Calculation of the ground state of a system of ultracold molecules

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Ultracold molecules gain more and more interest in current research, since they offer many possibilities to explore novel many–body phenomena. The most interesting part of these systems is, that they allow for control of the interaction, for example by applying external electric fields. The method of choice in this work, to study the ground state of these systems theoretically, is the hypernetted–chain Euler Lagrange (HNC/EL) method. This is a variational method that allows for the inclusion of two–body correlations in the wave function, therefore yielding much better results than mean field theory, especially for systems well beyond the weakly interacting limit. In this work we have, for the first time, included the rotational degrees of freedom of the ultracold molecules in the derivation of the equations.

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Part I.
Introduction

The first experimental realization of Bose–Einstein condensation (BEC) in magneto–optical traps [1, 2, 3], which was awarded the Nobel prize in 2001 to W. Ketterle, C. E. Wieman and E. A. Cornell, has lead to a large growth of the field of ultracold atoms. The reason for the growing interest in these systems is that they exhibit many interesting properties. For example macroscopic matter–wave interference [4] or BEC–BCS crossover [5, 6, 7] can be observed in these systems. Also, by using Feshbach resonances, the strength of the isotropic interaction can be tuned, which makes it possible to probe a whole range of different interactions with one BEC.

Dipolar quantum gases make up a rather new field within the quantum gas research since the experimental realization of ultracold gases of atoms [8, 9, 10] or molecules [11, 12, 13] with electric or magnetic dipole moment has been achieved only recently. Nevertheless this field has been growing ever since, because of the unique possibilities these systems offer to explore new many–body phenomena. This is the case because of the unique nature of the dipole–dipole interaction:

$$V_{dd}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{1}{4\pi} \frac{\boldsymbol{d}_1 \cdot \boldsymbol{d}_2 - 3\,(\boldsymbol{d}_1 \cdot \hat{\boldsymbol{r}})\,(\boldsymbol{d}_2 \cdot \hat{\boldsymbol{r}})}{r^3} \tag{1}$$

where $\boldsymbol{d}_i$ is the dipole moment of particle i, $r = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$ is the distance between the two particles and $\hat{\boldsymbol{r}} = (\boldsymbol{r}_1 - \boldsymbol{r}_2)/r$ is the unit vector pointing along the connecting line between the particles. This interaction is both long ranged, because of the $1/r^3$ dependence, and anisotropic, because it depends on the orientation of the dipoles. For example two parallel dipoles observe an attractive force, when they are aligned on top of each other, head–to–tail, and they repel each other if they are aligned next to each other, side–by–side. Additionally the interaction can be controlled, by applying for example an electric or magnetic field, which makes these systems excellent model systems for many–body physics. One can for example use external fields to partially polarize the dipole moments of the particles. Or by varying the confinement of the particles, the strength of the interaction can be tuned, because thereby the region of the interaction that the particles can explore changes. Because of this, and the long ranged nature of the interaction, it is crucial that the method to describe these systems theoretically, allows for the inclusion of correlations. Another very interesting aspect of systems of dipolar particles lies in their internal degrees of freedom. These particles can, additionally to their translational degrees of freedom, rotate. The study of how these rotational degrees of freedom affect the behavior of these strongly correlated many–body systems is the main motivation for this work. For further details on dipolar quantum gases see [14].

1. The hypernetted–chain Euler Lagrange method

The method we use in this work, to calculate the ground state of a system of strongly correlated dipolar bosons, is the hypernetted–chain Euler Lagrange (HNC/EL) method. This is a variational method where the ground state wave function is approximated using up to three–body correlation functions, which reproduces the correct short– and long–range behavior.

The properties of the desired wave function are:

- $r_i - r_j$ small $\rightarrow$ wave function reduces to effective two–body wave function
- $r_i - r_j$ large $\rightarrow$ particle i and j are no longer correlated

This is fulfilled for a product wave function of the form:

$$\psi_0(1,\ldots,N) = F_N(1,\ldots,N)\phi_0(1,\ldots,N) \tag{2}$$

with:

$$F_N(1,\ldots,N) \quad \ldots\ldots \quad \textit{Jastrow–Feenberg correlation operator}$$

which is the symmetric N–particle correlation operator. $\phi_0(1,\ldots,N)$ is a wave function of a weakly interacting model of the system and determines the symmetry of the ground state wave function. Because we are dealing here with a Bose fluid ϕ_0 is chosen to be unity.

The correlation operator assumes the Jastrow–Feenberg form given below because of the demanded properties of the wave function:

$$F_N(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N) = \exp\left[\frac{1}{2}\sum_{n=1}^{m}\left(\sum_{1\le i_1<\cdots<i_n\le N} u_n(\boldsymbol{i}_1,\ldots,\boldsymbol{i}_n)\right)\right] \tag{3}$$

One can include up to n–body functions $u_n(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_n)$ in the exponent but in this work we considered only up to two–body functions. It should be mentioned that the highest n numerically feasible is $n = 3$ [15]. The correlation operator including up to two–body functions, which is used in this work, is given by:

$$F_N(1,\ldots,N) = \exp\left[\frac{1}{2}\sum_{i=1}^{N} u_1(i) + \frac{1}{2}\sum_{1\le i<j\le N} u_2(i,j)\right] \tag{4}$$

$$= \prod_{i=1}^{N}\phi(i)\prod_{1\le i<j\le N} f(i,j). \tag{5}$$

Using this ansatz the expectation value of the Hamiltonian of the many–body system is calculated. To obtain a connection between the n–body correlation functions and physical properties, like the density or the pair distribution function, the hypernetted–chain (HNC) equations are used.

The procedure that is used to derive the HNC equations is called Mayer–Cluster expansion and is a technique known from classical statistical mechanics [16]. There it is used to rewrite the high dimensional integrals of the grand partition function in terms of graphs or 'diagrams' and then use theorems for these diagrams to calculate e.g. the density (see [16]). This expansion will not be described in detail here, just a short description of the nomenclature is given. For details on the derivation of the HNC equations see [17, 15].

HNC equations:

The calculation of the pair distribution function includes the calculation of high dimensional integrals

$$g(1,2) = \frac{\frac{N(N-1)}{I_0}\int d^3 3\ldots d^3N\,|\psi_0(1,\ldots,N)|^2}{\frac{N}{I_0}\int d^3 2\ldots d^3N\,|\psi_0(1,\ldots,N)|^2\frac{N}{I_0}\int d^3 1 d^3 3\ldots d^3N\,|\psi_0(1,\ldots,N)|^2}. \tag{6}$$

These high dimensional integrals can be expanded in graphs, where each graph can have three different elements which are:

- *open circle*: denotes the multiplication with the function $\phi(i)$; (*external point*)
- *filled circle*: denotes a multiplication with the function $\phi(i)$ and an integration over the corresponding coordinate namely $\int d^3 i\, \phi(i)$; (*internal point*)
- *line*: stands for the correlation $h_c(i, j)$; (*correlation line*)

where the correlation h_c is defined as

$$h_c(i, j) \equiv f^2(i, j) - 1 = \exp[u_2(i, j)] - 1. \tag{7}$$

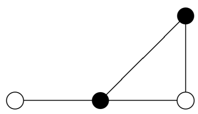
For example:

$$\int d^3 1 d^3 2\, \phi(1)\phi(2) h_c(1, 2) = \bullet\!\!-\!\!\bullet\ . \tag{8}$$

These graphs can be categorized into *different types of diagrams*:

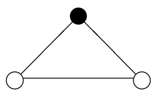
- Nodal diagrams: $N(1, 2)$: contain one or more *nodes* which are internal points through which all paths from one external point to the other must pass.

  Example:

- Non–nodal diagrams: $X(1, 2)$: do not contain any nodes.

  Example:

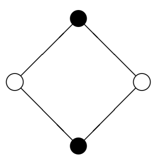
  Nodal diagrams can be constructed from non–nodal diagrams by sticking non–nodal diagrams together which is described by the following equation:

$$\begin{aligned} N(1, 2) &= \int d^3 3\, \rho(3) X(1, 3) X(3, 2) + \int d^3 3 d^3 4\, \rho(3)\rho(4) X(1, 3) X(3, \boldsymbol{r}_4) X(\boldsymbol{r}_4, 2) + \ldots \\ &= \int d^3 3\, \rho(3) X(1, 3) \left[X(3, 2) + N(3, 2)\right] \end{aligned} \tag{9}$$

  This is the Ornstein–Zernicke relation.

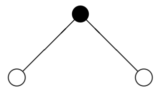
- Composite diagrams: $C(1, 2)$: can be factorized into two or more independent functions of 1 and 2.

  Example:

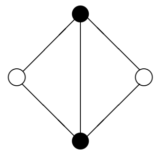
- Simple diagrams: $S_d(1,2)$: are all that can not be factorized.

  Example:



- Elementary diagrams: $E(1,2)$ are those which are neither composite nor nodal.

  Example:



  Therefore it holds that:

$$S_d(1,2) = N(1,2) + E(1,2) \tag{10}$$

From these diagrams we get relations for the pair distribution function which are:

$$\begin{aligned} g(1,2) &= \exp\left[u_2(1,2) + S_d(1,2)\right] && (11) \\ &= \exp\left[u_2(1,2) + N(1,2) + E(1,2)\right] && (12) \\ g(1,2) &= X(1,2) + N(1,2) + 1 && (13) \end{aligned}$$

and these are called HNC equations. From these equations further relations can be derived. In this work we neglect the contribution of the elementary diagrams.

After having expressed the expectation value of the Hamiltonian in terms of physically meaningful quantities, i.e. density and pair distribution function, we vary it with respect to these quantities and obtain a one– and a two–body equation, respectively. These equations can then be solved numerically.

Part II. Theoretical description

2. Definitions and equations

Here is a short summary of some of the important formulas and definitions used in this work.

Notation:

$$\begin{aligned} (\boldsymbol{r}_1, \Omega_1) &\equiv 1 && (14) \\ \int d\boldsymbol{r}_1 d\Omega_1 &\equiv \int d^3 r_1 d\Omega_1 = \int d^3 1 && (15) \\ f(\boldsymbol{r}_1, \boldsymbol{r}_2, \Omega_1, \Omega_2, \dots) &\equiv f(1,2,\dots) && (16) \end{aligned}$$

Normalization integral:

$$I_0 = \int d^3 1 \dots d^3 N \, |\psi_0(1, \dots, N)|^2 \tag{17}$$

One–body density:

$$\rho(1) = \frac{N}{I_0} \int d^3 2 \dots d^3 N \, |\psi_0(1, \dots, N)|^2 \tag{18}$$

Two–body density:

$$\rho(1,2) = \frac{N(N-1)}{I_0} \int d^3 3 \dots d^3 N \, |\psi_0(1, \dots, N)|^2 \tag{19}$$

Pair distribution function:

$$g(1,2) = \frac{\rho(1,2)}{\rho(1)\rho(2)} \tag{20}$$

Energy expectation value:

$$\langle H \rangle = \frac{1}{I_0} \int d^3 1 \dots d^3 N \, \psi_0(1, \dots, N) H \psi_0(1, \dots, N) \tag{21}$$

The following equation is valid for a wave function of the form used below (see [18]).

Born–Green–Yvon (BGY) equation:

$$\boldsymbol{\nabla}_1 u_1(1) = \frac{\boldsymbol{\nabla}_1 \rho(1)}{\rho(1)} - \int d^3 2 \, \rho(2) g(1,2) \boldsymbol{\nabla}_1 u_2(1,2) \tag{22}$$

3. Homogeneous system

In the following we do not specify the geometry of the system. But to give an example: A homogeneous system that we are interested in in this work, is for example a two–dimensional system of dipolar particles.

