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Wigner High Electron Correlation Regime in Nonuniform Electron Density Systems: Kinetic and Correlation-Kinetic Aspects

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Abstract

The Wigner high electron correlation regime is characterized in the literature by an electron-interaction energy much greater than the kinetic energy. Via the ‘quantal Newtonian’ first law, we discover that for a nonuniform electron density system in this regime, there is a ‘quantal compression’ of the kinetic energy density. The explanation of this compression provides a fundamental understanding for why the kinetic energy is a smaller fraction of the total energy relative to the same ratio in the low correlation regime. We also discover by application of quantal density functional theory, that the contribution of electron correlations to the kinetic energy – the correlation-kinetic effects – and to the total energy is very significant. We propose that in addition to a high electron-interaction energy, the Wigner regime must thus also be characterized by a high correlation-kinetic energy.

The Wigner high correlation regime of a system of N electrons in the presence of an external field $\mathcal{F}^{ext} = -\nabla v(\mathbf{r})$ is a new state of matter that has been observed experimentally. It is characterized by very low electronic density $\rho(\mathbf{r})$, and an electron-interaction energy significantly larger than the kinetic energy. For weakly confining external potentials $v(\mathbf{r})$, the kinetic energy then constitutes an even smaller fraction of the sum of the electron-interaction and external potential energies, thereby leading to a localization of the charge. A study of the Wigner regime of an electronic system can thus provide insights into the correlations between the electrons; the contributions of these correlations to the kinetic energy – the correlation-kinetic effects; and to why the kinetic energy is a smaller fraction of the total energy. This Letter is a brief description of such a study of the Wigner regime for an inhomogeneous electron density system with a focus on the kinetic and correlation kinetic aspects.

The crystallization of such a low density electron gas in the presence of a uniform positive charge background – the jellium – model, was originally proposed by Wigner [1, 2]. With a large lattice constant, and low kinetic energy, the potential energy is minimized with the electrons localized in a body-centered cubic lattice. Studies of the system have determined the energy, specific heat, and magnetic properties [3, 4]. There has also been work on the transition density for the onset of Wigner crystallization [5–7]. The Wigner crystal has been

observed experimentally in the two-dimensional electron systems on the surface of liquid helium, and in GaAs - GaAlAs heterostructures in the presence of strong magnetic fields [8–10]. Another model that allows for a study of the Wigner regime in a nonuniform electron density system is the Hooke's atom [11–13]. This atom is comprised of two electrons that interact Coulombically but are confined harmonically, the regime being achieved for weak confinement. The principal attribute of the model is that for particular, denumerably infinite set of the harmonic force constants, closed-form analytical solutions of the Schrödinger equation can be obtained [13] for both ground and excited states. Work on the Wigner regime employing this model has been performed [13–17] including the determination of the critical force constant k for transition to this regime ($k_{crit} \approx 1.6093 \times 10^{-3}$), and the determination of the natural orbitals in the limit of vanishing force constant. As shown in Fig. 1, drawn for a ground state corresponding to $k \approx 3.00891 \times 10^{-4}$, the regime is characterized by a density surrounding the nucleus that is less than the maximum value, with a local minimum at the nucleus – the 'fat attractor' profile [15]. (In contrast, for the low correlation regime, the density is a maximum at the nucleus.)

In this Letter we consider the Hooke's atom in the Wigner regime for the force constant of Fig. 1, and focus principally on the kinetic and correlation-kinetic components. (The discussion of the electron-interaction energy, and its Hartree, Pauli, and Coulomb components, and their corresponding quantal sources, is to be given elsewhere [18].) Employing the 'quantal Newtonian' first law [19–21] which involves the fields acting on each electron, we explain how the decrease in kinetic energy, relative to the electron-interaction and total energy, is a consequence of a 'quantal compression' of the kinetic energy density near the nucleus. Then, by mapping this interacting system to one of *noninteracting* fermions in a ground state with the same density $\rho(\mathbf{r})$ via quantal density functional theory [19, 20] (QDFT), we discover that although there is a decrease in the kinetic energy, there is a substantial increase in the correlation-kinetic contribution. Thus, in the Wigner regime, not only do electron correlations dominate as reflected in the electron-interaction energy, they contribute significantly to the kinetic energy.

