A Green's function quantum average atom model

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A quantum average atom model is reformulated using Green's functions. This allows integrals along the real energy axis to be deformed into the complex plane. The advantage being that sharp features such as resonances and bound states are broadened by a Lorentzian with a half-width chosen for numerical convenience. An implementation of this method therefore avoids numerically challenging resonance tracking and the search for weakly bound states, without changing the physical content or results of the model. A straightforward implementation results in up to a factor of 5 speed-up relative to an optimized orbital based code.

Keywords: average atom, greens function, warm dense matter, dense plasmas, density functional theory

I. INTRODUCTION

Average atom models are widely used to calculate equation of state [1–5] and other properties [6–11] of dense plasmas. They are density functional theory based models, and despite being less physically realistic than corresponding density functional theory molecular dynamics based methods [12–14], they are still very useful as they give a reasonable description of the plasma over a wide range of temperatures and densities and are much less computationally expensive.

Average atoms models come in a wide variety. They can be purely orbital free in character, for example using the Thomas-Fermi approximation [15], or use orbital based, Kohn-Sham density functional theory [1, 4, 10, 16, 17]. For a long time orbital based models had numerical problems due to the presence of narrow resonances in the continuum of free states. This led to erroneous discontinuities in the predicted pressure when resonance states occurred. Sophisticated algorithms were developed to track and accurately sample these resonances [2], resulting in a continuous prediction of pressure. These resonance trackers increase the computational cost and are complicated to program.

In this article we reformulate an orbital based average atom model in terms of the single-particle Green's function. The Green's function has a useful property that it is analytic in the upper half energy plane and has a non-negative imaginary part (i.e. the Hergoltz property). This means that integrals over energy along the real axis can instead be deformed into the complex energy plane, along any (numerically convenient) contour. The advantage to this is that the Green's function lying along the real axis is broadened at complex energies by a Lorentzian of half-width equal to the imaginary part of the complex energy. Therefore any structures that need to be resolved for accurate real energy integrations, including narrow resonances, are broadened automatically in the complex plane. The contour integration over energy can therefore be easily evaluated without adaptive grids for resonance tracking.

As an added benefit, bound states are treated numerically in exactly the same way as continuum states in

the Green's function approach. Along the real energy axis, the density of states (DOS) of a bound state is a Dirac delta function at the bound state eigen-energy, and a search algorithm must be used to find all bound states. In the complex plane the DOS becomes a continuous Lorentzian, so no search algorithm is necessary.

While this reformulation is interesting in its own right, for the reasons just discussed it also offers a significant numerical speed-up and a reduction in computational complexity, without changing the physical content or indeed the results. For clarity, let us repeat; the converged results from this Green's function approach are identical to the corresponding orbital based model (within numerical tolerance).

To our knowledge this is the first formulation and numerical evaluation of an average atom model in terms of Green's functions, though it has been noted previously that the average atom orbitals can be interpreted as spectral functions of the Green's functions [18]. However, the Green's function formulation of a 'single-center' problem and the use of complex energy integration is not new, and has been extensively used in solid-state physics for many decades [19–21]. There it is part of a broader method known as Korringa-Kohn-Rostoker Green's Function (KKR-GF), which has recently found its first application in dense plasma physics [22].

The structure of this article is as follows: In section II we briefly review the average atom model that is used throughout this article to demonstrate the Green's function method. However the method is equally applicable to other Kohn-Sham based average atom models [1–3, 10, 11, 23]. In section III we give the main equations for the Green's function formulation. We demonstrate the contour integration method and the broadening of resonances and bound states both theoretically and in a numerical example. In section IV we give our conclusions. Two appendices are provided, discussing the calculation of wavefunctions and automatic contour generation.