3.1. Hamiltonian

The Hamiltonian of a homogeneous system of freely rotating dipoles is:

$$H = -\frac{\hbar^2}{2M} \sum_i \nabla_i^2 - \frac{\hbar^2}{2I} \sum_i \Lambda_i^2 + \sum_{i<j} V_{dd}(i,j) \tag{23}$$

with

$$\boldsymbol{\Lambda}_i = \boldsymbol{e}_{\vartheta_i} \frac{\partial}{\partial \vartheta_i} + \boldsymbol{e}_{\varphi_i} \frac{1}{\sin \vartheta_i} \frac{\partial}{\partial \varphi_i}, \tag{24}$$

$$\Lambda_i^2 = \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta_i} \sin \vartheta_i \frac{\partial}{\partial \vartheta_i} + \frac{1}{\sin^2 \vartheta_i} \frac{\partial^2}{\partial \varphi_i^2}, \tag{25}$$

where I is the moment of inertia for one dipole and V_{dd} is the dipole–dipole interaction.

3.2. Ansatz

The ansatz for the wave function we make is:

$$\psi = \prod_{i<j} e^{\frac{1}{2}u(i,j)} = \prod_{i<j} e^{\frac{1}{2}u(\boldsymbol{r}_i-\boldsymbol{r}_j,\Omega_i,\Omega_j)}. \tag{26}$$

3.3. Calculation of $\langle H \rangle$

For the expectation value of the Hamiltonian we get:

$$\begin{aligned}
\langle H \rangle &= \frac{1}{I_0}\int d^3 1 \dots d^3 2N \prod_{i<j} e^{\frac{1}{2}u(i,j)} \left\{-\frac{\hbar^2}{2M}\sum_i \nabla_i^2 - \frac{\hbar^2}{2I}\sum_i \Lambda_i^2 + \sum_{i<j} V_{dd}(i,j)\right\} \prod_{i<j} e^{\frac{1}{2}u(i,j)} && (27)\\
&= \frac{N(N-1)}{2I_0}\int d^3 1 \dots d^3 2N \, |\psi|^2 \left\{-\frac{\hbar^2}{8M}\left(\nabla_1^2+\nabla_2^2\right)u(1,2) - \frac{\hbar^2}{8I}\left(\Lambda_1^2+\Lambda_2^2\right)u(1,2) + V_{dd}(1,2)\right\} && (28)\\
&= \frac{1}{2}\int d^3 1 d^3 2 \, \rho(1,2)\left\{-\frac{\hbar^2}{8M}\left(\nabla_1^2+\nabla_2^2\right) - \frac{\hbar^2}{8I}\left(\Lambda_1^2+\Lambda_2^2\right)\right\} u(1,2) + \frac{1}{2}\int d^3 1 d^3 2 \, \rho(1,2) V_{dd}(1,2) && (29)
\end{aligned}$$

where I_0 is the normalization integral and we used the Jackson–Feenberg Identity

$$F\nabla^2 F = \frac{1}{2}\left(\nabla^2 F^2 + F^2\nabla^2\right) + \frac{1}{2}F^2\left[\boldsymbol{\nabla},\left[\boldsymbol{\nabla},\ln F\right]\right] - \frac{1}{4}\left[\boldsymbol{\nabla},\left[\boldsymbol{\nabla},F^2\right]\right], \tag{30}$$

which is valid for any local Operator F.

3.3.1. Center of mass coordinates

Now we can change to center of mass coordinates

$$\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2 \tag{31}$$

from which follows

$$\begin{aligned}
\int d^3 r_1 d^3 r_2 &\rightarrow V\int d^3 r && (32)\\
-\frac{\hbar^2}{2M}\left(\nabla_1^2+\nabla_2^2\right) &\rightarrow -\frac{\hbar^2}{m}\nabla^2 && (33)
\end{aligned}$$

where $m = 2\mu$ is twice the reduced mass. Because we are dealing with identical particles here $m = M$.

With this we get for $\langle H \rangle$:

$$\begin{aligned}
\frac{\langle H \rangle}{V\rho^2} &= \int d^3 r d\Omega_1 d\Omega_2 \, g(\boldsymbol{r},\Omega_1,\Omega_2)\left\{-\frac{\hbar^2}{8M}\nabla^2 - \frac{\hbar^2}{16I}\left(\Lambda_1^2+\Lambda_2^2\right)\right\} u(\boldsymbol{r},\Omega_1,\Omega_2) && (34)\\
&+ \frac{1}{2}\int d^3 r d\Omega_1 d\Omega_2 \, g(\boldsymbol{r},\Omega_1,\Omega_2) V_{dd}(\boldsymbol{r},\Omega_1,\Omega_2). && (35)
\end{aligned}$$

3.3.2. Rewrite $\langle H \rangle$ in terms of g

By using the HNC equation

$$u(1,2) = \ln(g(1,2)) - N(1,2) \tag{36}$$

we can reformulate $\langle H \rangle$ in terms of the pair distribution function g.

$$\frac{\langle H \rangle}{V\rho^2} = \int d^3r d\Omega_1 d\Omega_2\, g(\boldsymbol{r},\Omega_1,\Omega_2)\left\{-\frac{\hbar^2}{8M}\nabla^2 - \frac{\hbar^2}{16I}\left(\Lambda_1^2+\Lambda_2^2\right)\right\}\ln(g(\boldsymbol{r},\Omega_1,\Omega_2)) \tag{37}$$

$$- \int d^3r d\Omega_1 d\Omega_2\, g(\boldsymbol{r},\Omega_1,\Omega_2)\left\{-\frac{\hbar^2}{8M}\nabla^2 - \frac{\hbar^2}{16I}\left(\Lambda_1^2+\Lambda_2^2\right)\right\}N(\boldsymbol{r},\Omega_1,\Omega_2) \tag{38}$$

$$+ \frac{1}{2}\int d^3r d\Omega_1 d\Omega_2\, g(\boldsymbol{r},\Omega_1,\Omega_2)V_{dd}(\boldsymbol{r},\Omega_1,\Omega_2). \tag{39}$$

and by integrating by parts and using the product rule we finally get:

$$\frac{\langle H \rangle}{V\rho^2} = 4\int d^3r d\Omega_1 d\Omega_2 \left\{\frac{\hbar^2}{8M}|\boldsymbol{\nabla}\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}|^2 + \frac{\hbar^2}{16I}\left(|\boldsymbol{\Lambda}_1\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}|^2 + |\boldsymbol{\Lambda}_2\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}|^2\right)\right\} \tag{40}$$

$$- \int d^3r d\Omega_1 d\Omega_2\, g(\boldsymbol{r},\Omega_1,\Omega_2)\left\{-\frac{\hbar^2}{8M}\nabla^2 - \frac{\hbar^2}{16I}\left(\Lambda_1^2+\Lambda_2^2\right)\right\}N(\boldsymbol{r},\Omega_1,\Omega_2) \tag{41}$$

$$+ \frac{1}{2}\int d^3r d\Omega_1 d\Omega_2\, g(\boldsymbol{r},\Omega_1,\Omega_2)V_{dd}(\boldsymbol{r},\Omega_1,\Omega_2). \tag{42}$$

3.4. Variation

Now we can vary the average of the Hamiltonian with respect to the pair distribution function.

$$\frac{\delta\langle H \rangle}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)} = 0 \tag{43}$$

For the first term (40) we get:

$$\frac{\delta(\text{eqn. (40)})}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)} = \frac{4}{\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)}}\left\{-\frac{\hbar^2}{8M}\nabla'^2 - \frac{\hbar^2}{16I}\left(\Lambda_3^2+\Lambda_4^2\right)\right\}\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)} \tag{44}$$

$$= \frac{4}{\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)}}H_k(\boldsymbol{r}',\Omega_3,\Omega_4)\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)} \tag{45}$$

where we defined

$$H_k(\boldsymbol{r},\Omega_1,\Omega_2) := \left\{-\frac{\hbar^2}{8M}\nabla^2 - \frac{\hbar^2}{16I}\left(\Lambda_1^2+\Lambda_2^2\right)\right\} \tag{46}$$

For the potential term (42) we get:

$$\frac{\delta(\text{eqn. (42)})}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)} = \frac{1}{2}V_{dd}(\boldsymbol{r}',\Omega_3,\Omega_4). \tag{47}$$

The third term (41) gives us two contributions:

$$\frac{\delta(\text{eqn. (41)})}{\delta g(\boldsymbol{r}', \Omega_3, \Omega_4)} = -H_k(\boldsymbol{r}', \Omega_3, \Omega_4) N(\boldsymbol{r}', \Omega_3, \Omega_4) \tag{48}$$

$$- \int d^3 r d\Omega_1 d\Omega_2 \frac{\delta N(\boldsymbol{r}, \Omega_1, \Omega_2)}{\delta g(\boldsymbol{r}', \Omega_3, \Omega_4)} H_k(\boldsymbol{r}, \Omega_1, \Omega_2) g(\boldsymbol{r}, \Omega_1, \Omega_2) \tag{49}$$

To calculate this term we have to calculate the variation of N with respect to g.

3.4.1. Variation of N with respect to g

We use the HNC equation to express N in terms of g and X

$$N(\boldsymbol{r}, \Omega_1, \Omega_2) = (g(\boldsymbol{r}, \Omega_1, \Omega_2) - 1) - X(\boldsymbol{r}, \Omega_1, \Omega_2). \tag{50}$$

After Fourier transforming we obtain

$$\tilde{N}(\boldsymbol{k}, \Omega_1, \Omega_2) = \left(\frac{1}{\rho} S(\boldsymbol{k}, \Omega_1, \Omega_2) - \delta(\Omega_1, \Omega_2)\right) - \tilde{X}(\boldsymbol{k}, \Omega_1, \Omega_2), \tag{51}$$

Where we used the definition of the static structure function

$$S(\boldsymbol{r}, \Omega_1, \Omega_2) = \delta(\boldsymbol{r})\delta(\Omega_1, \Omega_2) + \rho\,(g(\boldsymbol{r}, \Omega_1, \Omega_2) - 1) \tag{52}$$

$$S(\boldsymbol{k}, \Omega_1, \Omega_2) = \rho\delta(\Omega_1, \Omega_2) + \rho FT\,\{g(\boldsymbol{r}, \Omega_1, \Omega_2) - 1\}. \tag{53}$$

To get an expression for X we look at the HNC equation

$$X(\boldsymbol{r}, \Omega_1, \Omega_2) = \int d^3\tilde{r} d\Omega_5\, S^{-1}(\boldsymbol{r}, \Omega_1, \Omega_5)\,(g(\boldsymbol{r} - \tilde{\boldsymbol{r}}, \Omega_5, \Omega_2) - 1) \tag{54}$$

and with the convolution theorem we get for $\tilde{X}(\boldsymbol{k}, \Omega_1, \Omega_2)$:

$$\tilde{X}(\boldsymbol{k}, \Omega_1, \Omega_2) = \frac{1}{\rho} \int d\Omega_5\, S^{-1}(\boldsymbol{k}, \Omega_1, \Omega_5) \left(\frac{1}{\rho} S(\boldsymbol{k}, \Omega_5, \Omega_2) - \delta(\Omega_5, \Omega_2)\right) \tag{55}$$

$$= \delta(\Omega_1, \Omega_2) - \frac{1}{\rho} S^{-1}(\boldsymbol{k}, \Omega_1, \Omega_2). \tag{56}$$

