# pyFTEGhf.py: Uniform electron gas at finite temperature in the Hartree-Fock approximation

F. G. Eich[1, *]
[1] *Max Planck Institute for the Structure and Dynamics of Matter,*
*Luruper Chaussee 149,*
*D-22761 Hamburg,*
*Germany*

(Dated: July 24, 2017)

This is the documentation for the **pyFTEGhf.py** code, which solves the Hartree-Fock self-consistency equations for the uniform electron gas in three dimensions at finite temperature. The intent is to provide the explicit derivation of the algorithm used to obtain the Hartree-Fock results, together with some hints about the structure of the **pyFTEGhf.py** code. If you find the **pyFTEGhf.py** code, or the algorithm outlined in this document useful, please cite our publication Eich *et al.*, 2017.

## I. INTRODUCTION

The **pyFTEGhf.py** code solves the self-consistency equations for the interacting electron gas at finite temperatures in the Hartree-Fock (HF) approximation. The code employs *Hartree* atomic units and assumes a spin-unpolarized electron gas with long-ranged Coulomb interactions. There are several "global" parameters which are set in the **params.py** file:

- **nSC**: maximum number of iterations for the solution of the self-consistency condition.

- **M**: $2^{\mathrm{M}}$ determines the number integration points.

- **C**: dimensionless coupling strength ($C = 0$ noninteracting, $C = 1$ fully interacting electrons).

- **dq**: convergence criterion for the wave vectors.

- **maxIterPotInv**: maximum number of iterations for the inversion from density to potential.

- **relErrPotInv**: convergence criterion for the inversion from density to potential.

- **debug**: flag to produce verbose output.

**pyFTEGhf.py** defines a class, **hfEG**, representing the uniform electron gas (EG) at finite temperature. The initialization of a **hfEG** object requires two out of the four quantities:

- **alpha**: $\alpha$ is the relative dimensionless chemical potential (not the physical chemical potential!).

---

\* florian.eich@mpsd.mpg.de

- **beta**: $\beta = (k_{\mathrm{B}}T)^{-1}$ is the inverse temperature.

- **n**: density of the uniform electron gas.

- **h**: energy density (not energy per particle!) of the uniform electron gas.

*Remark: Currently only the pairs (alpha, beta) or (n, beta) are implemented.* Both inputs need to be arrays with the same shape.

Upon successful initialization the object **hfEG** contains the following variables:

- **mu**: physical chemical potential.

- **beta**: inverse temperature.

- **n**: density of the EG.

- **h**: energy density of the EG.

- **alpha**: relative dimensionless chemical potential (defined below).

- **s**: entropy density of the EG .

- **f**: free energy density of the EG.

- **w**: grand potential density of the EG.

All of the above variables have the same shape as the input variables. Furthermore **hfEG** stores the six differential $2 \times 2$ matrices corresponding to:

- **dNdV**: density and energy density viewed as functions of the chemical potential and inverse temperature, i.e.,

$$\mathbf{dNdV} = \begin{pmatrix} \left[\mathbf{dNdV}\right]_{00} & \left[\mathbf{dNdV}\right]_{01} \\ \left[\mathbf{dNdV}\right]_{10} & \left[\mathbf{dNdV}\right]_{11} \end{pmatrix} = \begin{pmatrix} \left.\partial_\mu n\right|_\beta & \left.\partial_\beta n\right|_\mu \\ \left.\partial_\mu h\right|_\beta & \left.\partial_\beta h\right|_\mu \end{pmatrix} \tag{1}$$

- **dVdN**: chemical potential and inverse temperature viewed as functions of the density and energy density (inverse of **dNdV**).

- **dMHdNB**: chemical potential and energy density viewed as functions of the density and inverse temperature.

- **dNBdMH**: density and inverse temperature viewed as functions of the chemical potential and energy density (inverse of **dMHdNB**).

- **dNMdHB**: density and chemical potential viewed as functions of the energy density and inverse temperature.

- **dHBdNM**: energy density and inverse temperature viewed as functions of density and chemical potential (inverse of **dNMdHB**).

