{n}_1^{(1)}$, and $\hat{g}_1^{(1)}$ (or $\hat{u}_1^{(1)}$).

From Eqs. (65) and (66), we find that both $\delta E_2^{(0)}/\delta\hat{n}_1^{(0)}(\mathbf{k})=0$ and $\delta E_2^{(1)}/\delta\hat{n}_1^{(1)}(\mathbf{k})=0$ yield

$$\hat{n}_1^{(0)}(\mathbf{k})=\frac{-4\bar{n}\hat{U}_{\text{ext}}(\mathbf{k})}{k^2} . \tag{71}$$

With Eq. (71), the dependence of $E_2^{(2)}$ on $\hat{n}_1^{(2)}$ also disappears. From $\delta E_2^{(2)}/\delta\hat{n}_1^{(1)}(\mathbf{k})=0$, then, we obtain

$$\hat{n}_1^{(1)}(\mathbf{k})=-4\bar{n}\,\hat{v}(k)\hat{n}_1^{(0)}(\mathbf{k})/k^2 . \tag{72}$$

From $\delta E_2^{(2)}/\delta\hat{g}_1^{(1)}(\mathbf{k}_1,\mathbf{k}_2)=0$, using Eqs. (59), (A6), and (A10), we find

$$\hat{g}_1^{(1)}(\mathbf{k}_1,\mathbf{k}_2)=\frac{2}{\bar{n}}\hat{n}_1^{(0)}(\mathbf{k}_2-\mathbf{k}_1)\left[\frac{\mathbf{k}_1\cdot\mathbf{k}_2\hat{v}(k_2)}{k_1^2k_2^2}-\frac{\hat{v}(k_1)}{k_1^2}\right] . \tag{73}$$

Substituting Eqs. (71), (72), and (73) into Eqs. (65), (66), and (67), after some mathematical manipulations we finally arrive at the optimized energy expressions,

$$E_2^{(0)}=\frac{-2\bar{n}}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\text{ext}}(\mathbf{k})|^2}{k^2} , \tag{74}$$

$$E_2^{(1)}=\frac{8\bar{n}^2}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\text{ext}}(\mathbf{k})|^2\hat{v}(k)}{k^4} , \tag{75}$$

and

$$E_2^{(2)}=\frac{-32\bar{n}^3}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\text{ext}}(\mathbf{k})|^2\hat{v}^2(k)}{k^6}-\frac{8\bar{n}^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\text{ext}}(\mathbf{k})|^2\hat{v}(q)}{k^4q^2}$$
$$+\frac{8\bar{n}^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\text{ext}}(\mathbf{q})|^2\hat{v}(k)\hat{v}(|\mathbf{k}+\mathbf{q}|)}{q^4|\mathbf{k}+\mathbf{q}|^2}-\frac{8\bar{n}^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\text{ext}}(\mathbf{q})|^2\hat{v}^2(k)}{q^4|\mathbf{k}+\mathbf{q}|^2}$$
$$+\frac{8\bar{n}^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\text{ext}}(\mathbf{q})|^2\hat{v}(k)\hat{v}(|\mathbf{k}+\mathbf{q}|)(\mathbf{k}\cdot\mathbf{q})}{q^4k^2|\mathbf{k}+\mathbf{q}|^2}-\frac{8\bar{n}^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\text{ext}}(\mathbf{q})|^2\hat{v}^2(k)(\mathbf{k}\cdot\mathbf{q})^2}{q^4k^2|\mathbf{k}+\mathbf{q}|^2} . \tag{76}$$

IV. DENSITY-FUNCTIONAL THEORY

Ebner and Saam[13] generalized the local-density-functional method (LDF) to treating Bose liquids. The ground-state energy functional

$$E[n]\approx\int e_H[n(\mathbf{r})]d\mathbf{r}+\varepsilon\int n(\mathbf{r})U_{\text{ext}}(\mathbf{r})d\mathbf{r}+\tfrac{1}{2}\int[\nabla\sqrt{n(\mathbf{r})}]^2d\mathbf{r} , \tag{77}$$

contains an energy density e_H of a homogeneous system at the local density $n(\mathbf{r})$. Apart from a constant,

$$e_H(\bar{n})=-\tfrac{1}{2}\bar{n}^2A\equiv\frac{-1}{2(2\pi)^3}\bar{n}^2\lambda^2\int d\mathbf{k}\frac{\hat{v}^2(k)}{k^2} . \tag{78}$$