Where we used the defining equation for S^{-1}, which is

$$\int d^3 r' d\Omega_3\, S^{-1}(\boldsymbol{r}, \Omega_1, \Omega_3) S(\boldsymbol{r} - \boldsymbol{r}', \Omega_3, \Omega_2) = \delta(\boldsymbol{r})\delta(\Omega_1, \Omega_2) \tag{57}$$

in real space and therefore after using the convolution theorem we get for the Fourier transform

$$\frac{1}{\rho} \int d\Omega_3\, S^{-1}(\boldsymbol{k}, \Omega_1, \Omega_3) S(\boldsymbol{k}, \Omega_3, \Omega_2) = \rho\delta(\Omega_1, \Omega_2). \tag{58}$$

We know that

$$\frac{\delta S(\boldsymbol{k},\Omega_1,\Omega_2)}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)} = \frac{\delta}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)}\left\{\rho\delta(\Omega_1,\Omega_2)+\rho^2\int d^3r\, e^{i\boldsymbol{kr}}\left(g(\boldsymbol{r},\Omega_1,\Omega_2)-1\right)\right\} \tag{59}$$

$$= \rho^2\int d^3r\, e^{i\boldsymbol{kr}}\delta(\boldsymbol{r},\boldsymbol{r}')\delta(\Omega_1,\Omega_3)\delta(\Omega_2,\Omega_4) \tag{60}$$

$$= \rho^2\, e^{i\boldsymbol{kr}'}\delta(\Omega_1,\Omega_3)\delta(\Omega_2,\Omega_4). \tag{61}$$

What we also need is the variation of S^{-1} with respect to g. To get this we again look at the defining equation for S^{-1} (58):

$$0 = \frac{\delta}{\delta g(\boldsymbol{r},\Omega_4,\Omega_5)}\frac{1}{\rho}\int d\Omega_3\, S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)S(\boldsymbol{k},\Omega_3,\Omega_2) \tag{62}$$

$$0 = \frac{1}{\rho}\int d\Omega_3\, S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\frac{\delta S(\boldsymbol{k},\Omega_3,\Omega_2)}{\delta g(\boldsymbol{r},\Omega_4,\Omega_5)}+\frac{1}{\rho}\int d\Omega_3\, S(\boldsymbol{k},\Omega_3,\Omega_2)\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)}{\delta g(\boldsymbol{r},\Omega_4,\Omega_5)}. \tag{63}$$

Now we use equation (61) and act with $\int d\Omega_2\, S^{-1}(\boldsymbol{k},\Omega_6,\Omega_2)$ on both sides of the above equation to obtain

$$\int d\Omega_3\, \rho\delta(\Omega_3,\Omega_6)\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)}{\delta g(\boldsymbol{r},\Omega_4,\Omega_5)} = -\rho\int d\Omega_2 d\Omega_3\, S^{-1}(\boldsymbol{k},\Omega_6,\Omega_2)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)e^{i\boldsymbol{kr}}\delta(\Omega_3,\Omega_4)\delta(\Omega_2,\Omega_5) \tag{64}$$

which finally leads to the desired relation:

$$\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_2)}{\delta g(\boldsymbol{r},\Omega_3,\Omega_4)} = -e^{i\boldsymbol{kr}}S^{-1}(\boldsymbol{k},\Omega_2,\Omega_4)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3) \tag{65}$$

With this we get

$$\frac{\delta N(\boldsymbol{r},\Omega_1,\Omega_2)}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)} = \frac{\delta}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)}\frac{1}{\rho}\int d^3k\, e^{-i\boldsymbol{kr}}\tilde{N}(\boldsymbol{k},\Omega_1,\Omega_2) \tag{66}$$

$$= \frac{\delta}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)}\frac{1}{\rho}\int d^3k\, e^{-i\boldsymbol{kr}}\left[\frac{1}{\rho}S(\boldsymbol{k},\Omega_1,\Omega_2)-2\delta(\Omega_1,\Omega_2)+\frac{1}{\rho}S^{-1}(\boldsymbol{k},\Omega_1,\Omega_2)\right] \tag{67}$$

$$= \frac{1}{\rho}\int d^3k\, e^{-i\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}\left(\rho\delta(\Omega_1,\Omega_3)\delta(\Omega_2,\Omega_4)-\frac{1}{\rho}S^{-1}(\boldsymbol{k},\Omega_2,\Omega_4)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\right). \tag{68}$$

Now let us define a new function

$$a(\boldsymbol{r}-\boldsymbol{r}',\Omega_1,\Omega_2,\Omega_3,\Omega_4) := \frac{1}{\rho}\int d^3k\, e^{-i\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}\left(\rho\delta(\Omega_1,\Omega_3)\delta(\Omega_2,\Omega_4)-\frac{1}{\rho}S^{-1}(\boldsymbol{k},\Omega_2,\Omega_4)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\right) \tag{69}$$

With this the variation of the third term (41) becomes:

$$\frac{\delta(\text{eqn. (41)})}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)} = -H_k(\boldsymbol{r}',\Omega_3,\Omega_4)N(\boldsymbol{r}',\Omega_3,\Omega_4) \tag{70}$$

$$- \int d^3r d\Omega_1 d\Omega_2\, a(\boldsymbol{r}-\boldsymbol{r}',\Omega_1,\Omega_2,\Omega_3,\Omega_4)H_k(\boldsymbol{r},\Omega_1,\Omega_2)g(\boldsymbol{r},\Omega_1,\Omega_2) \tag{71}$$

Finally we can rewrite this to obtain:

$$\frac{\delta(\text{eqn. (41)})}{\delta g(\boldsymbol{r}', \Omega_3, \Omega_4)} = -H_k(\boldsymbol{r}', \Omega_3, \Omega_4) N(\boldsymbol{r}', \Omega_3, \Omega_4) \quad (72)$$

$$- \left[H_k g * a\right](\boldsymbol{r}', \Omega_3, \Omega_4) \quad (73)$$

where the convolution asterisk $*$ represents the following operation

$$\left[f * g\right](\boldsymbol{r}, \Omega_3, \Omega_4) = \int d^3\tilde{r} d\Omega_1 d\Omega_2 \; f(\boldsymbol{r}, \Omega_1, \Omega_2) g(\boldsymbol{r} - \tilde{\boldsymbol{r}}, \Omega_1, \Omega_2, \Omega_3, \Omega_4). \quad (74)$$

This leads to the final form of our two–body equation:

$$0 = \frac{1}{2} V_{dd}(\boldsymbol{r}, \Omega_1, \Omega_2) + \frac{4}{\sqrt{g(\boldsymbol{r}, \Omega_1, \Omega_2)}} H_k(\boldsymbol{r}, \Omega_1, \Omega_2) \sqrt{g(\boldsymbol{r}, \Omega_1, \Omega_2)} \quad (75)$$

$$- H_k(\boldsymbol{r}, \Omega_1, \Omega_2) N(\boldsymbol{r}, \Omega_1, \Omega_2) - \left[H_k g * a\right](\boldsymbol{r}, \Omega_1, \Omega_2) \quad (76)$$

3.4.2. Alternative formulation

An alternative formulation of the two–body equation (76) can be obtained by Fourier transforming to get rid of the convolution in the last term and of the space derivatives.

To do so we first reformulate the last term

$$\begin{aligned}
&\int d^3r d\Omega_3 d\Omega_4 \, a(\boldsymbol{r} - \boldsymbol{r}', \Omega_3, \Omega_4, \Omega_1, \Omega_2) H_k(\boldsymbol{r}, \Omega_3, \Omega_4) \left(g(\boldsymbol{r}, \Omega_3, \Omega_4) - 1\right) \\
&= \int d^3r d\Omega_3 d\Omega_4 \left[H_k(\boldsymbol{r}, \Omega_3, \Omega_4) \frac{1}{\rho} \int d^3k \, e^{-i\boldsymbol{k}\boldsymbol{r}} \left(\frac{1}{\rho} S(\boldsymbol{k}, \Omega_3, \Omega_4) - \delta(\Omega_3, \Omega_4)\right)\right] \frac{1}{\rho} \int d^3k' \, e^{-i\boldsymbol{k}'(\boldsymbol{r}-\boldsymbol{r}')} \tilde{a}(\boldsymbol{k}', \Omega_3, \Omega_4, \Omega_1, \Omega_2) \\
&= \frac{1}{\rho^2} \int d^3r d\Omega_3 d\Omega_4 d^3k d^3k' \, e^{-i(\boldsymbol{k}+\boldsymbol{k}')\boldsymbol{r}} e^{i\boldsymbol{k}'\boldsymbol{r}'} \left[\tilde{H}_k(\boldsymbol{k}, \Omega_3, \Omega_4) \left(\frac{1}{\rho} S(\boldsymbol{k}, \Omega_3, \Omega_4) - \delta(\Omega_3, \Omega_4)\right)\right] \tilde{a}(\boldsymbol{k}', \Omega_3, \Omega_4, \Omega_1, \Omega_2) \quad (77)
\end{aligned}$$

where we defined

$$\tilde{H}_k(\boldsymbol{k}, \Omega_1, \Omega_2) := \left\{\frac{\hbar^2 k^2}{8M} - \frac{\hbar^2}{16I}\left(\Lambda_1^2 + \Lambda_2^2\right)\right\} \quad (78)$$

and used that

$$H_k(\boldsymbol{r}, \Omega_1, \Omega_2) g(\boldsymbol{r}, \Omega_1, \Omega_2) = H_k(\boldsymbol{r}, \Omega_1, \Omega_2) \left(g(\boldsymbol{r}, \Omega_1, \Omega_2) - 1\right). \quad (79)$$

We know that

$$\int d^3r \, e^{-i(\boldsymbol{k}+\boldsymbol{k}')\boldsymbol{r}} = \delta(\boldsymbol{k} + \boldsymbol{k}') \quad (80)$$

and if we use this and the fact that

$$\tilde{a}(-\boldsymbol{k}, \Omega_1, \Omega_2, \Omega_3, \Omega_4) = \tilde{a}(\boldsymbol{k}, \Omega_1, \Omega_2, \Omega_3, \Omega_4) \quad \text{because} \quad a(\boldsymbol{r} - \boldsymbol{r}', \Omega_1, \Omega_2, \Omega_3, \Omega_4) = a(\boldsymbol{r}' - \boldsymbol{r}, \Omega_1, \Omega_2, \Omega_3, \Omega_4) \quad (81)$$

we get for the last term of equation (76):

$$\begin{aligned} &\tfrac{1}{\rho^2} \int d^3k d\Omega_3 d\Omega_4\, e^{-i\boldsymbol{k}\boldsymbol{r}} \left[\tilde{H}_k(\boldsymbol{k},\Omega_3,\Omega_4)\left(\frac{1}{\rho}S(\boldsymbol{k},\Omega_3,\Omega_4)-\delta(\Omega_3,\Omega_4)\right)\right]\tilde{a}(\boldsymbol{k},\Omega_3,\Omega_4,\Omega_1,\Omega_2) \\ = \;& \frac{1}{\rho}FT^{-1}\left\{\int d\Omega_3 d\Omega_4 \left[\tilde{H}_k(\boldsymbol{k},\Omega_3,\Omega_4)\left(\frac{1}{\rho}S(\boldsymbol{k},\Omega_3,\Omega_4)-\delta(\Omega_3,\Omega_4)\right)\right]\tilde{a}(\boldsymbol{k},\Omega_3,\Omega_4,\Omega_1,\Omega_2)\right\}. \end{aligned} \tag{82}$$

We can perform similar manipulations to rewrite the second to last term of equation (76) and with this our new formulation of the two–body equation becomes:

$$0 = \frac{1}{2}g(\boldsymbol{r},\Omega_1,\Omega_2)V_{dd}(\boldsymbol{r},\Omega_1,\Omega_2) + 4\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}H_k(\boldsymbol{r},\Omega_1,\Omega_2)\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)} \tag{83}$$

$$- g(\boldsymbol{r},\Omega_1,\Omega_2)FT^{-1}\left\{\tilde{H}_k(\boldsymbol{k},\Omega_1,\Omega_2)\tilde{N}(\boldsymbol{k},\Omega_1,\Omega_2)\right\} \tag{84}$$

$$- \frac{1}{\rho}g(\boldsymbol{r},\Omega_1,\Omega_2)FT^{-1}\left\{\int d\Omega_3 d\Omega_4 \left[\tilde{H}_k(\boldsymbol{k},\Omega_3,\Omega_4)\left(\frac{1}{\rho}S(\boldsymbol{k},\Omega_3,\Omega_4)-\delta(\Omega_3,\Omega_4)\right)\right]\tilde{a}(\boldsymbol{k},\Omega_3,\Omega_4,\Omega_1,\Omega_2)\right\} \tag{85}$$

where we additionally multiplied the whole equation with $g(\boldsymbol{r},\Omega_1,\Omega_2)$.