The Hooke's atom Hamiltonian in atomic units ($e = \hbar = m = 1$) is $\hat{H} = \hat{T} + \hat{U} + \hat{V}$; $\hat{T} = \frac{1}{2} \sum_i \nabla_i^2$, $\hat{U} = \frac{1}{2} \sum_{i,j} 1 / |\mathbf{r}_i - \mathbf{r}_j|$, $\hat{V} = \frac{k}{2} \sum_i r_i^2$; $i = 1, 2$. In our calculations, we employ the *exact* Wigner regime ground state wave function of the Schrödinger equation $\hat{H}\Psi = E\Psi$ which is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = N e^{-\omega R^2} e^{-\frac{1}{4}\omega s^2} \left[1 + \frac{s}{2} + \sum_{j=2}^4 a_j \left(s \sqrt{\frac{\omega}{2}} \right)^j \right], \quad (1)$$

where $R = |\mathbf{r}_1 + \mathbf{r}_2|/2$, $s = |\mathbf{r}_1 - \mathbf{r}_2|$, $N = 8.94669 \times 10^{-6}$, $\omega = \sqrt{k} = 1.73462 \times 10^{-2}$, $a_2 = 8.274917$, $a_3 = 4.720056$, $a_4 = 0.879153$.

In order to explain the concept of 'quantal compression' of the kinetic energy density that occurs in the Wigner regime, we present in Table I our results for energy component

expectation values together with those for the low correlation regime corresponding to $k = \frac{1}{4}$ [19, 22]. It is evident that in the high-correlation regime, the electron-interaction energy E_{ee} contributes a much greater fraction (43.4% vs 22.4%), and the kinetic energy T a much smaller fraction (17.4% vs 33.2%), of the total energy E , in comparison to the low correlation regime. The weakness of the external binding potential in the high correlation regime is evidenced by a comparison of the external E_{ext} and E_{ee} energies in each regime.

We next explain how the reduction in density surrounding the nucleus leads to a decrease in the kinetic energy. According to the ‘quantal Newtonian’ first law [19–21], the sum of the fields experienced by each electron must vanish: $\mathcal{F}^{ext} + \mathcal{F}^{int}(\mathbf{r}) = 0$, where the internal field $\mathcal{F}^{int}(\mathbf{r})$ is the sum of the electron-interaction, $\mathcal{E}_{ee}(\mathbf{r})$, kinetic $\mathcal{Z}(\mathbf{r})$, and differential density

$\mathcal{D}(\mathbf{r})$ fields: $\mathcal{F}^{int}(\mathbf{r}) = \mathcal{E}_{ee}(\mathbf{r}) - \mathcal{Z}(\mathbf{r}) - \mathcal{D}(\mathbf{r})$ with $\mathcal{E}_{ee}(\mathbf{r}) = \mathbf{e}_{ee}(\mathbf{r}) / \rho(\mathbf{r})$, $\mathcal{Z}(\mathbf{r}) = \mathbf{z}(\mathbf{r}) / \rho(\mathbf{r})$,

$\mathcal{D}(\mathbf{r}) = \mathbf{d}(\mathbf{r}) / \rho(\mathbf{r})$. The corresponding ‘forces’ are $\mathbf{e}_{ee}(\mathbf{r}) = \int d\mathbf{r}' P(\mathbf{r}\mathbf{r}')(\mathbf{r} - \mathbf{r}')/|\mathbf{r} - \mathbf{r}'|^3$ (Coulomb’s law); $\mathbf{z}_\alpha(\mathbf{r}) = 2 \sum_\beta t_{\alpha\beta}(\mathbf{r}) / r_\beta$,