The various differential matrices contain the same information and are explicitly included for the users convenience. For example, if one is interested in the heat capacity (per particle) of the EG,

$$c_{\mathrm{V}} \equiv \partial_T \epsilon(n, T)|_n \ , \tag{2}$$

i.e., the derivative of the energy per particle ($\epsilon \equiv h/n$) with respect to the temperature, keeping the number of particles fixed, this can be simply obtained by

$$c_{\mathrm{V}}/k_{\mathrm{B}} = -\left(\mathbf{beta}\right)^2 \left[\mathbf{dMHdNB}\right]_{11}/\mathbf{n} \ . \tag{3}$$

## II. SELF-ENERGY

The dispersion relation for the electrons is given by

$$\tilde{\epsilon}_{\boldsymbol{k}}^{\mathrm{C}} = \frac{1}{2}k^2 + \mathrm{C}\tilde{\Sigma}^{\mathrm{C}}(\boldsymbol{k}) \ , \tag{4}$$

with the frequency independent self-energy

$$\tilde{\Sigma}^{\mathrm{C}}(\boldsymbol{k}) = -\int \frac{\mathrm{d}^3 q}{(2\pi)^3} \frac{4\pi}{|\boldsymbol{k} - \boldsymbol{q}|^2} f_{\alpha,\beta}(\tilde{\epsilon}_{\boldsymbol{q}}^{\mathrm{C}}) \ , \tag{5}$$

where $f_{\alpha,\beta}(\epsilon) = \left(e^{\beta\epsilon-\alpha} + 1\right)^{-1}$ is the usual Fermi-Dirac distribution with the inverse temperature $\beta = (k_{\mathrm{B}}T)^{-1}$ and the dimensionless chemical potential $\alpha = \mu\beta$. The parameter C is the coupling constant of the electron–electron interaction, which we will set to one in the following. Equations (4) and (5) have to be solved self-consistently.

Let us start by evaluating the expression for the self-energy. The self-energy depends only on the magnitude of the wave vector and, hence, one angular integration can be performed trivially,

$$\tilde{\Sigma}(k) = -\frac{1}{\pi} \int_0^\infty \mathrm{d}q \ f_{\alpha,\beta}(\tilde{\epsilon}_q) \int_{-1}^1 \mathrm{d}x \ \frac{k^2}{k^2 + q^2 - 2kqx} \ . \tag{6}$$

The Fermi function can be rewritten as

$$f_{\alpha,\beta}(\epsilon) = -\int_\epsilon^\infty \mathrm{d}\nu \ \partial_\nu f_{\alpha,\beta}(\nu) = -\int_{-\infty}^\infty \mathrm{d}\nu \ [\partial_\nu f_{\alpha,\beta}(\nu)] \ \Theta(\nu - \epsilon) \ , \tag{7}$$

where $\Theta(x)$ is the Heaviside step function. Using Eq. (7) we can rewrite Eq. (6) as

$$\tilde{\Sigma}(k) = -\int_{\tilde{\epsilon}_0}^\infty \mathrm{d}\nu \ [\partial_\nu f_{\alpha,\beta}(\nu)] \ \tilde{S}(k, q_\nu) \ , \tag{8a}$$

$$\tilde{S}(k, q_\nu) = -\frac{1}{\pi} \int_0^{q_\nu} \mathrm{d}q \int_{-1}^1 \mathrm{d}x \ \frac{k^2}{k^2 + q^2 - 2kqx} \ . \tag{8b}$$

Equation (8b) is just the Hartree-Fock self-energy at zero temperature with the Fermi wave vector replaced by $q_\nu$, i.e,

$$S(k, q) = -\frac{1}{\pi} \left[ q - \frac{k}{4} \left[ 1 - \left(\frac{q}{k}\right)^2 \right] \ln\left(\frac{(k+q)^2}{(k-q)^2}\right) \right] \ . \tag{9}$$