4. Additional external field

If we additionally have an external field that acts on the dipole moments only, like for example an electric or magnetic field, we get an additional term in the Hamiltonian.

The new Hamiltonian looks as follows:

$$H = -\frac{\hbar^2}{2M}\sum_i \nabla_i^2 - \frac{\hbar^2}{2I}\sum_i \Lambda_i^2 + \sum_i U_{ext}(\Omega_i) + \sum_{i<j} V_{dd}(i,j). \tag{86}$$

The density in coordinate space is still constant, since the external potential does not affect the particle coordinates. But the density in angular space, corresponding to the dipole moment distribution of one particle, is not constant, since the external potential influences the orientation of the dipole moments. Therefore we need an additional one–body term in our ansatz that depends on the dipolar angle.

4.1. Ansatz

The new ansatz looks as follows:

$$\psi = \prod_i e^{\frac{1}{2}u(i)} \prod_{i<j} e^{\frac{1}{2}u(i,j)} = \prod_i e^{\frac{1}{2}u(\Omega_i)} \prod_{i<j} e^{\frac{1}{2}u(\boldsymbol{r}_i-\boldsymbol{r}_j,\Omega_i,\Omega_j)}. \tag{87}$$

The density is given by

$$\rho(i) = \rho_0\,\rho(\Omega_i) \qquad \text{with} \qquad \rho_0 = \frac{N}{V}. \tag{88}$$

4.2. Calculation of $\langle H\rangle$

The expectation value of the potential energy is given by

$$\begin{aligned}\langle U\rangle &= \frac{1}{I_0}\int d^3 1\ldots d^3 2N \prod_i e^{\frac{1}{2}u(\Omega_i)}\prod_{i<j} e^{\frac{1}{2}u(\boldsymbol{r}_i-\boldsymbol{r}_j,\Omega_i,\Omega_j)}\left\{\sum_k U_{ext}(\Omega_k)+\sum_{l<m}V_{dd}(l,m)\right\}\prod_i e^{\frac{1}{2}u(\Omega_i)}\prod_{i<j} e^{\frac{1}{2}u(\boldsymbol{r}_i-\boldsymbol{r}_j,\Omega_i,\Omega_j)}\\ &= \int d^3 1\,\rho(1)U_{ext}(\Omega_1)+\frac{1}{2}\int d^3 1 d^3 2\,\rho(1,2)V_{dd}(1,2) \qquad (89)\\ &= V\rho_0\int d^3\Omega_1\,\rho(\Omega_1)U_{ext}(\Omega_1)+\frac{1}{2}V\rho_0^2\int d^3 r d^3\Omega_1 d^3\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)g(\boldsymbol{r},\Omega_1,\Omega_2)V_{dd}(\boldsymbol{r},\Omega_1,\Omega_2) \qquad (90)\end{aligned}$$

where we used the definition of the one– and two–body density (18) and (19), respectively and introduced center of mass coordinates (see section 3.3.1).

The expectation value of the kinetic energy operator is almost the same as for the homogeneous case, since the one–body correlation function in the ansatz does not depend on the spatial coordinate. The expectation value is given by

$$\begin{aligned}\langle T\rangle &= \frac{1}{I_0}\int d^3 1\ldots d^3 2N \prod_i e^{\frac{1}{2}u(\Omega_i)}\prod_{i<j} e^{\frac{1}{2}u(\boldsymbol{r}_i-\boldsymbol{r}_j,\Omega_i,\Omega_j)}\left\{-\frac{\hbar^2}{2M}\sum_i\nabla_i^2\right\}\prod_i e^{\frac{1}{2}u(\Omega_i)}\prod_{i<j} e^{\frac{1}{2}u(\boldsymbol{r}_i-\boldsymbol{r}_j,\Omega_i,\Omega_j)} \qquad (91)\\ &= \frac{N(N-1)}{2I_0}\int d^3 1\ldots d^3 2N\,|\psi|^2\left\{-\frac{\hbar^2}{8M}\left(\nabla_1^2+\nabla_2^2\right)u(1,2)\right\} \qquad (92)\\ &= -\frac{\hbar^2}{16M}\int d^3 1 d^3 2\,\rho(1,2)\left(\nabla_1^2+\nabla_2^2\right)u(1,2) \qquad (93)\\ &= -\frac{\hbar^2}{8M}V\rho_0^2\int d^3 r d\Omega_1 d^3\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)g(\boldsymbol{r},\Omega_1,\Omega_2)\nabla^2 u(\boldsymbol{r},\Omega_1,\Omega_2) \qquad (94)\\ &= \frac{\hbar^2}{8M}V\rho_0^2\int d^3 r d\Omega_1 d\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)\left\{4|\boldsymbol{\nabla}\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}|^2+g(\boldsymbol{r},\Omega_1,\Omega_2)\nabla^2 N(\boldsymbol{r},\Omega_1,\Omega_2)\right\} \qquad (95)\end{aligned}$$

where we already reformulated it in terms of the pair distribution function g and introduced center of mass coordinates.

Next we calculate the expectation value of the kinetic energy operator for the rotations

$$\langle R\rangle = \frac{1}{I_0}\int d^3 1\ldots d^3 2N \prod_i e^{\frac{1}{2}u(\Omega_i)}\prod_{i<j} e^{\frac{1}{2}u(\boldsymbol{r}_i-\boldsymbol{r}_j,\Omega_i,\Omega_j)}\left\{-\frac{\hbar^2}{2I}\sum_i\Lambda_i^2\right\}\prod_i e^{\frac{1}{2}u(\Omega_i)}\prod_{i<j} e^{\frac{1}{2}u(\boldsymbol{r}_i-\boldsymbol{r}_j,\Omega_i,\Omega_j)}. \qquad (96)$$

If we do so, we get two terms, one for the one–body correlation function and one for the two–body correlation function

$$\begin{aligned}
\langle R\rangle &= -\frac{\hbar^2}{8I}\int d^3 1\ldots d^3 2N|\psi|^2\left\{\frac{N}{I_0}\Lambda_1^2 u(\Omega_1)+\frac{N(N-1)}{2I_0}\left(\Lambda_1^2+\Lambda_2^2\right)u(1,2)\right\} \quad (97)\\
&= -\frac{\hbar^2}{8I}\left\{\int d^3 1\,\rho(1)\Lambda_1^2 u(1)+\frac{1}{2}\int d^3 1 d^3 2\,\rho(1,2)\left(\Lambda_1^2+\Lambda_2^2\right)u(1,2)\right\} \quad (98)\\
&= -\frac{\hbar^2}{8I}V\rho_0\left\{\int d\Omega_1\,\rho(\Omega_1)\Lambda_1^2 u(\Omega_1)+\frac{\rho_0}{2}\int d^3 r d\Omega_1 d\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)g(\boldsymbol{r},\Omega_1,\Omega_2)\left(\Lambda_1^2+\Lambda_2^2\right)u(\boldsymbol{r},\Omega_1,\Omega_2)\right\}\\
&= -\frac{\hbar^2}{8I}V\rho_0\left\{\underbrace{-\int d\Omega_1\ (\boldsymbol{\Lambda}_1\rho(\Omega_1))\,\boldsymbol{\Lambda}_1 u(\Omega_1)}_{①}+\frac{\rho_0}{2}\int d^3 r d\Omega_1 d\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)g(\boldsymbol{r},\Omega_1,\Omega_2)\left(\Lambda_1^2+\Lambda_2^2\right)u(\boldsymbol{r},\Omega_1,\Omega_2)\right\}
\end{aligned}$$

where we integrated by parts once.

We continue by reformulating the first term ① of the last line of the above equation by using a variation of the BGY–equation (22) that holds for the rotation operator:

$$\boldsymbol{\Lambda}_1 u(\Omega_1)=\frac{\boldsymbol{\Lambda}_1\rho(\Omega_1)}{\rho(\Omega_1)}-\int d^3 r d\Omega_2\,\rho_0\rho(\Omega_2)g(\boldsymbol{r},\Omega_1,\Omega_2)\boldsymbol{\Lambda}_1 u(\boldsymbol{r},\Omega_1,\Omega_2). \quad (99)$$

With this we get

$$\begin{aligned}
① &= -\int d\Omega_1\,\frac{(\boldsymbol{\Lambda}_1\rho(\Omega_1))^2}{\rho(\Omega_1)}+\rho_0\int d^3 r d\Omega_1 d\Omega_2\ (\boldsymbol{\Lambda}_1\rho(\Omega_1))\,\rho(\Omega_2)g(\boldsymbol{r},\Omega_1,\Omega_2)\boldsymbol{\Lambda}_1 u(\boldsymbol{r},\Omega_1,\Omega_2) \quad (100)\\
&= -\int d\Omega_1\,\frac{(\boldsymbol{\Lambda}_1\rho(\Omega_1))^2}{\rho(\Omega_1)}+\frac{\rho_0}{2}\int d^3 r d\Omega_1 d\Omega_2\ (\boldsymbol{\Lambda}_1\rho(\Omega_1))\,\rho(\Omega_2)g(\boldsymbol{r},\Omega_1,\Omega_2)\boldsymbol{\Lambda}_1 u(\boldsymbol{r},\Omega_1,\Omega_2) \quad (101)\\
&+ \frac{\rho_0}{2}\int d^3 r d\Omega_1 d\Omega_2\ (\boldsymbol{\Lambda}_2\rho(\Omega_2))\,\rho(\Omega_1)g(\boldsymbol{r},\Omega_1,\Omega_2)\boldsymbol{\Lambda}_2 u(\boldsymbol{r},\Omega_1,\Omega_2) \quad (102)
\end{aligned}$$

where we used the pair–symmetry, which means that all two–particle quantities are symmetric under exchange of the two particle coordinates, to get from the first to the second line.