II. AVERAGE ATOM PHYSICAL MODEL

In the present average atom model we consider a sphere of radius R (volume V) containing an nucleus of charge Z at its center (the origin) and electrons of density $n_e(\mathbf{r})$. The sphere is charge neutral, i.e.

$$\int_V d\mathbf{r} n_e(\mathbf{r}) = Z \quad (1)$$

The non-relativistic Kohn-Sham Hamiltonian is

$$\mathcal{H}(\mathbf{r}) = -\frac{\hbar^2}{2m_e} \nabla^2 + V^{eff}(\mathbf{r}) \quad (2)$$

Here the effective interaction is given by

$$V^{eff}(\mathbf{r}) = (V^{el}(\mathbf{r}) + V^{xc}(\mathbf{r})) e^2 \quad (3)$$

where the electrostatic part is

$$V^{el}(\mathbf{r}) = -\frac{Z}{r} + \int_V d\mathbf{r}' \frac{n_e(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \quad (4)$$

and the exchange and correlation part is

$$V^{xc}(\mathbf{r}) = \frac{\delta F^{xc}}{\delta n_e(\mathbf{r})} \quad (5)$$

For the exchange and correlation free energy F^{xc} we have used the finite temperature expression of [24]. By construction the potentials and electron densities are spherically symmetric.

In orbital based average atom calculations one solves the Schrödinger equation for the one-electron orbitals $\psi_\epsilon(\mathbf{r})$ at energy ϵ , and constructs the electron density with

$$n_e(r) = 2 \int_{-\infty}^{\infty} d\epsilon f(\epsilon) |\psi_\epsilon(\mathbf{r})|^2 \quad (6)$$

where f_ϵ is the Fermi-Dirac occupation factor

$$f(\epsilon) = \frac{1}{\exp(\beta(\epsilon - \mu)) + 1} \quad (7)$$

and $\beta = 1/(k_B T)$ is the inverse temperature. μ is the ideal (non-interacting) contribution to the electronic chemical potential. The part of the integral in equation (6) from $-\infty$ to 0 reduces to a finite summation over all bound states since their density of states are Dirac delta functions at their eigen-energies [25]. The integral from 0 to ∞ is over the continuum of positive energy states.

The self-consistent procedure for solving these equations is as follows:

1. start with an initial guess at the potential $V^{eff}(r)$
2. solve the Schrödinger equation for the orbitals ψ_ϵ

3. construct an electron density from these orbitals (equation (6)) and vary μ until charge neutrality is satisfied (equation (1))
4. calculate a new potential from this electron density using equations (3), (4) and (5)
5. using a linear combination of the new and old potentials as a new guess for V^{eff} , iterate steps 2 through 4 until the new potential is the same as the old one to within a numerical tolerance.

Calculation of the electron density with equation (6) requires searching for bound states and accurately evaluating the integral over continuum states. The integrand for this latter can be highly structured and therefore require a large number of energy points and a sophisticated algorithm to make sure that sharp features are found and accurately resolved [2].

In the following section it is shown that the electron density can be evaluated using a Green's function approach which guarantees that structures in the continuum integration are smooth and slowly varying and moreover, ameliorates the search for bound states.

III. GREEN'S FUNCTION FORMULATION

In terms of the one-electron Green's function $G(\mathbf{r}, \mathbf{r}', z)$, the spherically symmetric electron density is given by [21]

$$n_e(r) = -\frac{2}{\pi} \text{Im} \int_{-\infty}^{\infty} dz f(z) G(r, r, z) \quad (8)$$

where the integral over (complex) energy z is along the real axis, $f(z)$ is the Fermi-Dirac occupation factor (equation (7)) and the Green's functions is given by

$$G(\mathbf{r}, \mathbf{r}', z) = -ip \sum_L R_l(r_<, z) H_l(r_>, z) Y_L(\mathbf{r}) Y_L^*(\mathbf{r}') \frac{4\pi\epsilon_0\hbar}{m_e e^4} \quad (9)$$

Here $\mathbf{r}$ and $\mathbf{r}'$ are spatial coordinates, $p = \sqrt{(2m_e z / \hbar^2)}$ is the momentum, $L = \{l, m\}$ is combined notation for the orbital angular momentum and magnetic quantum numbers, Y_L are the spherical harmonics, and $r_{<(>) } = \min(\max)(r, r')$. $R_l(r) = P_l(r)/r$ and $H_l(r) = I_l(r)/r$, where P_l and I_l are the regular and irregular solutions of the radial Schrödinger equation (appendix A)

$$\left[-\frac{\hbar^2}{2m_e} \left(\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} \right) + V^{eff}(r) - z \right] \begin{Bmatrix} P_l(r) \\ I_l(r) \end{Bmatrix} = 0 \quad (10)$$