$t_{\alpha\beta}(\mathbf{r}) = \frac{1}{4} \left[\partial^2 \left(\partial r'_\alpha \partial r''_\beta + \partial^2 \left(\partial'_\beta \partial r''_\alpha \right) \gamma(\mathbf{r}'\mathbf{r}'') \right) \right]_{\mathbf{r}' = \mathbf{r}'' = \mathbf{r}}$; $\mathbf{d}(\mathbf{r}) = -\frac{1}{4} \nabla \nabla^2 \rho(\mathbf{r})$. The quantal

sources of these fields are expectations taken with respect to the wave function of Hermitian operators: the pair function $P(\mathbf{r}\mathbf{r}') = \langle \hat{P}(\mathbf{r}\mathbf{r}') \rangle$, $\hat{P}(\mathbf{r}\mathbf{r}') = \sum_{i \neq j} \delta(\mathbf{r}_i - \mathbf{r}) \delta(\mathbf{r}_j - \mathbf{r}')$; the single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}') = \langle \hat{\gamma}(\mathbf{r}\mathbf{r}') \rangle$, $\hat{\gamma}(\mathbf{r}\mathbf{r}') = \hat{A} + i\hat{B}$,

$\hat{A} = \frac{1}{2} \sum_j [\delta(\mathbf{r}_j - \mathbf{r}) T_j(\mathbf{a}) + \delta(\mathbf{r}_j - \mathbf{r}') T_j(-\mathbf{a})]$, $\hat{B} = -\frac{i}{2} \sum_j [\delta(\mathbf{r}_j - \mathbf{r}) T_j(\mathbf{a}) - \delta(\mathbf{r}_j - \mathbf{r}') T_j(-\mathbf{a})]$,

$T_j(\mathbf{a})$ is a translation operator $T_j(\mathbf{a}) \psi(\dots \mathbf{r}_j \dots) = \psi(\dots \mathbf{r}_j + \mathbf{a}, \dots)$, $\mathbf{a} = \mathbf{r}' - \mathbf{r}$; the density

$\rho(\mathbf{r}) = \langle \hat{\rho}(\mathbf{r}) \rangle$, $\hat{\rho}(\mathbf{r}) = \sum_i \delta(\mathbf{r}_i - \mathbf{r})$. For the Hooke’s atom in its ground state, the individual

fields are each conservative. The corresponding energies are $E_{ee} = \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{E}_{ee}(\mathbf{r}) / d\mathbf{r}$,

$T = -\frac{1}{2} \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{Z}(\mathbf{r}) d\mathbf{r}$, and $E_{ext} = \int \rho(\mathbf{r}) \mathbf{r}(\mathbf{r}) d\mathbf{r}$. The field $\mathcal{E}_{ee}(\mathbf{r})$ accounts for electron

correlations due to the Pauli exclusion principle and Coulomb repulsion.

In Fig. 2 we plot the kinetic ‘force’ $\mathbf{z}(\mathbf{r})$. Observe that since the density surrounding the nucleus ($r \leq 5$ a.u.) is less than the maximum value, the kinetic ‘force’ is negative in this region. Since there also exists a strong negative gradient with respect to the kinetic ‘force’ in this region, the divergence must also be negative there. This divergence plotted in Fig. 3, thus reflects a net flow of kinetic ‘force’ directed towards the interior of any infinitesimal spherical volume surrounding the Hooke’s atom nucleus in its proximate vicinity. As its global extremum is achieved at the nucleus, this implies a ‘quantal compression’ of the kinetic energy density $\kappa(r) = \text{Tr } t_{\alpha\beta}(\mathbf{r})$ in this region as shown in Fig 4. In the region $5.5 \leq r \leq 12$ a.u., the divergence is positive thereby resulting in a depletion of the kinetic ‘force’ vector from this region, leading to a decrease in $\kappa(r)$. The divergence is again negative for $12 \leq r \leq 19$ a.u. giving rise to another though weaker ‘quantal compression’ in this region. The ‘quantal compression’ of the kinetic energy density near the nucleus explains why the kinetic energy contribution in the Wigner regime is small. For small values of r , the kinetic energy density is large. Thus, from the alternate definition of $T = \int \kappa(\mathbf{r}) d\mathbf{r}$, it becomes evident why this is the case. This also explains why the kinetic energy as a fraction of the total energy is small. In contrast (see Fig. 5), for the low correlation regime, there is a

‘quantal decompression’ of the kinetic energy density near and about the nucleus with the maximum of this function occurring for larger values of the radius. Correspondingly, the kinetic energy value relative to the total energy is larger (see Table I).