We know that

$$(\boldsymbol{\Lambda}\rho)\boldsymbol{\Lambda}u_2+\rho\boldsymbol{\Lambda}^2 u_2=\boldsymbol{\Lambda}\rho\boldsymbol{\Lambda}u_2 \qquad \text{and} \qquad |\boldsymbol{\Lambda}\ln\rho|^2=\rho^{-2}(\boldsymbol{\Lambda}\rho)^2 \quad (103)$$

therefore we obtain for the expectation value

$$\begin{aligned}
\langle R\rangle &= \frac{\hbar^2}{8I}V\rho_0\int d\Omega_1\,\rho(\Omega_1)|\boldsymbol{\Lambda}_1\ln\rho(\Omega_1)|^2 \quad (104)\\
&- \frac{\hbar^2 V\rho_0^2}{16I}\underbrace{\int d^3 r d\Omega_1 d\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)g(\boldsymbol{r},\Omega_1,\Omega_2)\left(\frac{1}{\rho(\Omega_1)}\boldsymbol{\Lambda}_1\rho(\Omega_1)\boldsymbol{\Lambda}_1+\frac{1}{\rho(\Omega_2)}\boldsymbol{\Lambda}_2\rho(\Omega_2)\boldsymbol{\Lambda}_2\right)u(\boldsymbol{r},\Omega_1,\Omega_2)}_{②}.
\end{aligned}$$

The next step is to reformulate the second term of this expression in terms of the pair distribution function and we do so by using the HNC equation

$$u(\boldsymbol{r},\Omega_1,\Omega_2)=\ln(g(\boldsymbol{r},\Omega_1,\Omega_2))-N(\boldsymbol{r},\Omega_1,\Omega_2) \quad (105)$$

and inserting it in the above equation.

$$\begin{aligned} \text{(II)} &= \int d^3r d\Omega_1 d\Omega_2\, \rho(\Omega_1)\rho(\Omega_2) g(\boldsymbol{r},\Omega_1,\Omega_2)\left(\frac{1}{\rho(\Omega_1)}\boldsymbol{\Lambda}_1\rho(\Omega_1)\boldsymbol{\Lambda}_1 + \frac{1}{\rho(\Omega_2)}\boldsymbol{\Lambda}_2\rho(\Omega_2)\boldsymbol{\Lambda}_2\right)\ln(g(\boldsymbol{r},\Omega_1,\Omega_2)) \\ &- \int d^3r d\Omega_1 d\Omega_2\, \rho(\Omega_1)\rho(\Omega_2) g(\boldsymbol{r},\Omega_1,\Omega_2)\left(\frac{1}{\rho(\Omega_1)}\boldsymbol{\Lambda}_1\rho(\Omega_1)\boldsymbol{\Lambda}_1 + \frac{1}{\rho(\Omega_2)}\boldsymbol{\Lambda}_2\rho(\Omega_2)\boldsymbol{\Lambda}_2\right)N(\boldsymbol{r},\Omega_1,\Omega_2) \quad (106) \end{aligned}$$

Now we integrate by parts and use

$$\left|\boldsymbol{\Lambda}\sqrt{g}\right|^2 = \frac{1}{4}\frac{(\boldsymbol{\Lambda}g)^2}{g} \quad (107)$$

to obtain

$$\begin{aligned} \text{(II)} = &- 4\int d^3r d\Omega_1 d\Omega_2\, \rho(\Omega_1)\rho(\Omega_2)\left(\left|\boldsymbol{\Lambda}_1\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}\right|^2 + \left|\boldsymbol{\Lambda}_2\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}\right|^2\right) \quad (108) \\ &- \int d^3r d\Omega_1 d\Omega_2\, \rho(\Omega_1)\rho(\Omega_2) N(\boldsymbol{r},\Omega_1,\Omega_2)\left(\frac{1}{\rho(\Omega_1)}\boldsymbol{\Lambda}_1\rho(\Omega_1)\boldsymbol{\Lambda}_1 + \frac{1}{\rho(\Omega_2)}\boldsymbol{\Lambda}_2\rho(\Omega_2)\boldsymbol{\Lambda}_2\right)g(\boldsymbol{r},\Omega_1,\Omega_2). \end{aligned}$$

The final result for the expectation value of the rotational energy is

$$\begin{aligned} \langle R\rangle &= \frac{\hbar^2}{8I}V\rho_0\int d\Omega_1\, \rho(\Omega_1)|\boldsymbol{\Lambda}_1\ln\rho(\Omega_1)|^2 \quad (109) \\ &+ \frac{\hbar^2 V\rho_0^2}{4I}\int d^3r d\Omega_1 d\Omega_2\, \rho(\Omega_1)\rho(\Omega_2)\left(\left|\boldsymbol{\Lambda}_1\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}\right|^2 + \left|\boldsymbol{\Lambda}_2\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}\right|^2\right) \\ &+ \frac{\hbar^2 V\rho_0^2}{16I}\int d^3r d\Omega_1 d\Omega_2\, \rho(\Omega_1)\rho(\Omega_2) N(\boldsymbol{r},\Omega_1,\Omega_2)\left(\frac{1}{\rho(\Omega_1)}\boldsymbol{\Lambda}_1\rho(\Omega_1)\boldsymbol{\Lambda}_1 + \frac{1}{\rho(\Omega_2)}\boldsymbol{\Lambda}_2\rho(\Omega_2)\boldsymbol{\Lambda}_2\right)g(\boldsymbol{r},\Omega_1,\Omega_2), \end{aligned}$$

and with this we get for $\langle H\rangle$:

$$\begin{aligned} \langle H\rangle &= V\rho_0\int d^3\Omega_1\, \rho(\Omega_1)U_{ext}(\Omega_1) + \frac{1}{2}V\rho_0^2\int d^3r d^3\Omega_1 d^3\Omega_2\, \rho(\Omega_1)\rho(\Omega_2)g(\boldsymbol{r},\Omega_1,\Omega_2)V_{dd}(\boldsymbol{r},\Omega_1,\Omega_2) \quad (110) \\ &+ \frac{\hbar^2}{8M}V\rho_0^2\int d^3r d\Omega_1 d\Omega_2\, \rho(\Omega_1)\rho(\Omega_2)\left\{4|\boldsymbol{\nabla}\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}|^2 + g(\boldsymbol{r},\Omega_1,\Omega_2)\nabla^2 N(\boldsymbol{r},\Omega_1,\Omega_2)\right\} \\ &+ \frac{\hbar^2}{8I}V\rho_0\int d\Omega_1\, \rho(\Omega_1)|\boldsymbol{\Lambda}_1\ln\rho(\Omega_1)|^2 \\ &+ \frac{\hbar^2 V\rho_0^2}{4I}\int d^3r d\Omega_1 d\Omega_2\, \rho(\Omega_1)\rho(\Omega_2)\left(\left|\boldsymbol{\Lambda}_1\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}\right|^2 + \left|\boldsymbol{\Lambda}_2\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}\right|^2\right) \\ &+ \frac{\hbar^2 V\rho_0^2}{16I}\int d^3r d\Omega_1 d\Omega_2\, \rho(\Omega_1)\rho(\Omega_2) N(\boldsymbol{r},\Omega_1,\Omega_2)\left(\frac{1}{\rho(\Omega_1)}\boldsymbol{\Lambda}_1\rho(\Omega_1)\boldsymbol{\Lambda}_1 + \frac{1}{\rho(\Omega_2)}\boldsymbol{\Lambda}_2\rho(\Omega_2)\boldsymbol{\Lambda}_2\right)g(\boldsymbol{r},\Omega_1,\Omega_2). \end{aligned}$$

4.3. Variation

Our independent variables are the pair distribution function g and the density ρ and we vary the expectation value of the Hamiltonian with respect to these two quantities to obtain the two–body equation and the one–body equation respectively.

4.3.1. Two–body equation

We obtain the two–body equation by varying the expectation value of the Hamiltonian with respect to the pair distribution function

$$\frac{\delta \langle H\rangle}{\delta g(\boldsymbol{r}', \Omega_3, \Omega_4)} = 0. \tag{111}$$

The variation of $\langle U\rangle$ and $\langle K\rangle$ is similar to the variation performed in section 3.4, except for some density–factors.

For the potential energy we instantly obtain

$$\frac{\delta \langle U\rangle}{\delta g(\boldsymbol{r}', \Omega_3, \Omega_4)} = \frac{1}{2} V\rho_0^2 \rho(\Omega_3)\rho(\Omega_4) V_{dd}(\boldsymbol{r}', \Omega_3, \Omega_4). \tag{112}$$

Next we calculate the variation of the kinetic energy

$$\begin{aligned}
\frac{\delta \langle T\rangle}{\delta g(\boldsymbol{r}', \Omega_3, \Omega_4)} &= \frac{\hbar^2}{8M} V\rho_0^2 \frac{\delta}{\delta g(\boldsymbol{r}', \Omega_3, \Omega_4)} \int d^3 r d\Omega_1 d\Omega_2\, \rho(\Omega_1)\rho(\Omega_2) \left\{4|\boldsymbol{\nabla} \sqrt{g(\boldsymbol{r}, \Omega_1, \Omega_2)}|^2 + g(\boldsymbol{r}, \Omega_1, \Omega_2)\nabla^2 N(\boldsymbol{r}, \Omega_1, \Omega_2)\right\} \\
&= \frac{\hbar^2}{8M} V\rho_0^2 \rho(\Omega_3)\rho(\Omega_4) \left\{ \frac{-4}{\sqrt{g(\boldsymbol{r}', \Omega_3, \Omega_4)}} \nabla'^2 \sqrt{g(\boldsymbol{r}', \Omega_3, \Omega_4)} + \nabla'^2 N(\boldsymbol{r}', \Omega_3, \Omega_4) \right\} && (113) \\
&+ \frac{\hbar^2}{8M} V\rho_0^2 \int d^3 r d\Omega_1 d\Omega_2\, \rho(\Omega_1)\rho(\Omega_2) \frac{\delta N(\boldsymbol{r}, \Omega_1, \Omega_2)}{\delta g(\boldsymbol{r}', \Omega_3, \Omega_4)} \nabla^2 g(\boldsymbol{r}, \Omega_1, \Omega_2). && (114)
\end{aligned}$$

To complete this calculation we need the variation of N with respect to g.

Variation of N with respect to g:

We follow the same procedure as for the homogeneous case:

We start by using the HNC equation to express N in terms of g and X which is exactly the same for the inhomogeneous and the homogeneous case

$$N(\boldsymbol{r}, \Omega_1, \Omega_2) = (g(\boldsymbol{r}, \Omega_1, \Omega_2) - 1) - X(\boldsymbol{r}, \Omega_1, \Omega_2). \tag{115}$$

The definition of the static structure function is different in the inhomogeneous case, namely

$$\begin{aligned}
S(\boldsymbol{r}, \Omega_1, \Omega_2) &= \delta(\boldsymbol{r})\delta(\Omega_1, \Omega_2) + \rho_0 \sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}\,(g(\boldsymbol{r}, \Omega_1, \Omega_2) - 1) && (116) \\
S(\boldsymbol{k}, \Omega_1, \Omega_2) &= \rho_0 \delta(\Omega_1, \Omega_2) + \rho_0 \sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)} FT\{g(\boldsymbol{r}, \Omega_1, \Omega_2) - 1\}. && (117)
\end{aligned}$$

Therefore the Fourier transform of the HNC equation is given by

$$\tilde{N}(\boldsymbol{k}, \Omega_1, \Omega_2) = \frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}} \left(\frac{1}{\rho_0} S(\boldsymbol{k}, \Omega_1, \Omega_2) - \delta(\Omega_1, \Omega_2) \right) - \tilde{X}(\boldsymbol{k}, \Omega_1, \Omega_2). \tag{118}$$

Now we need an expression for X which we get from the HNC equation

$$\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)} X(\boldsymbol{r}, \Omega_1, \Omega_2) = \int d^3\tilde{r} d\Omega_5\, S^{-1}(\boldsymbol{r}, \Omega_1, \Omega_5) \sqrt{\rho(\Omega_5)}\sqrt{\rho(\Omega_2)}\,(g(\boldsymbol{r} - \tilde{\boldsymbol{r}}, \Omega_5, \Omega_2) - 1) \tag{119}$$

and we use the convolution theorem to get for $\tilde{X}(\boldsymbol{k},\Omega_1,\Omega_2)$:

$$\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}\tilde{X}(\boldsymbol{k},\Omega_1,\Omega_2) = \frac{1}{\rho_0}\int d\Omega_5\, S^{-1}(\boldsymbol{k},\Omega_1,\Omega_5)\left(\frac{1}{\rho_0}S(\boldsymbol{k},\Omega_5,\Omega_2)-\delta(\Omega_5,\Omega_2)\right) \quad (120)$$

$$\tilde{X}(\boldsymbol{k},\Omega_1,\Omega_2) = \frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}}\left(\delta(\Omega_1,\Omega_2)-\frac{1}{\rho_0}S^{-1}(\boldsymbol{k},\Omega_1,\Omega_2)\right). \quad (121)$$