At zero momentum we have $\lim_{k\to 0} \tilde{S}(q, k) = -\frac{2q}{\pi}$. $q_\nu$ itself is given by the solution of $\tilde{\epsilon}_q = \nu$ and, similarly the lower bound for the integral in Eq. (8a) is determined by the energy at zero momentum. It turns out to be crucial for

numerical stability to include the $k \to 0$ limit of the self-energy in the chemical potential. Accordingly, we define a modified self-energy by removing the constant contribution in the $k \to 0$ limit, i.e.,

$$S(k, q) = \tilde{S}(q, k) + \frac{2q}{\pi} = \frac{1}{\pi} \left[ q + \frac{k}{4} \left[ 1 - \left( \frac{q}{k} \right)^2 \right] \ln \left( \frac{(k+q)^2}{(k-q)^2} \right) \right] . \tag{10}$$

A consequence of this redefinition is that the lower bound in Eq. (8a) is trivially zero. However, it has to be kept in mind that $\alpha$ in the Fermi function is not simply the dimensionless chemical potential. Instead, we have the relation

$$\mu = \frac{\alpha}{\beta} + \frac{2\lambda}{\pi} \int_0^\infty d\nu \, \left[ \partial_\nu f_{\alpha,\beta}(\nu) \right] q_\nu \, , \tag{11}$$

which yields the *physical* chemical potential as function of the inverse temperature $\beta$ and the *relative* dimensionless chemical potential $\alpha$. The notion of "relative" dimensionless chemical potential stems from the fact that $\frac{\alpha}{\beta}$ measures, in fact, the dimensionless chemical potential from the bottom of the self-consistent Hartree-Fock quasi-particle dispersion.

## A. Discretization of energy integral

Central part of the **pyFTEGhf** code is to evaluate numerically integrals of the form

$$I = - \int_0^\infty d\nu \, \left[ \partial_\nu f_{\alpha,\beta}(\nu) \right] F(\nu) . \tag{12}$$

This means that a natural choice to perform the numerical integration is to include the derivative of the Fermi function in the integration weight, i.e., to define

$$ds = d\nu \left[ \partial_\nu f_{\alpha,\beta}(\nu) \right] . \tag{13}$$

This implies the substitution

$$\nu(s) = \frac{\ln \left( \frac{1-s}{s} \right) + \alpha}{\beta} \, , \tag{14}$$

which turns integral (12) into

$$I = \int_0^{s_0} ds \, F \left[ \nu(s) \right] \, , \tag{15}$$

with $s_0 = (\exp(-\alpha) + 1)^{-1}$. We note in passing that the integration limit $s_0$ depends on the physical chemical potential and the inverse temperature, as can be seen by inverting Eq. (11) formally to define $\alpha(\mu, \beta)$. Hence, if we are interested in evaluating the derivatives of integral $I$ with respect to $\mu$ or $\beta$ we have to take the variation of the integration interval into account. For this variation we have explicitly

$$\partial_{s_0} I = F(\nu(s_0)) = F(0) \, , \tag{16}$$

which means that this contribution is identically zero provided the integrand vanishes for $\nu \to 0$.

Numerically we evaluate integral (15) by first transforming it into the standard range $x \in [-1, 1]$ and then employing a Gauss-Legendre quadrature rule, i.e.,

$$I = \frac{s_0}{2} \int_{-1}^1 dx \, F \left[ \nu \left( \frac{s_0}{2} (x + 1) \right) \right] \approx \sum_{i=1}^N \Delta_i F_i \, , \tag{17}$$

where we defined $F_i = F(\nu_i)$, $\nu_i = \nu(s_i)$, $s_i = \frac{s_0}{2}(x_i + 1)$, and $\Delta_i = \frac{s_0}{2}dx_i$. The $dx_i$ and $x_i$ are the integration weights and points of the $N$th order Gauss-Legendre quadrature rule. Defining furthermore $q_i = q_{\nu_i}$ we arrive at the approximation for the self-energy,

$$\Sigma(k) \approx \sum_{i=1}^{N} \Delta_i S(k, q_i) \ . \tag{18}$$

Equipped with the approximation for the self-energy we can formulate the self-consistency condition as

$$\nu_i = \frac{1}{2}q_i^2 + \lambda \sum_{j=1}^{N} \Delta_j S(q_i, q_j) \ . \tag{19}$$