We note that since z is in general complex, so are P_l and I_l . The wave functions R_l and H_l are normalized such that for $r \geq R$ they take the field free form, i.e.

$$R_l(r) = j_l(pr) - ip h_l^+(pr) t_l(p) \quad (11)$$

$$H_l(r) = h_l^+(pr) \quad (12)$$

FIG. 1: (Color online) Schematic example of a contour for energy integration. The dashed blue line is the integration contour C in equation (16).

where $h^+ = j_l + i\eta_l$ is the spherical Hankel function, j_l is the spherical Bessel function and η_l is the spherical Neumann function. t_l is the so-called t-matrix element, defined in appendix A. It is straightforward to show that the Green's function expression for the electron density (equation (8)) recovers the usual orbital based expression by noting that on the real axis the wave functions can be chosen to be real.

For the present spherically symmetric system the expression for the Green's function simplifies to

$$G(r, r, z) = -ip \sum_{l=0}^{\infty} \frac{(2l+1)}{4\pi} R_l(r) H_l(r) \frac{4\pi\epsilon_0\hbar}{m_e e^4} \quad (13)$$

where we have dropped explicit reference to the energy z in R_l and H_l . When the interaction potential $V^{eff}(r)$ is identically zero the t-matrix also becomes zero and the Greens function is given by

$$G^0(r, r, z) = -ip \sum_{l=0}^{\infty} \frac{(2l+1)}{4\pi} j_l(pr) h_l^+(pr) \frac{4\pi\epsilon_0\hbar}{m_e e^4} \quad (14)$$

We note also that the density of states (DOS) is given in terms of the Green's function by

$$\chi(z) = -\frac{2}{\pi} \text{Im} \int_V d\mathbf{r} G(r, r, z) \quad (15)$$

If we were to use equations (8) and (13) to evaluate the electron density there would be no advantage over the orbital based approach. However, because of the analytic properties of the Green's function and the Fermi-Dirac function in the upper half z -plane, the integral along the real energy axis in equation (8) can be rewritten using Cauchy's residue theorem. The resulting expression for the electron density is [26, 27]

$$n_e(r) = \frac{2}{\pi} \text{Im} \int_C dz f(z) G(r, r, z) + 4k_B T \text{Re} \left[\sum_{j=1}^{N_m} G(r, r, z_j) \right] \quad (16)$$

FIG. 2: (Color online) Example of a density of states (DOS), for aluminum at 1.35 g/cm³ and 400 eV. The dashed black lines show the result of the orbital based approach along the real axis. For $\text{Re}(z) < 0$ the 4s, 4p and 4d bound states are seen, while for $\text{Re}(z) > 0$ we find a sharp resonance feature that must be tracked numerically (note the logarithmic scale). Adding a small imaginary component (0.05 E_H) to the energy, the DOS is broadened as shown by the solid red line. For a larger imaginary component (1 E_H) all structure is completely smoothed out and the numerical integral is much easier (and quicker) to perform.

where the integral is in the counter-clockwise direction along a contour C , and the sum is over the residues of the N_m poles enclosed by this contour and the real axis. There are no poles in the Green's function for $\text{Im}(z) > 0$, but the Fermi-Dirac function has poles at the so-called Matsubara frequencies z_j

$$z_j = \mu + (2j-1)i\pi k_B T \quad (17)$$

for $j = 1, 2, \dots$, with residues of $-k_B T$. In principle the contour C should join the real axis at $\pm\infty$. In practice however, the integral along the real axis has effective lower and upper bounds E_{min} and E_{max} . E_{max} is chosen so that the Fermi-Dirac function has decayed sufficiently. For E_{min} it is convenient to choose it such that very deeply bound states are treated with the usual search methods [28], while more loosely bound states are included with the Green's function calculation. A schematic example of a contour illustrating these concepts is shown in figure 1. Due to the integral theorem, one is free to choose whichever contour one wishes provided it rejoins the real axis at E_{min} and E_{max} . The main challenge in the numerical implementation of this Green's function approach is the automatic generation of a contour that requires a small number of integration points and avoids the Matsubara poles. In appendix B we address this issue.