Where we used the defining equation for S^{-1} (57) which is, in Fourier space,

$$\frac{1}{\rho_0}\int d\Omega_3\, S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)S(\boldsymbol{k},\Omega_3,\Omega_2) = \rho_0\delta(\Omega_1,\Omega_2). \quad (122)$$

Next we need the variation of S:

$$\frac{\delta S(\boldsymbol{k},\Omega_1,\Omega_2)}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)} = \frac{\delta}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)}\left\{\rho_0\delta(\Omega_1,\Omega_2)+\rho_0^2\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}\int d^3r\, e^{i\boldsymbol{k}\boldsymbol{r}}\left(g(\boldsymbol{r},\Omega_1,\Omega_2)-1\right)\right\} \quad (123)$$

$$= \rho_0^2\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}\int d^3r\, e^{i\boldsymbol{k}\boldsymbol{r}}\delta(\boldsymbol{r},\boldsymbol{r}')\delta(\Omega_1,\Omega_3)\delta(\Omega_2,\Omega_4) \quad (124)$$

$$= \rho_0^2 e^{i\boldsymbol{k}\boldsymbol{r}'}\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}\delta(\Omega_1,\Omega_3)\delta(\Omega_2,\Omega_4), \quad (125)$$

and the variation of S^{-1} with respect to g. To do so we use the defining equation for S^{-1} (122):

$$0 = \frac{\delta}{\delta g(\boldsymbol{r},\Omega_4,\Omega_5)}\frac{1}{\rho_0}\int d\Omega_3\, S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)S(\boldsymbol{k},\Omega_3,\Omega_2) \quad (126)$$

$$0 = \frac{1}{\rho_0}\int d\Omega_3\, S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\frac{\delta S(\boldsymbol{k},\Omega_3,\Omega_2)}{\delta g(\boldsymbol{r},\Omega_4,\Omega_5)}+\frac{1}{\rho_0}\int d\Omega_3\, S(\boldsymbol{k},\Omega_3,\Omega_2)\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)}{\delta g(\boldsymbol{r},\Omega_4,\Omega_5)}. \quad (127)$$

By using equation (125) and acting with $\int d\Omega_2\, S^{-1}(\boldsymbol{k},\Omega_6,\Omega_2)$ on both sides of the above equation we obtain

$$\int d\Omega_3 \quad \rho_0 \quad \delta(\Omega_3,\Omega_6)\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)}{\delta g(\boldsymbol{r},\Omega_4,\Omega_5)} =$$

$$- \quad \rho_0 \quad \int d\Omega_2 d\Omega_3\, S^{-1}(\boldsymbol{k},\Omega_6,\Omega_2)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)e^{i\boldsymbol{k}\boldsymbol{r}}\sqrt{\rho(\Omega_3)}\sqrt{\rho(\Omega_2)}\delta(\Omega_3,\Omega_4)\delta(\Omega_2,\Omega_5) \quad (128)$$

which gives the result:

$$\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_2)}{\delta g(\boldsymbol{r},\Omega_3,\Omega_4)} = -e^{i\boldsymbol{k}\boldsymbol{r}}\sqrt{\rho(\Omega_3)}\sqrt{\rho(\Omega_4)}S^{-1}(\boldsymbol{k},\Omega_2,\Omega_4)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3). \quad (129)$$

Now we return to the variation of N:

$$\frac{\delta N(\boldsymbol{r},\Omega_1,\Omega_2)}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)} = \frac{\delta}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)}\frac{1}{\rho_0}\int d^3k\, e^{-i\boldsymbol{k}\boldsymbol{r}}\tilde{N}(\boldsymbol{k},\Omega_1,\Omega_2) \quad (130)$$

$$= \frac{\delta}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)}\frac{1}{\rho_0}\int d^3k\, e^{-i\boldsymbol{k}\boldsymbol{r}}\frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}}\left[\frac{1}{\rho_0}S(\boldsymbol{k},\Omega_1,\Omega_2)-2\delta(\Omega_1,\Omega_2)+\frac{1}{\rho_0}S^{-1}(\boldsymbol{k},\Omega_1,\Omega_2)\right]$$

$$= \frac{1}{\rho_0}\int d^3k\, e^{-i\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}\frac{\sqrt{\rho(\Omega_3)\rho(\Omega_4)}}{\sqrt{\rho(\Omega_1)\rho(\Omega_2)}}\left(\rho_0\delta(\Omega_1,\Omega_3)\delta(\Omega_2,\Omega_4)-\frac{1}{\rho_0}S^{-1}(\boldsymbol{k},\Omega_2,\Omega_4)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\right) \quad (131)$$

Again we define a new function

$$a(\boldsymbol{r}-\boldsymbol{r}',\Omega_1,\Omega_2,\Omega_3,\Omega_4) := \frac{1}{\rho_0}\int d^3k\, e^{-ik(r-r')}\frac{\sqrt{\rho(\Omega_3)\rho(\Omega_4)}}{\sqrt{\rho(\Omega_1)\rho(\Omega_2)}}\left(\rho_0\delta(\Omega_1,\Omega_3)\delta(\Omega_2,\Omega_4) - \frac{1}{\rho_0}S^{-1}(\boldsymbol{k},\Omega_2,\Omega_4)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\right). \tag{132}$$

Now we can return to the calculation of the variation of the kinetic energy and we get:

$$\begin{aligned}\frac{\delta\langle T\rangle}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)} &= \frac{\hbar^2}{8M}V\rho_0^2\rho(\Omega_3)\rho(\Omega_4)\left\{\frac{-4}{\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)}}\nabla'^2\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)} + \nabla'^2 N(\boldsymbol{r}',\Omega_3,\Omega_4)\right\}\\ &+ \frac{\hbar^2}{8M}V\rho_0^2\int d^3r d\Omega_1 d\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)a(\boldsymbol{r}-\boldsymbol{r}',\Omega_1,\Omega_2,\Omega_3,\Omega_4)\nabla^2 g(\boldsymbol{r},\Omega_1,\Omega_2).\end{aligned} \tag{133}$$

We again define a convolution asterisk $*$

$$[f*g](\boldsymbol{r},\Omega_3,\Omega_4) = \int d^3\tilde{r} d\Omega_1 d\Omega_2\ \rho(\Omega_1)\rho(\Omega_2)f(\boldsymbol{r},\Omega_1,\Omega_2)g(\boldsymbol{r}-\tilde{\boldsymbol{r}},\Omega_1,\Omega_2,\Omega_3,\Omega_4). \tag{134}$$

and with this we can rewrite equation (133) to finally get

$$\begin{aligned}\frac{\delta\langle T\rangle}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)} &= \frac{\hbar^2}{8M}V\rho_0^2\rho(\Omega_3)\rho(\Omega_4)\left\{\frac{-4}{\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)}}\nabla'^2\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)} + \nabla'^2 N(\boldsymbol{r}',\Omega_3,\Omega_4)\right\}\\ &+ \frac{\hbar^2}{8M}V\rho_0^2\left[a*(\nabla^2 g)\right](\boldsymbol{r}',\Omega_3,\Omega_4).\end{aligned} \tag{135}$$

The last thing we need for the two–body equation, is the variation of the rotational energy. The calculation is similar to that of the variation of the kinetic energy and the result is:

$$\frac{\delta\langle R\rangle}{\delta g(\boldsymbol{r}',\Omega_3,\Omega_4)} = -\frac{\hbar^2}{4I}V\rho_0^2\rho(\Omega_3)\rho(\Omega_4)\frac{1}{\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)}}\left(\Lambda_1{}^2+\Lambda_2^2\right)\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)} \tag{136}$$

$$\begin{aligned}&+ \frac{\hbar^2}{16I}V\rho_0^2\left(\frac{1}{\rho(\Omega_3)}\boldsymbol{\Lambda}_3\rho(\Omega_3)\boldsymbol{\Lambda}_3 + \frac{1}{\rho(\Omega_4)}\boldsymbol{\Lambda}_4\rho(\Omega_4)\boldsymbol{\Lambda}_4\right)N(\boldsymbol{r}',\Omega_3,\Omega_4)\\ &+ \frac{\hbar^2}{16I}V\rho_0^2\left[a*(\boldsymbol{L}g)\right](\boldsymbol{r}',\Omega_3,\Omega_4),\end{aligned} \tag{137}$$

where we defined a new operator:

$$\boldsymbol{L}\,f(\boldsymbol{r},\Omega_1,\Omega_2) = \left(\frac{1}{\rho(\Omega_1)}\boldsymbol{\Lambda}_1\rho(\Omega_1)\boldsymbol{\Lambda}_1 + \frac{1}{\rho(\Omega_2)}\boldsymbol{\Lambda}_2\rho(\Omega_2)\boldsymbol{\Lambda}_2\right)f(\boldsymbol{r},\Omega_1,\Omega_2). \tag{138}$$

Finally we get the following two–body equation:

$$
\begin{aligned}
0 &= \frac{1}{2}\rho(\Omega_3)\rho(\Omega_4)V_{dd}(\boldsymbol{r}',\Omega_3,\Omega_4) &(139)\\
&+ \frac{\hbar^2}{8M}\rho(\Omega_3)\rho(\Omega_4)\left\{\frac{-4}{\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)}}\nabla'^2\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)}+\nabla'^2 N(\boldsymbol{r}',\Omega_3,\Omega_4)\right\}\\
&+ \frac{\hbar^2}{8M}\left[a*(\nabla^2 g)\right](\boldsymbol{r}',\Omega_3,\Omega_4) &(140)\\
&- \frac{\hbar^2}{4I}\rho(\Omega_3)\rho(\Omega_4)\frac{1}{\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)}}\left(\Lambda_1{}^2+\Lambda_2^2\right)\sqrt{g(\boldsymbol{r}',\Omega_3,\Omega_4)} &(141)\\
&+ \frac{\hbar^2}{16I}\left(\frac{1}{\rho(\Omega_3)}\boldsymbol{\Lambda}_3\rho(\Omega_3)\boldsymbol{\Lambda}_3+\frac{1}{\rho(\Omega_4)}\boldsymbol{\Lambda}_4\rho(\Omega_4)\boldsymbol{\Lambda}_4\right)N(\boldsymbol{r}',\Omega_3,\Omega_4)\\
&+ \frac{\hbar^2}{16I}\left[a*(\boldsymbol{L}g)\right](\boldsymbol{r}',\Omega_3,\Omega_4). &(142)
\end{aligned}
$$

4.3.2. One–body equation

To get the one–body equation we have to vary the expectation value of the Hamiltonian (110) with respect to the density ρ. We also have to take into account the constraint that the particle number is fixed:

$$N=\int d^3r d\Omega_1\,\rho(\boldsymbol{r},\Omega_1)=V\rho_0\int d\Omega_1\,\rho(\Omega_1). \tag{143}$$

Therefore what we calculate is:

$$\frac{\delta\left(\langle H\rangle-\mu N\right)}{\delta\sqrt{\rho(\Omega_3)}}=\left[\frac{\delta\langle U\rangle}{\delta\rho(\Omega_3)}+\frac{\delta\langle T\rangle}{\delta\rho(\Omega_3)}+\frac{\delta\langle R\rangle}{\delta\rho(\Omega_3)}-V\rho_0\,\mu\right]2\sqrt{\rho(\Omega_3)}=0 \tag{144}$$

First we vary the potential energy (90)

$$
\begin{aligned}
\frac{\delta\langle U\rangle}{\delta\rho(\Omega_3)} &= \frac{\delta}{\delta\rho(\Omega_3)}V\rho_0\left[\int d\Omega_1\,\rho(\Omega_1)U_{ext}(\Omega_1)+\frac{1}{2}\rho_0\int d^3r d\Omega_1 d\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)g(\boldsymbol{r},\Omega_1,\Omega_2)V_{dd}(\boldsymbol{r},\Omega_1,\Omega_2)\right]\\
&= V\rho_0 U_{ext}(\Omega_3)+V\rho_0^2\int d^3r d\Omega_1\,\rho(\Omega_1)g(\boldsymbol{r},\Omega_1,\Omega_3)V_{dd}(\boldsymbol{r},\Omega_1,\Omega_3) &(145)
\end{aligned}
$$

where we used the pair–symmetry. Note that

$$\frac{\delta g(\boldsymbol{r},\Omega_1,\Omega_2)}{\delta\rho(\Omega_3)}=0 \tag{146}$$

since g and ρ are our independent variables.