Suppose that the $q_i$ do not fulfill the self-consistency condition (19), we can find wave vector shifts $dq_i$ by linearizing the self-consistency condition (19), i.e.,

$$\nu_i - \left[ \frac{1}{2}(q_i)^2 + \lambda \sum_{j=1}^{N} \Delta_j S(q_i, q_j) \right] = \left[ q_i + \lambda \sum_{j=1}^{N} \Delta_j \ \partial_k S(k, q_j)|_{k=q_i} \right] dq_i + \lambda \sum_{j=1}^{N} \Delta_j \ \partial_q S(q_i, q)|_{q=q_j} \ dq_j \ . \tag{20}$$

We can solve the self-consistency condition with any suitable root-finding (or minimization) algorithm. The Jacobian matrix on the right hand side of (20) is analytically given in terms of the derivatives of $S(k, q)$,

$$\partial_q S(k, q) = \frac{2}{\pi} - \frac{1}{2\pi} \frac{q}{k} \ln\left( \frac{(k+q)^2}{(k-q)^2} \right) \ , \tag{21a}$$

$$\partial_k S(k, q) = -\frac{1}{\pi} \left[ \frac{q}{k} - \frac{1}{4} \left[ 1 + \left( \frac{q}{k} \right)^2 \right] \ln\left( \frac{(k+q)^2}{(k-q)^2} \right) \right] \ . \tag{21b}$$

It is worth noting that both derivatives diverge on the diagonal, i.e., for $k \to q$. [1] However, in the diagonal of the Jacobian we only need the sum of both derivatives, which is well behaved,

$$\lim_{k \to q} [\partial_q S(k, q) + \partial_k S(k, q)] = \frac{1}{\pi} \ . \tag{22}$$

## III. OBSERVABLES

In the previous section we have described how the self-consistency condition is solved, providing us with the discretized wave vectors $q_i$. Using these wave vectors we can compute a number of physical quantities. For example, the density is given by

$$
\begin{aligned}
n &= 2 \int \frac{d^3 k}{(2\pi)^3} \ f_{\alpha\beta}(\epsilon_{\boldsymbol{k}}) \\
&= \frac{1}{\pi^2} \int_0^\infty dk \ k^2 f_{\alpha\beta}(\epsilon_k) \\
&= -\frac{1}{\pi^2} \int_0^\infty d\nu \ [\partial_\nu f_{\alpha,\beta}(\nu)] \int_0^{q_\nu} dk \ k^2 \\
&= -\frac{1}{3\pi^2} \int_0^\infty d\nu \ [\partial_\nu f_{\alpha,\beta}(\nu)] (q_\nu)^3 \\
&\approx \frac{1}{3\pi^2} \sum_{i=1}^{N} \Delta_i \ [q_i]^3 \ .
\end{aligned} \tag{23}
$$

---

[1] This is a reflection of the fact that the derivative of the self-energy with respect to the wave vector diverges at the Fermi wave vector logarithmically in the Hartree-Fock approximation at zero temperature.

Similarly the kinetic energy density is given by

$$t = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \, k^2 f_{\alpha\beta}(\epsilon_{\boldsymbol{k}}) \approx \frac{1}{10\pi^2} \sum_{i=1}^{N} \Delta_i \left[q_i\right]^5 \ , \tag{24}$$

and the chemical potential (cf. Eq. (11)) by

$$\mu = \frac{\alpha}{\beta} - \frac{2\lambda}{\pi} \sum_{i=1}^{N} \Delta_i q_i \ . \tag{25}$$

The evaluation of the electron–electron interaction density will be deferred to the next section. In order to compute the entropy we start with its definition in terms of the single-particle occupation functions, i.e.,