For complex energy $z = \epsilon + i\gamma$ the Greens function can be expressed in terms of the imaginary part of the Green's function along the real axis [26]. In turn the density of states (DOS) at complex energies can be related to the

FIG. 3: (Color online) Example of an integrand of equation (16) along a contour, for aluminum at 1.35 g/cm³ and 400 eV. Note that for this case $\mu = -73.1 E_H$ so there are no Matsubara poles ($N_m = 0$) within the contour.

DOS along the real axis as

$$\chi(z) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\epsilon' \frac{\gamma}{(\epsilon - \epsilon')^2 + \gamma^2} \chi(\epsilon') \quad (18)$$

This remarkable result means that any sharp features in the DOS along the real axis (including bound states and resonances) are automatically broadened by a Lorentzian of half-width γ . To illustrate this point an example is given in figure 2. Sharp structure in the DOS on the real energy axis is caused by both bound states and a resonance. Both are completely smoothed out by using $\gamma = 1 E_H$. One might think that electron states have been lost through this method, until it is remembered that the contour must return to the real axis.

In figure 3 we give an example of an integrand of equation (16) that must be numerically integrated. Clearly the integrand is smoothly varying and can be easily integrated numerically. In contrast, for the real energy integration we must track the bound and resonance states (see figure 2). In practice we calculate the difference between the the Green's function and its free electron counter part (equation (14)). This allows for more rapid convergence of the orbital angular momentum summation in equation (13). This is the same numerical trick that is used in the orbital-based average atom models [25, 29, 30].

In summary, we use equations (13) and (16) to calculate the electron density, with the contour described in appendix B. The computational cost of our implementation of this method ranges from 40 seconds to 5 minutes on a single Intel Xeon 2.60GHz processor for aluminum at 1.35 and 80 g/cm³ at 1 and 500 eV. The time depends on the maximum orbital angular momentum needed which increases with temperature and as density is lowered. No particular effort was made to make the implementation

as efficient as possible, so it is possible that significant computational cost savings could be found. For the same accuracy (agreement on μ to <0.01%), on the same machine, our optimized orbital based implementation takes 2.5 – 25 minutes.

Perhaps the main purpose of average atom models is for equation of state calculations. Using the Green's function approach the calculation of most of the terms contributing to the free energy does not change as they depend only on the electron density [1]. However, the entropic contribution to the free energy F_s is given by the expression

$$F_s = -k_B T \int_{-\infty}^{\infty} dz \left(\frac{\hbar^2}{m_e} \right) S(z) \chi(z) \quad (19)$$

where

$$S(z) = f(z) \ln(f(z)) + (1 - f(z)) \ln(1 - f(z)) \quad (20)$$

The energy integral in equation (19) is along the real energy axis. It cannot be deformed onto any arbitrary contour due to the presence of the multi-valued natural logarithm. We cannot cross the branch-cut parallel to the real axis at the first Matsubara energy, i.e. it is required that $\text{Im}(z) < \pi k_B T$ at all points of the contour. However, since the entropy is only needed at the end of the self-consistent calculation, once convergence has already been reached, this does not present a serious problem. Either a one-off integration along the real axis or a contour satisfying this restriction can be used. Moreover, for high enough temperature ($\gtrsim 13$ eV) the same contour as is described in appendix B for the self-consistent calculation can be used, since the first Matsubara energy is far enough away from the real axis.

IV. CONCLUSIONS

We have demonstrated that a Green's function method widely used in solid state physics [21, 31–33] can be used to reformulate Kohn-Sham density functional theory based average atom models. Aside from the elegance of the method, it has been shown that significant numerical advantages are found, without changing the physical content or results of the model. In particular the Green's function method circumvents the need for numerically costly resonance tracking. The method applies to bound and continuum states equally. A simple implementation of the method was found to result in up to a factor of 5 speed-up relative to an optimized orbital based implementation. Finally, we note that while the present implementation is non-relativistic, a relativistic, Dirac equation based treatment is also possible [31].

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Appendix A: Calculation of wavefunctions

To calculate the regular solution of the Schrödinger equation $R_l(r) = P_l(r)/r$ standard methods that are analogous to the usual methods for orbital based calculations [28] can be used. The complex nature of the solution does not seriously complicate matters. A good description of an algorithm is found in [31]. Calculation of the irregular solution $H_l(r) = I_l(r)/r$ is similar with the key difference being that one should integrate inwards from the cell boundary, using the free wave solution (equation (12)) to initialize the calculation.