Next we calculate the variation of the kinetic energy (95)

$$\begin{aligned}
\frac{\delta\langle T\rangle}{\delta\rho(\Omega_3)} &= \frac{\hbar^2}{8M}V\rho_0^2\frac{\delta}{\delta\rho(\Omega_3)}\int d^3r d\Omega_1 d\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)\left\{4|\boldsymbol{\nabla}\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_2)}|^2+g(\boldsymbol{r},\Omega_1,\Omega_2)\nabla^2 N(\boldsymbol{r},\Omega_1,\Omega_2)\right\} \\
&= \frac{\hbar^2}{4M}V\rho_0^2\int d^3r d\Omega_1\,\rho(\Omega_1)\left\{4|\boldsymbol{\nabla}\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_3)}|^2+g(\boldsymbol{r},\Omega_1,\Omega_3)\nabla^2 N(\boldsymbol{r},\Omega_1,\Omega_3)\right\} \qquad (147)\\
&+ \frac{\hbar^2}{8M}V\rho_0^2\int d^3r d\Omega_1 d\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)\nabla^2 g(\boldsymbol{r},\Omega_1,\Omega_2)\frac{\delta N(\boldsymbol{r},\Omega_1,\Omega_2)}{\delta\rho(\Omega_3)} \qquad (148)
\end{aligned}$$

where we again used the pair–symmetry. To proceed we need the variation of N with respect to ρ.

Variation of N with respect to ρ:

We start again by finding expressions for the variation of the structure function S and its inverse S^{-1}.

For S we get:

$$\begin{aligned}
\frac{\delta S(\boldsymbol{k},\Omega_1,\Omega_2)}{\delta\rho(\Omega_3)} &= \frac{\delta}{\delta\rho(\Omega_3)}\left\{\rho_0\delta(\Omega_1,\Omega_2)+\rho_0^2\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}\int d^3r\,e^{i\boldsymbol{kr}}\,(g(\boldsymbol{r},\Omega_1,\Omega_2)-1)\right\} \qquad (149)\\
&= \frac{1}{2}\rho_0^2\int d^3r\,e^{i\boldsymbol{kr}}\,(g(\boldsymbol{r},\Omega_1,\Omega_2)-1)\left[\frac{\sqrt{\rho(\Omega_2)}}{\sqrt{\rho(\Omega_1)}}\delta(\Omega_1,\Omega_3)+\frac{\sqrt{\rho(\Omega_1)}}{\sqrt{\rho(\Omega_2)}}\delta(\Omega_2,\Omega_3)\right] \qquad (150)\\
&= \frac{1}{2}\left[\frac{1}{\rho(\Omega_1)}\delta(\Omega_1,\Omega_3)+\frac{1}{\rho(\Omega_2)}\delta(\Omega_2,\Omega_3)\right]\left[S(\boldsymbol{k},\Omega_1,\Omega_2)-\rho_0\delta(\Omega_1,\Omega_2)\right]. \qquad (151)
\end{aligned}$$

The variation of the defining relation of S^{-1} (122) leads to the desired expression for the variation of S^{-1} with respect to ρ:

$$\begin{aligned}
0 &= \frac{\delta}{\delta\rho(\Omega_3)}\frac{1}{\rho_0}\int d\Omega_4\,S^{-1}(\boldsymbol{k},\Omega_1,\Omega_4)S(\boldsymbol{k},\Omega_4,\Omega_2) \qquad (152)\\
0 &= \frac{1}{\rho_0}\int d\Omega_4\,S^{-1}(\boldsymbol{k},\Omega_1,\Omega_4)\frac{\delta S(\boldsymbol{k},\Omega_4,\Omega_2)}{\delta\rho(\Omega_3)}+\frac{1}{\rho_0}\int d\Omega_4\,S(\boldsymbol{k},\Omega_4,\Omega_2)\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_4)}{\delta\rho(\Omega_3)} \qquad (153)\\
0 &= \frac{1}{2}\int d\Omega_4\,S^{-1}(\boldsymbol{k},\Omega_1,\Omega_4)\left[\frac{1}{\rho(\Omega_4)}\delta(\Omega_4,\Omega_3)+\frac{1}{\rho(\Omega_2)}\delta(\Omega_2,\Omega_3)\right]\left[S(\boldsymbol{k},\Omega_4,\Omega_2)-\rho_0\delta(\Omega_4,\Omega_2)\right]\\
&+ \int d\Omega_4\,S(\boldsymbol{k},\Omega_4,\Omega_2)\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_4)}{\delta\rho(\Omega_3)} \qquad (154)\\
0 &= \frac{1}{2}\int d\Omega_2 d\Omega_4\,S^{-1}(\boldsymbol{k},\Omega_2,\Omega_5)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_4)\left[\frac{1}{\rho(\Omega_4)}\delta(\Omega_4,\Omega_3)+\frac{1}{\rho(\Omega_2)}\delta(\Omega_2,\Omega_3)\right]\left[S(\boldsymbol{k},\Omega_4,\Omega_2)-\rho_0\delta(\Omega_4,\Omega_2)\right]\\
&+ \rho_0^2\int d\Omega_4\,\delta(\Omega_5,\Omega_4)\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_4)}{\delta\rho(\Omega_3)} \qquad (155)
\end{aligned}$$

$$
\begin{aligned}
0 &= \frac{1}{2}\int d\Omega_2\, S^{-1}(\boldsymbol{k},\Omega_2,\Omega_5)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\frac{1}{\rho(\Omega_3)}S(\boldsymbol{k},\Omega_3,\Omega_2) && (156)\\
&+ \frac{1}{2}\int d\Omega_4\, S^{-1}(\boldsymbol{k},\Omega_3,\Omega_5)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_4)\frac{1}{\rho(\Omega_3)}S(\boldsymbol{k},\Omega_4,\Omega_3) && (157)\\
&- \rho_0\, S^{-1}(\boldsymbol{k},\Omega_3,\Omega_5)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\frac{1}{\rho(\Omega_3)} && (158)\\
&+ \rho_0^2\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_5)}{\delta\rho(\Omega_3)} && (159)\\
0 &= \frac{1}{2}\rho_0^2\,\delta(\Omega_3,\Omega_5)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\frac{1}{\rho(\Omega_3)} + \frac{1}{2}\rho_0^2\, S^{-1}(\boldsymbol{k},\Omega_3,\Omega_5)\delta(\Omega_1,\Omega_3)\frac{1}{\rho(\Omega_3)} && (160)\\
&- \rho_0\, S^{-1}(\boldsymbol{k},\Omega_3,\Omega_5)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\frac{1}{\rho(\Omega_3)} && (161)\\
&+ \rho_0^2\,\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_5)}{\delta\rho(\Omega_3)}, && (162)
\end{aligned}
$$

where we used equation (151) and (122). We obtain the relation:

$$
\begin{aligned}
\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_5)}{\delta\rho(\Omega_3)} &= -\frac{1}{2\rho(\Omega_3)}S^{-1}(\boldsymbol{k},\Omega_1,\Omega_5)\,[\delta(\Omega_3,\Omega_5)+\delta(\Omega_1,\Omega_3)] && (163)\\
&+ \frac{1}{\rho_0\rho(\Omega_3)}S^{-1}(\boldsymbol{k},\Omega_3,\Omega_5)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3). && (164)
\end{aligned}
$$

Now we can calculate the variation of N where we use the HNC equation (118):

$$
\begin{aligned}
\frac{\delta N(\boldsymbol{r},\Omega_1,\Omega_2)}{\delta\rho(\Omega_3)} &= \frac{\delta}{\delta\rho(\Omega_3)}\frac{1}{\rho_0}\int d^3k\, e^{-i\boldsymbol{kr}}\tilde{N}(\boldsymbol{k},\Omega_1,\Omega_2) && (165)\\
&= \frac{\delta}{\delta\rho(\Omega_3)}\frac{1}{\rho_0}\int d^3k\, e^{-i\boldsymbol{kr}}\frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}}\left[\frac{1}{\rho_0}S(\boldsymbol{k},\Omega_1,\Omega_2)-2\delta(\Omega_1,\Omega_2)+\frac{1}{\rho_0}S^{-1}(\boldsymbol{k},\Omega_1,\Omega_2)\right]\\
&= -\frac{1}{2}N(\boldsymbol{r},\Omega_1,\Omega_2)\left(\frac{1}{\rho(\Omega_1)}\delta(\Omega_1,\Omega_3)+\frac{1}{\rho(\Omega_2)}\delta(\Omega_2,\Omega_3)\right) && (166)\\
&+ \frac{1}{\rho_0}\int d^3k\, e^{-i\boldsymbol{kr}}\frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}}\frac{\delta}{\delta\rho(\Omega_3)}\left[\frac{1}{\rho_0}S(\boldsymbol{k},\Omega_1,\Omega_2)-2\delta(\Omega_1,\Omega_2)+\frac{1}{\rho_0}S^{-1}(\boldsymbol{k},\Omega_1,\Omega_2)\right]\\
&= -\frac{1}{2}N(\boldsymbol{r},\Omega_1,\Omega_2)\left(\frac{1}{\rho(\Omega_1)}\delta(\Omega_1,\Omega_3)+\frac{1}{\rho(\Omega_2)}\delta(\Omega_2,\Omega_3)\right) && (167)\\
&+ \frac{1}{\rho_0^2}\int d^3k\, e^{-i\boldsymbol{kr}}\frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}}\left[\frac{\delta S(\boldsymbol{k},\Omega_1,\Omega_2)}{\delta\rho(\Omega_3)}+\frac{\delta S^{-1}(\boldsymbol{k},\Omega_1,\Omega_2)}{\delta\rho(\Omega_3)}\right]
\end{aligned}
$$

$$
\begin{aligned}
\frac{\delta N(\boldsymbol{r},\Omega_1,\Omega_2)}{\delta\rho(\Omega_3)} &= -\frac{1}{2}N(\boldsymbol{r},\Omega_1,\Omega_2)\left(\frac{1}{\rho(\Omega_1)}\delta(\Omega_1,\Omega_3)+\frac{1}{\rho(\Omega_2)}\delta(\Omega_2,\Omega_3)\right) \\
&+ \frac{1}{2\rho_0^2}\int d^3k\, e^{-i\boldsymbol{k}\boldsymbol{r}}\frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}}\left[\frac{1}{\rho(\Omega_1)}\delta(\Omega_1,\Omega_3)+\frac{1}{\rho(\Omega_2)}\delta(\Omega_2,\Omega_3)\right]\left[S(\boldsymbol{k},\Omega_1,\Omega_2)-\rho_0\delta(\Omega_1,\Omega_2)\right] \\
&- \frac{1}{2\rho_0^2}\int d^3k\, e^{-i\boldsymbol{k}\boldsymbol{r}}\frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}}S^{-1}(\boldsymbol{k},\Omega_1,\Omega_2)\left[\frac{1}{\rho(\Omega_3)}\delta(\Omega_3,\Omega_2)+\frac{1}{\rho(\Omega_3)}\delta(\Omega_1,\Omega_3)\right] \\
&+ \frac{1}{\rho_0^2}\int d^3k\, e^{-i\boldsymbol{k}\boldsymbol{r}}\frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}}\left[\frac{1}{\rho_0\rho(\Omega_3)}S^{-1}(\boldsymbol{k},\Omega_3,\Omega_2)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\right].
\end{aligned}
\tag{168}
$$