Another key difference is that since in the high correlation regime, the electrons are localized to a spherical shell, the angular contribution to the kinetic energy density tensor is as significant as the radial component and in fact an order of magnitude greater near the nucleus. By sphericalization and rotation the kinetic energy density tensor $t_{\alpha\beta}(\mathbf{r})$ in $\mathbb{R}^3$ space can be reduced [18] to a new high symmetry 2nd rank tensor in $\mathbb{R}^2$ space which is

$$\tau_{\mu\nu} = \begin{bmatrix} \tau_{rr}(r) & 0 \\ 0 & \tau_{\theta\theta}(r) \end{bmatrix}, \quad (2)$$

where the radial component $\tau_{rr}(r) = (1/8\pi) \int \gamma_{r'r''}(r, \theta) d\Omega$, the angular component $\tau_{\theta\theta}(r) = (1/8\pi^2) \int \gamma_{\theta'\theta''}(r, \theta) d\Omega$, and $\gamma_{r'r''}(r, \theta) = \frac{\partial}{\partial r'} (\frac{\partial}{\partial r''} \gamma(r', \theta'; r'', \theta'')) \big|_{r'=r''=r, \theta'=\theta''=\theta}$

$\gamma_{\theta'\theta''} = \frac{\partial}{\partial \theta'} (\frac{\partial}{\partial \theta''} \gamma(r', \theta'; r'', \theta'')) \big|_{r'=r''=r, \theta'=\theta''=\theta}$. The radial $\tau_{rr}(r)$ and the angular $\tau_{\theta\theta}(r)$ components

are plotted in Fig. 6. Note how much more significant the angular component is near and about the nucleus.

In the low correlation regime, the angular component is less significant [18, 19, 22]. These details too are to be given in [18]. We conclude this section by noting that while the choice of different force constant can explain the reduction in the kinetic energy in the Wigner regime, it cannot explain the remarkable suppression of the kinetic energy to total energy ratio experienced by this regime. The more fundamental understanding thus required is achieved via the ‘quantal Newtonian’ first law perspective. It is the knowledge of the kinetic field via its divergence that explains the change in the structure of the kinetic energy density – the ‘quantal compression’ – in the Wigner regime, as opposed to the ‘quantal decompression’ in the low correlation case.

To determine the correlation-kinetic energy T_c contribution to the kinetic energy T , we map the interacting system to one of noninteracting fermions – the S system – in a ground state with the same density $\rho(\mathbf{r})$ via QDFT. (The reason for this choice of property for the equivalence is because the density is a basic variable of quantum mechanics [23, 24]: it is a gauge invariant property that uniquely determines the external potential, thereby the Hamiltonian, and by solution of the Schrödinger equation, the wave function.) With the assumption that the model fermions experience the same external field, the corresponding Schrödinger equation is $[-\frac{1}{2}\nabla^2 + v(\mathbf{r}) + v_{ee}(\mathbf{r})]\phi_i = \epsilon_i\phi_i (i = 1, 2)$, the wave function is the Slater determinant $\Phi\{\phi_i\}$ and where $v_{ee}(\mathbf{r})$ is the local (multiplicative) potential that incorporates the many body correlations due to the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects. (The correlation-kinetic contribution is a consequence of the difference in the kinetic energy of the interacting and model systems having the same density $\rho(\mathbf{r})$.) The corresponding S -system ‘quantal Newtonian’ first law is