$$\begin{aligned}
s &= -2 \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \left( f_{\alpha\beta}(\epsilon_{\boldsymbol{k}}) \ln(f_{\alpha\beta}(\epsilon_{\boldsymbol{k}})) + [1 - f_{\alpha\beta}(\epsilon_{\boldsymbol{k}})] \ln(1 - f_{\alpha\beta}(\epsilon_{\boldsymbol{k}})) \right) \\
&= -\frac{1}{\pi^2} \int_0^\infty \mathrm{d}k \, k^2 \left( f_{\alpha\beta}(\epsilon_k) \ln(f_{\alpha\beta}(\epsilon_k)) + [1 - f_{\alpha\beta}(\epsilon_k)] \ln(1 - f_{\alpha\beta}(\epsilon_k)) \right) \\
&= -\frac{1}{\pi^2} \int_0^\infty \mathrm{d}\nu \, [q_\nu]^2 \left[ \frac{\partial q_\nu}{\partial \nu} \right] \left( f_{\alpha\beta}(\nu) \ln(f_{\alpha\beta}(\nu)) + [1 - f_{\alpha\beta}(\nu)] \ln(1 - f_{\alpha\beta}(\nu)) \right) \ .
\end{aligned} \tag{26}$$

Now we use the identity

$$\frac{1}{\beta} \left[ \partial_\nu f_{\alpha\beta}(\nu) \right] = f_{\alpha\beta}(\nu) \left[ f_{\alpha\beta}(\nu) - 1 \right] \ , \tag{27}$$

to rewrite Eq. (26) as

$$\begin{aligned}
s &= -\frac{1}{\pi^2 \beta} \int_0^\infty \mathrm{d}\nu \, [\partial_\nu f_{\alpha,\beta}(\nu)] \, [q_\nu]^2 \left[ \frac{\partial q_\nu}{\partial \nu} \right] \left( \frac{\ln(f_{\alpha\beta}(\nu))}{f_{\alpha\beta}(\nu) - 1} - \frac{\ln(1 - f_{\alpha\beta}(\nu))}{f_{\alpha\beta}(\nu)} \right) \\
&\approx -\frac{1}{\pi^2 \beta} \sum_{i=1}^{N} \Delta_i \frac{[q_i]^2}{q_i + \Sigma_i'} \left( \frac{\ln(s_i)}{s_i - 1} - \frac{\ln(1 - s_i)}{s_i} \right) \ ,
\end{aligned} \tag{28}$$

where we have defined

$$\Sigma_i' = \sum_{j=1}^{N} \Delta_j \, \partial_k S(k, q_j)|_{k=q_j} \ . \tag{29}$$

## A. Derivatives

We are also interested in computing the derivatives of observables with respect to the chemical potential and the inverse temperature. In the previous section we have shown how the numerical approximations for the observables are given in terms of the discretized $\Delta_i$, $s_i$ and $q_i$. In principle all these quantities change when the relative dimensionless chemical potential, $\alpha$, and the inverse temperature, $\beta$, are changed. However, $\Delta_i$ and $s_i$ only depend on $\alpha$ and $\beta$ through the upper integration limit $s_0$ and, as discussed in Sec. II.A (cf. Eq. (16)), this dependency does not contribute to the derivative. Accordingly, we only have to derive the derivatives of the $q_i$ with respect to $\alpha$ and $\beta$. Using the self-consistency condition (19) we have

$$\partial_\alpha \nu_i = q_i \left[ \partial_\alpha q_i \right] + \lambda \sum_{j=1}^{N} \Delta_j \left( \partial_k S(k, q_j)|_{k=q_i} \left[ \partial_\alpha q_i \right] + \partial_q S(q_i, q)|_{q=q_j} \left[ \partial_\alpha q_j \right] \right) \ , \tag{30a}$$

$$\partial_\beta \nu_i = q_i \left[ \partial_\beta q_i \right] + \lambda \sum_{j=1}^{N} \Delta_j \left( \partial_k S(k, q_j)|_{k=q_i} \left[ \partial_\beta q_i \right] + \partial_q S(q_i, q)|_{q=q_j} \left[ \partial_\beta q_j \right] \right) \ . \tag{30b}$$