This expression can be reformulated by using equation (118) and (121) and we finally obtain:

$$
\begin{aligned}
\frac{\delta N(\boldsymbol{r},\Omega_1,\Omega_2)}{\delta\rho(\Omega_3)} &= \frac{1}{2\rho_0}\int d^3k\, e^{-i\boldsymbol{k}\boldsymbol{r}}\frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}}\left[\frac{1}{\rho(\Omega_1)}\delta(\Omega_1,\Omega_3)+\frac{1}{\rho(\Omega_2)}\delta(\Omega_2,\Omega_3)\right]\delta(\Omega_1,\Omega_2) \\
&- \frac{1}{\rho_0^2}\int d^3k\, e^{-i\boldsymbol{k}\boldsymbol{r}}\frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}}\left[\frac{1}{\rho(\Omega_1)}\delta(\Omega_1,\Omega_3)+\frac{1}{\rho(\Omega_2)}\delta(\Omega_2,\Omega_3)\right]S^{-1}(\boldsymbol{k},\Omega_1,\Omega_2) \\
&+ \frac{1}{\rho_0^2}\int d^3k\, e^{-i\boldsymbol{k}\boldsymbol{r}}\frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}}\left[\frac{1}{\rho_0\rho(\Omega_3)}S^{-1}(\boldsymbol{k},\Omega_3,\Omega_2)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)\right].
\end{aligned}
\tag{169}
$$

Let us define a new function

$$
\begin{aligned}
\tilde{b}(\boldsymbol{k},\Omega_1,\Omega_2,\Omega_3) :=& - \frac{1}{\sqrt{\rho(\Omega_1)}\sqrt{\rho(\Omega_2)}\rho(\Omega_3)}\left\{\frac{1}{\rho_0}\left(\delta(\Omega_1,\Omega_3)+\delta(\Omega_2,\Omega_3)\right)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_3)-\delta(\Omega_1,\Omega_3)\delta(\Omega_2,\Omega_3)\right\} \\
&+ \frac{1}{\rho_0^2\sqrt{\rho(\Omega_1)\rho(\Omega_2)}\rho(\Omega_3)}S^{-1}(\boldsymbol{k},\Omega_3,\Omega_2)S^{-1}(\boldsymbol{k},\Omega_1,\Omega_2).
\end{aligned}
\tag{170}
$$

This expression can be reformulated by using equation (121) and what we get is:

$$
\tilde{b}(\boldsymbol{k},\Omega_1,\Omega_2,\Omega_3) = \tilde{X}(\boldsymbol{k},\Omega_1,\Omega_3)\tilde{X}(\boldsymbol{k},\Omega_3,\Omega_2). \tag{171}
$$

Now we return to the calculation of the variation of the kinetic energy. We obtain:

$$
\frac{\delta\langle T\rangle}{\delta\rho(\Omega_3)} = \frac{\hbar^2}{4M}V\rho_0^2\int d^3r d\Omega_1\,\rho(\Omega_1)\left\{4|\boldsymbol{\nabla}\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_3)}|^2+g(\boldsymbol{r},\Omega_1,\Omega_3)\nabla^2 N(\boldsymbol{r},\Omega_1,\Omega_3)\right\} \tag{172}
$$

$$
+ \frac{\hbar^2}{8M}V\rho_0^2\int d^3r d\Omega_1 d\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)b(\boldsymbol{r},\Omega_1,\Omega_2,\Omega_3)\nabla^2 g(\boldsymbol{r},\Omega_1,\Omega_2). \tag{173}
$$

Next we calculate the variation of the rotational energy $\langle R\rangle$ given in equation (109).

$$
\begin{aligned}
\frac{\delta\langle R\rangle}{\delta\rho(\Omega_3)} &= -\frac{\hbar^2}{I}V\rho_0\int d\Omega_1\left(\Lambda_1^2\sqrt{\rho(\Omega_1)}\right)\frac{\delta\sqrt{\rho(\Omega_1)}}{\delta\rho(\Omega_3)} \\
&+ \frac{\hbar^2V\rho_0^2}{2I}\int d^3rd\Omega_1\,\rho(\Omega_1)\left(\left|\mathbf{\Lambda}_1\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_3)}\right|^2+\left|\mathbf{\Lambda}_3\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_3)}\right|^2\right) \\
&+ \frac{\hbar^2V\rho_0^2}{8I}\int d^3rd\Omega_1\,N(\boldsymbol{r},\Omega_1,\Omega_3)\mathbf{\Lambda}_1\rho(\Omega_1)\mathbf{\Lambda}_1 g(\boldsymbol{r},\Omega_1,\Omega_3) \\
&- \frac{\hbar^2V\rho_0^2}{8I}\int d^3rd\Omega_1\,\rho(\Omega_1)\left(\mathbf{\Lambda}_3N(\boldsymbol{r},\Omega_1,\Omega_3)\right)\left(\mathbf{\Lambda}_3 g(\boldsymbol{r},\Omega_1,\Omega_3)\right) \\
&+ \frac{\hbar^2V\rho_0^2}{16I}\int d^3rd\Omega_1d\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)\frac{\delta N(\boldsymbol{r},\Omega_1,\Omega_2)}{\delta\rho(\Omega_3)}\left(\frac{1}{\rho(\Omega_1)}\mathbf{\Lambda}_1\rho(\Omega_1)\mathbf{\Lambda}_1+\frac{1}{\rho(\Omega_2)}\mathbf{\Lambda}_2\rho(\Omega_2)\mathbf{\Lambda}_2\right)g(\boldsymbol{r},\Omega_1,\Omega_2)
\end{aligned}
\tag{174}
$$

To get to the above expression we used the pair–symmetry and integration by parts. Now we insert the variation of N with respect to ρ (169) and rewrite the third and fourth term by integrating by parts and we get:

$$
\begin{aligned}
\frac{\delta\langle R\rangle}{\delta\rho(\Omega_3)} &= -\frac{\hbar^2}{2I}V\rho_0\frac{1}{\sqrt{\rho(\Omega_3)}}\left(\Lambda_3^2\sqrt{\rho(\Omega_3)}\right) \\
&+ \frac{\hbar^2V\rho_0^2}{2I}\int d^3rd\Omega_1\,\rho(\Omega_1)\left(\left|\mathbf{\Lambda}_1\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_3)}\right|^2+\left|\mathbf{\Lambda}_3\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_3)}\right|^2\right) \\
&- \frac{\hbar^2V\rho_0^2}{8I}\int d^3rd\Omega_1\,\rho(\Omega_1)\left[\left(\mathbf{\Lambda}_1N(\boldsymbol{r},\Omega_1,\Omega_3)\right)\left(\mathbf{\Lambda}_1g(\boldsymbol{r},\Omega_1,\Omega_3)\right)+\left(\mathbf{\Lambda}_3N(\boldsymbol{r},\Omega_1,\Omega_3)\right)\left(\mathbf{\Lambda}_3g(\boldsymbol{r},\Omega_1,\Omega_3)\right)\right] \\
&+ \frac{\hbar^2V\rho_0^2}{16I}\int d^3rd\Omega_1d\Omega_2\,b(\boldsymbol{r},\Omega_1,\Omega_2,\Omega_3)\left(\rho(\Omega_2)\mathbf{\Lambda}_1\rho(\Omega_1)\mathbf{\Lambda}_1+\rho(\Omega_1)\mathbf{\Lambda}_2\rho(\Omega_2)\mathbf{\Lambda}_2\right)g(\boldsymbol{r},\Omega_1,\Omega_2).
\end{aligned}
\tag{175}
$$

Finally, we combine the different results to obtain the one–body equation:

$$
\begin{aligned}
\mu &= U_{ext}(\Omega_3)\sqrt{\rho(\Omega_3)}+\rho_0\sqrt{\rho(\Omega_3)}\int d^3rd\Omega_1\,\rho(\Omega_1)g(\boldsymbol{r},\Omega_1,\Omega_3)V_{dd}(\boldsymbol{r},\Omega_1,\Omega_3) \\
&+ \frac{\hbar^2}{4M}\rho_0\sqrt{\rho(\Omega_3)}\int d^3rd\Omega_1\,\rho(\Omega_1)\left\{4|\mathbf{\nabla}\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_3)}|^2+g(\boldsymbol{r},\Omega_1,\Omega_3)\nabla^2N(\boldsymbol{r},\Omega_1,\Omega_3)\right\} \\
&+ \frac{\hbar^2}{8M}\rho_0\sqrt{\rho(\Omega_3)}\int d^3rd\Omega_1d\Omega_2\,\rho(\Omega_1)\rho(\Omega_2)b(\boldsymbol{r},\Omega_1,\Omega_2,\Omega_3)\nabla^2g(\boldsymbol{r},\Omega_1,\Omega_2)-\frac{\hbar^2}{2I}\left(\Lambda_3^2\sqrt{\rho(\Omega_3)}\right) \\
&+ \frac{\hbar^2\rho_0}{2I}\sqrt{\rho(\Omega_3)}\int d^3rd\Omega_1\,\rho(\Omega_1)\left(\left|\mathbf{\Lambda}_1\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_3)}\right|^2+\left|\mathbf{\Lambda}_3\sqrt{g(\boldsymbol{r},\Omega_1,\Omega_3)}\right|^2\right) \\
&- \frac{\hbar^2\rho_0}{8I}\sqrt{\rho(\Omega_3)}\int d^3rd\Omega_1\,\rho(\Omega_1)\left[\left(\mathbf{\Lambda}_1N(\boldsymbol{r},\Omega_1,\Omega_3)\right)\left(\mathbf{\Lambda}_1g(\boldsymbol{r},\Omega_1,\Omega_3)\right)+\left(\mathbf{\Lambda}_3N(\boldsymbol{r},\Omega_1,\Omega_3)\right)\left(\mathbf{\Lambda}_3g(\boldsymbol{r},\Omega_1,\Omega_3)\right)\right] \\
&+ \frac{\hbar^2\rho_0}{16I}\sqrt{\rho(\Omega_3)}\int d^3rd\Omega_1d\Omega_2\,b(\boldsymbol{r},\Omega_1,\Omega_2,\Omega_3)\left(\rho(\Omega_2)\mathbf{\Lambda}_1\rho(\Omega_1)\mathbf{\Lambda}_1+\rho(\Omega_1)\mathbf{\Lambda}_2\rho(\Omega_2)\mathbf{\Lambda}_2\right)g(\boldsymbol{r},\Omega_1,\Omega_2).
\end{aligned}
\tag{176}
$$

Part III.
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