$\mathcal{F}^{ext}(\mathbf{r}) + \mathcal{F}_s^{int}(\mathbf{r}) = 0$ with $\mathcal{F}_s^{int}(\mathbf{r}) = -\nabla v_{ee}(\mathbf{r}) - \mathcal{Z}_s(\mathbf{r}) - \mathcal{D}(\mathbf{r})$ with the $\mathcal{S}$ -system kinetic field $\mathcal{Z}_s(\mathbf{r}) = \mathbf{z}_s(\mathbf{r}) / \rho(\mathbf{r})$. The kinetic ‘force’ $\mathbf{z}_s(\mathbf{r})$ is defined as for the interacting system, but its quantal source is the Dirac density matrix $\gamma_s(\mathbf{r}\mathbf{r}')$ which is the expectation $\langle \hat{\gamma}(\mathbf{r}\mathbf{r}') \rangle$ taken with respect to $\Phi\{\phi_j\}$. The potential $v_{ee}(\mathbf{r})$ is the work done on the model fermion in the conservative effective field $\mathcal{F}^{eff}(\mathbf{r}) = \mathcal{E}_{ee}(\mathbf{r}) + \mathcal{Z}_t(\mathbf{r})$, where $\mathcal{Z}_t(\mathbf{r}) = \mathcal{Z}_s(\mathbf{r}) - \mathcal{Z}(\mathbf{r})$ is the correlation-kinetic field.

The $\mathcal{S}$ -system kinetic ‘force’ $\mathbf{z}_s(\mathbf{r})$ and kinetic energy density $t_s(\mathbf{r})$ are plotted in Figs 2 and 4, respectively. Observe the cancelation of the ‘forces’ $\mathbf{z}(\mathbf{r})$ and $\mathbf{z}_s(\mathbf{r})$ in the asymptotic region away from the nucleus. In the region near the nucleus, the fields are distinctly different. Also observe that $t_s(\mathbf{r})$ is an order of magnitude smaller than $t(\mathbf{r})$. The correlation-kinetic field $\mathcal{Z}_t(\mathbf{r})$ is plotted in Fig 7. Note that this field is positive. Thus, the correlation-kinetic energy

$T_c = \frac{1}{2} \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{Z}_t(\mathbf{r}) d\mathbf{r}$ or equivalently $T_c = \int [t(\mathbf{r}) - t_s(\mathbf{r})] d\mathbf{r}$ (see Fig 4) is also positive (see

Table I) as must be the case for a mapping to the model system in its ground state [20]. What is remarkable is that the correlation contribution T_c to the kinetic energy T is 27%, and 4.5% of the total energy E . Furthermore, the *total* contribution of electron correlations ($T_c + E_{ee}$) to the energy E is 48%.

Yet another comparison that can be made is via analogy to the uniform electron gas jellium model. In this model, the contributions of the potential due to the (external) jellium positive charge background and the Hartree component of the electron-interaction potential cancel. As such, the Hartree term is absent in the final energy expression, and thus so too in subsequent comparisons between the high and low correlation regimes. In the nonuniform electron gas case, there is no such cancellation between the external and Hartree terms. However, to draw a parallel with the uniform gas case, we include in Table I, a comparison of the ratio $(E_{ee} - E_H + T_c)/T_s$ in which the Hartree energy E_H is eliminated. As may be observed, the value of this ratio in the Wigner regime is an order of magnitude greater than that for the low correlation regime. This difference will increase as one ventures further into the Wigner regime of smaller density. Thus, this ratio can be employed to further categorize the Wigner regime for the nonuniform density system.

As a consequence of the above comparisons, we propose that one must now define the Wigner high correlation regime of an inhomogeneous electron gas as one characterized not *solely* by a high electron-interaction energy value but also as one that possesses a high correlation-kinetic energy relative to the total energy.

We conclude by noting that in order to perform the above calculations, we have developed accurate numerical codes employing in particular the Fourier and Chebyshev pseudo-spectral method [25, 26]. This allows for the rapid determination of the nonlocal quantal sources of the pair function and the interacting system density matrix, and various derivatives of the latter. This work too is to be described elsewhere [18].