Using the expansion formula (42) and the property (ii) of Eq. (46), casting $E[n]$ in momentum representation, and varying E with respect to $\hat{n}_1(\mathbf{k})$, we find order by order in the expansion

$$n(\mathbf{r})=n_0+\sum_{\alpha=1}^{\infty}\varepsilon^\alpha n_\alpha(\mathbf{r}),\quad \hat{n}_\alpha(\mathbf{k})=\sum_{m=0}^{\infty}\hat{n}_\alpha^{(m)}(\mathbf{k})\lambda^m , \tag{79}$$

$$\hat{n}_1^{(0)}(\mathbf{k})=\frac{-4\bar{n}\hat{U}_{\text{ext}}(\mathbf{k})}{k^2} , \tag{80}$$

$$\hat{n}_1^{(1)}(\mathbf{k})=0 , \tag{81}$$

$$\hat{n}_1^{(2)}(\mathbf{k})=\frac{4\bar{n}\,\hat{n}_1^{(0)}(\mathbf{k})}{k^2}\int d\mathbf{q}\frac{\hat{v}^2(q)}{q^2} . \tag{82}$$

Also, $E_1^{(m)}=0$, for all $m=0,1,2,\ldots,\infty$;

$$E_2^{(0)}=\frac{-2\bar{n}}{(2\pi)^3}\int\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2}{k^2}d\mathbf{k}\ , \tag{83}$$

$$E_2^{(1)}=0\ , \tag{84}$$

$$E_2^{(2)}=\frac{-8\bar{n}^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}^2(q)}{k^4q^2}\ . \tag{85}$$

Going beyond local-density approximation, one adds a nonlocal correction term to the energy functional, $\delta E[n]$:

$$\delta E[n]\approx-\tfrac{1}{4}\int\int\int[n(\mathbf{r}_1)-n(\mathbf{r}_2)]^2e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}[\chi_{\mathbf{k}}^{-1}(\bar{n})-(\chi_{\mathbf{k}}^{(0)})^{-1}(\bar{n})]d\mathbf{k}\,d\mathbf{r}_1\,d\mathbf{r}_2\ ,$$

or (86)

$$\delta E[n_\alpha(\mathbf{k})]\approx\tfrac{1}{2}\varepsilon^2\int d\mathbf{k}\hat{n}_1(\mathbf{k})\hat{n}_1(-\mathbf{k})[\chi_{\mathbf{k}}^{-1}(\bar{n})-(\chi_{\mathbf{k}}^{(0)})^{-1}(\bar{n})]\ ,$$

where

$$\begin{aligned}\chi_{\mathbf{k}}^{-1}(\bar{n})-(\chi_{\mathbf{k}}^{(0)})^{-1}(\bar{n})&=\frac{k^2}{4\bar{n}}[S_0^{-2}(k)-1]\\&=\lambda\frac{-k^2}{2}\hat{g}_0^{(1)}(k)+\lambda^2\frac{k^2}{4}\{-2\hat{g}_0^{2}(k)+3\bar{n}[\hat{g}_0^{(1)}(k)]^2\}+O(\lambda^3)\ .\end{aligned} \tag{87}$$

$S_0(k)$ denotes the liquid structure factor of the homogeneous Bose system, and $g_0^{(m)}(k)$ represents the mth term in the expansion of $1/\bar{n}[S_0(k)-1]$ in powers of λ. $[g_0^{(m)}(k)]$ are taken then from the exact expressions given in Ref. 5.