Now the left hand sides of Eqs. (30a) and (30b) can be evaluated directly using Eq. (14) yielding $\partial_\alpha \nu_i = \frac{1}{\beta}$ and $\partial_\beta \nu_i = -\frac{\nu_i}{\beta}$, respectively, where we ignored, again, the dependence on $s_0$. The linear system of equations (30a) and (30b) can be solve to obtain $\partial_\alpha q_i$ and $\partial_\beta q_i$. It follows that the derivatives for the density and kinetic-energy density are given by

$$\partial_X n = \frac{1}{\pi^2} \sum_{i=1}^{N} \Delta_i \left[q_i\right]^2 \left[\partial_X q_i\right] \ , \tag{31a}$$

$$\partial_X t = \frac{1}{2\pi^2} \sum_{i=1}^{N} \Delta_i \left[q_i\right]^4 \left[\partial_X q_i\right] \ , \tag{31b}$$

where $X = \alpha, \beta$. Finally we can also compute the derivatives of the physical chemical potential, i.e.,

$$\partial_\alpha \mu = \frac{1}{\beta} - \frac{2\lambda}{\pi} \sum_{i=1}^{N} \Delta_i \left[\partial_\alpha q_i\right] \ , \tag{32a}$$

$$\partial_\beta \mu = -\frac{\alpha}{\beta^2} - \frac{2\lambda}{\pi} \sum_{i=1}^{N} \Delta_i \left[\partial_\beta q_i\right] \ . \tag{32b}$$

Moreover from the total differential

$$d\mu = \partial_\alpha \mu d\alpha + \partial_\beta \mu d\beta \ , \tag{33}$$

we can derive the derivatives of the relative dimensionless chemical potential with respect to the physical chemical potential and the inverse temperature:

$$\partial_\mu \alpha = \frac{1}{\partial_\alpha \mu} = \frac{\beta}{1 - \frac{2\lambda\beta}{\pi} \sum_{i=1}^{N} \Delta_i \left[\partial_\alpha q_i\right]} \ , \tag{34a}$$

$$\partial_\beta \alpha = -\frac{\partial_\beta \mu}{\partial_\alpha \mu} = \frac{\frac{\alpha}{\beta} + \frac{2\lambda\beta}{\pi} \sum_{i=1}^{N} \Delta_i \left[\partial_\beta q_i\right]}{1 - \frac{2\lambda\beta}{\pi} \sum_{i=1}^{N} \Delta_i \left[\partial_\alpha q_i\right]} \ , \tag{34b}$$

Accordingly the derivatives of a generic observable $D$ with respect to the physical chemical potential and the inverse temperature are given by

$$d_\mu D = \left[\partial_\alpha D\right] \partial_\mu \alpha \ , \tag{35a}$$

$$d_\beta D = \partial_\beta D + \left[\partial_\alpha D\right] \partial_\beta \alpha \ . \tag{35b}$$

## IV. INTERACTION ENERGY

The Hartree-Fock approximation for the interaction-energy density of the uniform electron gas is given by

$$h_{\text{int}} = -\int \frac{d^3 k_1}{(2\pi)^3} \int \frac{d^3 k_2}{(2\pi)^3} \frac{4\pi}{|\mathbf{k}_1 - \mathbf{k}_2|^2} f_{\alpha,\beta}(\tilde{\epsilon}_{\mathbf{k}_1}) f_{\alpha,\beta}(\tilde{\epsilon}_{\mathbf{k}_2}) \ . \tag{36}$$

Using the same steps that lead to Eq. (8) we can rewrite

$$h_{\text{int}} = \int_{\epsilon_0^\lambda}^{\infty} d\nu_1 \int_{\epsilon_0^\lambda}^{\infty} d\nu_2 \ \left[\partial_{\nu_1} f_{\alpha,\beta}(\nu_1)\right] \left[\partial_{\nu_2} f_{\alpha,\beta}(\nu_2)\right] E(q^\lambda(\nu_1), q^\lambda(\nu_2)) \ , \tag{37a}$$

$$E(q^\lambda(\nu_1), q^\lambda(\nu_1)) = -\frac{1}{2\pi^3} \int_0^{q_{\nu_1}^\lambda} dk_1 \int_0^{q_{\nu_2}^\lambda} dk_2 \int_{-1}^{1} dx \ \frac{k_1^2 k_2^2}{k_1^2 + k_2^2 - 2k_1 k_2 x} \ . \tag{37b}$$