Let the unnormalized regular and irregular numerical solutions be denoted $\bar{R}_l$ and $\bar{H}_l$ respectively. At the sphere boundary ($r = R$), in general we have

$$\begin{aligned} R_l(r) &= a_l \bar{R}_l(r) \\ &= j_l(pr) - \imath p h_l^+(pr) t_l(p) \\ H_l(r) &= b_l \bar{R}_l(r) + c_l \bar{H}_l(r) \\ &= h_l^+(pr) \end{aligned}$$

because the irregular solution diverges at the origin, but the regular does not. Requiring continuity of R_l and H_l and their radial derivatives with their free solutions at the boundary allows one to determine the energy dependent constants a_l , b_l and c_l as well as the t-matrix element t_l . The result for the t-matrix is

$$t_l = \frac{1}{\imath p} \frac{j_l'(pr) \bar{R}_l(r) - j_l(pr) \bar{R}_l'(r)}{h_l^{+\prime}(pr) \bar{R}_l(r) - h_l^+(pr) \bar{R}_l'(r)}$$

where the prime indicates differentiation with respect to r . This normalization and the corresponding expression for the Green's function (equation (9)) are sometimes called the Jülich convention [21]. A frequently used alternative formulation, sometimes known as the Oak Ridge-Bristol convention, uses the so-called scattering solutions [34] $\{Z_l, J_l\}$. The regular scattering solution is normalized so that at the sphere boundary ($r = R$)

$$Z_l(r) = j_l(pr) t_l^{-1} - \imath p h_l^+(pr)$$

We have found this normalization to be numerically unstable for plasma applications where we frequently encounter solutions such that $t_l \rightarrow 0$. However, it is important to note that both conventions formally give exactly the same results.

Appendix B: Automatic contour generation

At each step in the self-consistent procedure we generate a contour that allows for an accurate energy integration. We have used the rectangular path illustrated in figure 1, though other choices are possible. To define this path we need to pick E_{min} , E_{max} and the imaginary part of the energy on the section parallel to the real axis E_I . Let us first address E_{min} . Bound states with energy less than E_{min} are treated with the usual search techniques [28]. Those with energy greater than E_{min} are treated with the Green's function formalism. Perhaps the simplest choice is $E_{min} = 0$. Then, by using standard methods to search for bound states one is guaranteed that no double counting of states will occur. However, we have found it to be more numerically efficient to choose E_{min} to lie at a negative energy, typically with magnitude of a few E_H or less. Using an initial guess for the interaction potential V^{eff} given by the Thomas-Fermi model [15], we first search for all bound states of that potential. This gives a good initial estimate of the final bound state structure. Next we select E_{min} so that it falls in a gap between (the energy ordered) bound states, which is sufficiently large ($\gtrsim 1E_H$) so that it is very unlikely that a bound state energy will change enough during the self-consistent procedure to be either missed or double counted.

E_{max} is chosen so that the Fermi-Dirac occupation factor has decayed to a very small number, e.g. 10^{-10} . The energy position that this occurs depends on the chemical potential μ , and we used the previous iterations' result.

For the choice of E_I we have opted for a scheme that attempts to pick $E_I = 1 E_H$. We are constrained however, by the necessity of avoiding the Matsubara energies. For sufficiently large temperatures ($\gtrsim 13\text{eV}$) the first Matsubara energy lies far enough above $E_I = 1 E_H$ that there is no problem. For lower temperatures we set $E_I = 2N_m \pi k_B T$, where N_m is the number of Matsubara energies inside the contour such that E_I is as close to $1 E_H$ as possible.

To integrate along the sections of the contour we divide each section into panels, and treat each panel using a 4-point Gauss-Legendre formula. The number of panels used depends on the accuracy required. Typically one might use 1 panel for the section of the contour going from $z = E_{max}$ to $z = E_{max} + \imath E_I$, 20 for $z = E_{max} + \imath E_I$ to $z = E_{min} + \imath E_I$ and 20 for the return to the real axis, i.e. 164 points in total. We have found this contour to give accurate and stable results for various elements from one-half to fifty times solid density and for temperatures ranging from 1 to 500 eV.

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