Variation of $E+\delta E$ with respect to $\hat{n}_1(\mathbf{k})$ and separating into various powers of λ as before give us a new set of $\{\hat{n}_1^{(m)}(\mathbf{k})\}$ and new energy expressions. While $E_2^{(0)}$ is unchanged, we find

$$E_2^{(1)}=\frac{8\bar{n}^2}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(k)}{k^4}\ , \tag{88}$$

and

$$\begin{aligned}E_2^{(2)}=&\frac{-8\bar{n}^2}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2}{k^4}\int d\mathbf{q}\frac{\hat{v}^2(q)}{q^2}+\frac{4\bar{n}^2}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2}{k^2}\int d\mathbf{q}\frac{\hat{v}^2(q)}{q^4}\\&-\frac{8\bar{n}^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(q)\hat{v}(|\mathbf{k}+\mathbf{q}|)}{k^4q^2}-\frac{8\bar{n}^2}{(2\pi)^6}\int d\mathbf{k}\int d\mathbf{q}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}(q)\hat{v}(|\mathbf{k}+\mathbf{q}|)}{k^2q^2|\mathbf{k}+\mathbf{q}|^2}\\&-\frac{32\bar{n}^3}{(2\pi)^3}\int d\mathbf{k}\frac{|\hat{U}_{\rm ext}(\mathbf{k})|^2\hat{v}^2(k)}{k^6}\ .\end{aligned} \tag{89}$$

V. COMPARISON AND CONCLUSIONS

In this work we have studied the ground-state properties of a weakly interacting Bose gas made inhomogeneous by the presence of a weak external field. Three different theories have been used to obtain the ground-state energy: the perturbation theory, CBF, and DFT. In each case the energy is calculated to order $\varepsilon^2\lambda^2$.

For the perturbation theory, a new and simpler method than that of Ref. 5 is used to obtain both the chemical potential and the ground-state energy. We have shown that for the homogeneous system ($\varepsilon=0$) this method gives identical results to those of Ref. 5 using a more conventional approach.

For our CBF calculation, only one- and two-particle factors are included in the trial wave function, and the Kirkwood superposition approximation has been used.

Comparing results from the CBF theory to perturbation theory, we find that in the first order of ε, Eqs. (54), (55), (61), and (63) agree with the results of the perturbation theory. In the CBF, however, we have not proved generally that $E_1^{(m)}=0$ for all m. To second order in ε, $E_2^{(0)}$ and $E_2^{(1)}$, as given in Eqs. (74) and (75), are identical to those of Eq. (34) from the perturbation theory. But for $E_2^{(2)}$, Eq. (76) is able to pick up only parts of the terms in Eq. (34). The last two terms in Eq. (76) cannot be expressed in terms of perturbation diagrams. There are two reasons. First, the choice of the trial wave function has been limited. It is not so much the omission of high-order correlating factors, but the artificial separation of the single-particle factors (which account for statistical correlations) from the two-particle factors (which account for dynamical correlations) that introduces inherent errors. For the ground state of a homogeneous Bose system, the single-particle factors reduce to unity, thus preserving the generality of the wave function. The inclusion of higher-order correlating factors would improve the description of the ground state, leading asymptotically toward an exact expression while continuing to preserve the generality of the wave function. It does not work in the same way for its excited states, or for an inhomogeneous system, or for the ground state of a Fermi system. (For example, for the excited states of a homogeneous Bose system, factorization leads to the Feynman theory, which is exact only in the long-wavelength limit. It fails to describe phonon dispersion. See the detailed discussions in Ref. 2.) The second reason is the use of the Kirkwood superposition approximation. At such low orders, this approximation scheme would have been acceptable (as seen in Ref. 5), were it not for the above-mentioned problem created by using such a trial wave function for an *inhomogeneous* system.

For the DFT calculation, we find $E_1^{(m)}=0$ for all m, in agreement with the perturbation theory. However, in the LDF, other than $O(\varepsilon^2\lambda^0)$ there is no similarity at all between results from the DFT and from the perturbation theory. A nonlocal correction term to the energy functional has to be included in order to get the correct result for $E_2^{(1)}$. $E_2^{(2)}$ remains far apart from the corresponding expression in the perturbation theory.

We conclude that in their simplest workable forms (meaning the renormalized theory by Ebner and Saam in the case of DFT) the CBF theory yields results which are better than DFT. In particular, it is superior to DFT in the local density approximation, even though the latter was designed to take care of systems with slow and small density variations such as the one considered here.