Explicitly we have

$$E(q_1, q_2) = -\frac{1}{(2\pi)^3}\left[q_1 q_2 \left(q_1^2 + q_2^2\right) - \frac{1}{4}\left(q_1^2 - q_2^2\right)^2 \ln\left(\frac{(q_1 + q_2)^2}{(q_1 - q_2)^2}\right)\right] \ . \tag{38}$$

Accordingly we get the approximation

$$h_{\text{int}} = \sum_{i=1}^{N}\sum_{j=1}^{N}\Delta_i\Delta_j E(q_i, q_j) \ . \tag{39}$$

Using the symmetry $E(q_1, q_2) = E(q_2, q_1)$ and the limit $E(q, q) = -\frac{1}{4\pi^3}q^4$ this can be rewritten as

$$h_{\text{int}} = \left[2\sum_{i=1}^{N}\sum_{j=1}^{i-1}\Delta_i\Delta_j E(q_i, q_j) - \frac{1}{4\pi^3}\sum_{i=1}^{N}\Delta_i^2\left(q_i\right)^4\right] \ . \tag{40}$$

Furthermore we are interested in the derivatives of the interaction-energy density with respect to $\beta$ and $\alpha$. It is straight forward to compute the required derivatives,

$$E_1(q_1, q_2) \equiv \partial_{q_1}E(q_1, q_2) = -\frac{1}{(2\pi)^3}q_1\left[4q_1 q_2 - \left(q_1^2 - q_2^2\right)\ln\left(\frac{(q_1 + q_2)^2}{(q_1 - q_2)^2}\right)\right] \ , \tag{41a}$$

$$E_2(q_1, q_2) \equiv \partial_{q_2}E(q_1, q_2) = -\frac{1}{(2\pi)^3}q_2\left[4q_1 q_2 - \left(q_2^2 - q_1^2\right)\ln\left(\frac{(q_1 + q_2)^2}{(q_1 - q_2)^2}\right)\right] \ , \tag{41b}$$

with the limiting behavior $\lim_{q_2 \to q_1} E_1(q_1, q_2) = \lim_{q_2 \to q_1} E_2(q_1, q_2) = -\frac{1}{2\pi^3}q_1^3$. Accordingly we have

$$\partial_\alpha h_{\text{int}} = \sum_{i=1}^{N}\sum_{j=1}^{N}\Delta_i\Delta_j\left(E_1(q_i, q_j)\left[\partial_\alpha q_i\right] + E_2(q_i, q_j)\left[\partial_\alpha q_j\right]\right) \ , \tag{42a}$$

$$\partial_\beta h_{\text{int}} = \sum_{i=1}^{N}\sum_{j=1}^{N}\Delta_i\Delta_j\left(E_1(q_i, q_j)\left[\partial_\beta q_i\right] + E_2(q_i, q_j)\left[\partial_\beta q_j\right]\right) \ . \tag{42b}$$

## V. FINAL REMARKS

In the derivation of the algorithm for the solution of the HF self-consistency equations for the EG presented in the previous sections we have taken the relative dimensionless chemical potential $\alpha$ and the inverse temperature $\beta$ as input. Suppose, instead, that we would like to specify the density $n$ and the (inverse) temperature $\beta$ as input. In this case we can guess an initial $\alpha_0$ and compute the corresponding density. Then we update iteratively

$$\alpha_n = \alpha_{n-1} + \frac{n - n(\alpha_{n-1})}{\partial_\alpha n(\alpha_{n_1})|_\beta} \ . \tag{43}$$

This is implemented in the routine **getAfromNB**. Furthermore, the function **SdS** returns the self energy as a function of the wave vector. Note that this relies on the presence of the internal variables $q_i$, which are determined during the solution of the self-consistency condition. Since the object **hfEG** contains, in general, a collection of observables for the EG for various parameters (e.g., various $n$ and $\beta$), the internal variables are removed after the initialization. If one wants to get the self energy via a call of **SdS** one first has to call the function **scCycle** (which constructs the internal variables $q_i$) with the specific parameters for which the self energy is computed.

## REFERENCES

Eich, F. G., M. Holzmann,  and G. Vignale (2017), Phys. Rev. B **96**, 035132.