APPENDIX

We expand E_0 of Eq. (50) in powers of λ using Eqs. (43) and (44). Writing E_0 as $E_0=\sum_{m=0}^{\infty}E_0^{(m)}\lambda^m$, we have, using property (iv), or Eq. (48),

$$E_0^{(0)}=0\ , \tag{A1}$$

$$\frac{E_0^{(1)}}{\Omega}=\frac{\bar{n}^2}{2}\hat{v}(0)\ , \tag{A2}$$

$$\begin{aligned}\frac{E_0^{(2)}}{\Omega}&=\frac{\bar{n}^2}{2}\int g_0^{(1)}(r)v(r)d\mathbf{r}+\frac{\bar{n}^2}{8}\int \nabla g_0^{(1)}(r)\cdot\nabla u_0^{(1)}(r)d\mathbf{r}\\&=\frac{\bar{n}^2}{2(2\pi)^3}\int \hat{g}_0^{(1)}(k)\hat{v}(k)d\mathbf{k}+\frac{\bar{n}^2}{8(2\pi)^3}\int k^2\hat{g}_0^{(1)}(k)\hat{u}_0^{(1)}(k)d\mathbf{k}\ ,\end{aligned} \tag{A3}$$

$$\begin{aligned}\frac{E_0^{(3)}}{\Omega}&=\frac{\bar{n}^2}{2}\int g_0^{(2)}(r)v(r)d\mathbf{r}+\frac{\bar{n}^2}{8}\int [\nabla g_0^{(2)}(r)\cdot\nabla u_0^{(1)}(r)+\nabla g_0^{(1)}(r)\cdot\nabla u_0^{(2)}(r)]d\mathbf{r}\\&=\frac{\bar{n}^2}{2(2\pi)^3}\int \hat{g}_0^{(2)}(k)v(k)d\mathbf{k}+\frac{\bar{n}^2}{8(2\pi)^3}\int [\hat{g}_0^{(2)}(k)\hat{u}_0^{(1)}(k)+\hat{g}_0^{(1)}(k)\hat{u}_0^{(2)}(k)]k^2d\mathbf{k}\ ,\end{aligned} \tag{A4}$$

$$\begin{aligned}\frac{E_0^{(4)}}{\Omega}&=\frac{\bar{n}^2}{2}\int g_0^{(3)}(r)v(r)d\mathbf{r}+\frac{\bar{n}^2}{8}\int [\nabla g_0^{(3)}(r)\cdot\nabla u_0^{(1)}(r)+\nabla g_0^{(2)}(r)\cdot\nabla u_0^{(2)}(r)+\nabla g_0^{(1)}(r)\cdot\nabla u_0^{(3)}(r)]d\mathbf{r}\\&=\frac{\bar{n}^2}{2(2\pi)^3}\int \hat{g}_0^{(3)}(k)\hat{v}(k)d\mathbf{k}+\frac{\bar{n}^2}{8(2\pi)^3}\int [\hat{g}_0^{(3)}(k)\hat{u}_0^{(1)}(k)+\hat{g}_0^{(2)}(k)\hat{u}_0^{(2)}(k)+\hat{g}_0^{(1)}(k)\hat{u}_0^{(3)}(k)]k^2d\mathbf{k}\ .\end{aligned} \tag{A5}$$

We now wish to determine the optimal $\{u_0^{(m)}(r)\}$ which minimize $\{E_0^{(m)}\}$. The relation between $g_0^{(m)}$ and $u_0^{(m)}$ can be obtained from the BBGKY Eq. (39). We use the Kirkwood superposition approximation $g(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\approx g(\mathbf{r}_1,\mathbf{r}_2)g(\mathbf{r}_2,\mathbf{r}_3)g(\mathbf{r}_3,\mathbf{r}_1)$ in Eq. (39) and expand both sides of this equation in powers of λ. Once again using property (iv), or Eq. (48), we find the following. To order λ:

$$\nabla g_0^{(1)}(r)=\nabla u_0^{(1)}(r),\quad \text{or}\ \hat{g}_0^{(1)}(k)=\hat{u}_0^{(1)}(k)\ . \tag{A6}$$

To order λ^2:

$$\begin{aligned}\nabla_1 g_0^{(2)}(|\mathbf{r}_1-\mathbf{r}_2|)=&\nabla_1 u_0^{(2)}(|\mathbf{r}_1-\mathbf{r}_2|)+g_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)\nabla_1 u_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)\\&+\bar{n}\int g_0^{(1)}(|\mathbf{r}_2-\mathbf{r}_3|)\nabla_1 u_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_3|)d\mathbf{r}_3\ ,\end{aligned}$$

or

$$\hat{g}_0^{(2)}(k)=\hat{u}_0^{(2)}(k)+\bar{n}\,\hat{g}_0^{(1)}(k)\hat{u}_0^{(1)}(k)+\frac{1}{(2\pi)^3}\int \frac{\mathbf{k}\cdot\mathbf{q}}{k^2}\hat{g}_0^{(1)}(|\mathbf{k}-\mathbf{q}|)\hat{g}_0^{(1)}(q)d\mathbf{q}\ . \tag{A7}$$

Using the relation

$$\int \frac{\mathbf{k}\cdot\mathbf{q}}{k^2}\hat{g}_0^{(1)}(|\mathbf{k}-\mathbf{q}|)\hat{g}_0^{(1)}(q)d\mathbf{q}=\int \frac{\mathbf{k}\cdot(\mathbf{k}-\mathbf{q})}{k^2}\hat{g}_0^{(1)}(q)\hat{g}_0^{(1)}(|\mathbf{k}-\mathbf{q}|)d\mathbf{q}\ ,$$

and Eq. (A6), Eq. (A7) can be written as

$$\Delta\hat{g}_0^{(2)}(k)\equiv\hat{g}_0^{(2)}(k)-u_0^{(2)}(k)=\bar{n}[\hat{g}_0^{(1)}(k)]^2+\frac{1}{2(2\pi)^3}\int \hat{g}_0^{(1)}(q)\hat{g}_0^{(1)}(|\mathbf{k}-\mathbf{q}|)d\mathbf{q}\ . \tag{A8}$$

To order λ^3:

$$\nabla_1 g_0^{(3)}(|\mathbf{r}_1-\mathbf{r}_2|)=\nabla_1 u_0^3(|\mathbf{r}_1-\mathbf{r}_2|)+g_0^{(2)}(|\mathbf{r}_1-\mathbf{r}_2|)\nabla_1 u_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)$$
$$+g_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)\nabla_1 u_0^{(2)}(|\mathbf{r}_1-\mathbf{r}_2|)+\bar{n}\int g^{(1)}(|\mathbf{r}_2-\mathbf{r}_3|)\nabla_1 u_0^{(2)}(|\mathbf{r}_1-\mathbf{r}_3|)d\mathbf{r}_3$$
$$+\bar{n}\int [g_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_2|)g_0^{(1)}(|\mathbf{r}_2-\mathbf{r}_3|)+g_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_3|)g_0^{(1)}(|\mathbf{r}_2-\mathbf{r}_3|)$$
$$+g_0^{(2)}(|\mathbf{r}_2-\mathbf{r}_3|)]\nabla_1 u_0^{(1)}(|\mathbf{r}_1-\mathbf{r}_3|)d\mathbf{r}_3 ,$$

or

$$\hat{g}_0^{(3)}(k)=\hat{u}_0^{(3)}(k)+\bar{n}\,\hat{g}_0^{(2)}(k)\hat{u}_0^{(1)}(k)+\bar{n}\,\hat{g}_0^{(1)}(k)\hat{u}_0^{(2)}(k)$$
$$+\frac{1}{(2\pi)^3}\int \frac{\mathbf{k}\cdot\mathbf{q}}{k^2}\hat{g}_0^{(2)}(|\mathbf{k}-\mathbf{q}|)\hat{g}_0^{(1)}(q)d\mathbf{q}+\frac{1}{(2\pi)^3}\int \frac{\mathbf{k}\cdot(\mathbf{k}-\mathbf{q})}{k^2}\hat{g}_0^{(1)}(q)\hat{u}_0^{(2)}(|\mathbf{k}-\mathbf{q}|)d\mathbf{q}$$
$$+\frac{1}{(2\pi)^3}\int \frac{\mathbf{k}\cdot\mathbf{q}}{k^2}\hat{g}_0^{(1)}(|\mathbf{k}-\mathbf{q}|)\hat{g}_0^{(1)}(q)\hat{u}_0^{(1)}(q)d\mathbf{q}+\frac{1}{(2\pi)^3}\int \frac{\mathbf{k}\cdot\mathbf{q}}{k^2}\hat{g}_0^{(1)}(|\mathbf{k}-\mathbf{q}|)\hat{g}_0^{(1)}(-k)\hat{u}_0^{(1)}(q)d\mathbf{q} . \quad \text{(A9)}$$

Substituting Eq. (A6) into Eq. (A4), and using $\delta E_0^{(2)}/\delta\hat{g}_0^{(1)}(k)=0$, we find

$$\hat{g}_0^{(1)}(k)=\frac{-2\hat{v}(k)}{k^2} . \quad \text{(A10)}$$

Using Eqs. (A6), (A8), and (A10), it can be shown that

$$\frac{\delta E_0^{(3)}}{\delta\hat{g}_0^{(2)}(k)}=\frac{\bar{n}^2}{2(2\pi)^3}[\hat{v}(k)+\tfrac{1}{2}\hat{g}_0^{(1)}(k)k^2]=0 . \quad \text{(A11)}$$

Now we consider the condition $\delta E_0^{(4)}/\delta g_0^{(2)}(k)=0$. From Eqs. (A5) and (A10) we have

$$\frac{\delta E_0^{(4)}}{\delta\hat{g}_0^{(2)}(k)}=\frac{\bar{n}^2}{8(2\pi)^3}\left[2k^2\hat{g}_0^{(2)}(k)-k^2\Delta\hat{g}_0^{(2)}(k)-\int \hat{g}_0^{(1)}(q)q^2\frac{\delta\Delta\hat{g}_0^{(3)}(q)}{\delta\hat{g}_0^{(2)}(k)}d\mathbf{q}\right] , \quad \text{(A12)}$$

where $\Delta\hat{g}^{(2)}(k)$ is as defined in Eq. (A8) and $\Delta g_0^3(q)$ is as defined by

$$\Delta\hat{g}_0^{(3)}(q)=\hat{g}_0^{(3)}(q)-\hat{u}_0^{(3)}(q) . \quad \text{(A13)}$$

From Eq. (A9), we have

$$\frac{\delta\Delta\hat{g}_0^{(3)}(q)}{\delta\hat{g}_0^{(2)}(k)}=2\bar{n}\,\hat{g}_0^{(1)}(q)\delta(\mathbf{q}-\mathbf{k})+\frac{1}{(2\pi)^3}\hat{g}_0^{(1)}(|\mathbf{q}-\mathbf{k}|) . \quad \text{(A14)}$$

Substituting Eq. (A14) into Eq. (A12), we have

$$\hat{g}_0^{(2)}(k)=\tfrac{1}{2}\Delta\hat{g}_0^{(2)}(k)+\bar{n}[\hat{g}_0^{(1)}(k)]^2+\frac{1}{2(2\pi)^3}\int \frac{q^2}{k^2}\hat{g}_0^{(1)}(q)\hat{g}_0^{(1)}(|\mathbf{q}-\mathbf{k}|)d\mathbf{q} . \quad \text{(A15)}$$

Using Eq. (A8), Eq. (A15) becomes

$$\hat{g}_0^{(2)}(k)=\frac{3\bar{n}}{2}[\hat{g}_0^{(1)}(k)]^2+\frac{1}{4(2\pi)^3}\int \hat{g}_0^{(1)}(q)\hat{g}_0^{(1)}(|\mathbf{k}-\mathbf{q}|)d\mathbf{q}+\frac{1}{2(2\pi)^3}\int \frac{q^2}{k^2}\hat{g}_0^{(1)}(q)\hat{g}_0^{(1)}(|\mathbf{k}-\mathbf{q}|)d\mathbf{q} . \quad \text{(A16)}$$

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