It is interesting to note that in the low correlation regime, correlation-kinetic effects also play a more significant role with a reduction in dimensionality as in quantum dots [27]. Thus, we expect that these effects will be even more pronounced in two-dimensional electron systems in the Wigner regime. (Other than [27], correlation-kinetic effects have not been previously considered [28] in such systems.) Work towards an analysis of the Hooke's atom in the presence of a magnetic field [29, 30] in this regime is in progress. Finally, the present results constitute part of a complete QDFT analysis [18] of the mapping from the interacting to the model system. Hence, all the properties of the latter including the potential $v_{ee}(\mathbf{r})$ and its Hartree, Pauli, Coulomb, and Correlation-kinetic components are known. These results can then be employed to test and further develop the various approximate Kohn-Sham theory [31] electron-interaction $E_{ee}[\rho]$ or 'exchange-correlation' $E_{xc}[\rho]$ energy functionals of the density in the literature [32]. More recently [33–38] there has been work on the construction of approximate energy functionals for strongly interacting electrons which too could be tested. Such tests would be meaningful particularly in light of the fact that correlation-kinetic effects play so significant a role in this regime. The results of the present work could also prove to be valuable in the construction of new $E_{xc}[\rho]$ functionals which must now explicitly account for the correlation-kinetic effects. As is evident from Table I, the value of the correlation-kinetic energy T_c diminishes as one proceeds further into the Wigner regime, but the ratio of this value relative to the kinetic energy T and the total energy E must increase. This structure must be replicated by these new functionals. The corresponding functional derivatives must replicate the local electron-interaction potential $v_{ee}(\mathbf{r})$ and its individual Hartree, Pauli, Coulomb, and Correlation-Kinetic components [18].

Finally, the relative contributions of the kinetic T and electron-interaction E_{ee} energies as explained in the context of the Hooke's atom in the Wigner regime, can be related to work [34] within standard density functional theory in the infinite electron-interaction coupling strength parameter λ limit i.e. in the limit of the high correlation Wigner regime. There, in an expansion about the classical potential minimum, there exists a zero-point kinetic energy term due to oscillations about the potential minimum (as in the original work of Wigner) that is proportional to $\sqrt{\lambda}$ and hence diverges in this limit, but the divergence is integrable. A similar expansion about the classical minimum for the Hooke's atom at small k also leads to a zero point kinetic energy term that is high. However, because of localization of the charge in this limit, the electron-interaction energy dominates (see Table I) as one proceeds further into the Wigner regime. On the other hand, as one approaches the low correlation regime (smaller values of λ), due to delocalization of the charge, the kinetic energy term then becomes more significant (see Table I). The localization and delocalization of the charge as a function of the strength of the coupling parameter λ is, of course, reflected by the sharp differences in the structure of the density. This then leads to the 'quantal compression' and 'quantal decompression' of the kinetic energy densities, and to the corresponding ratios T/E_{ee} (see Table I), as explained previously.

In summary, we have explained via the 'quantal Newtonian' first law why in the Wigner high correlation regime of a nonuniform electron gas there is a 'quantal compression' of the kinetic energy density. This in turn explains why in this regime the kinetic energy is a smaller fraction of the total energy. We further conclude, that in addition to a high electron-

interaction energy value, the Wigner regime must also be characterized by a high value of the correlation-kinetic energy.

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FIG. 1:
The electron density $\rho(r)$ for $k \approx 3.00891 \times 10^{-4}$.

FIG. 2:

Wigner regime ($k \approx 3.00891 \times 10^{-4}$) kinetic 'force' for the interacting ($z(r)$) and noninteracting ($z_s(r)$) systems.

FIG. 3:
The divergence of the kinetic 'force' of the interacting system in the Wigner regime ($k \approx 3.00891 \times 10^{-4}$).

FIG. 4: Wigner regime ($k \approx 3.00891 \times 10^{-4}$) kinetic energy densities for the interacting ($t(r)$) and noninteracting ($t_s(r)$) systems.

FIG. 5: Low correlation regime ($k = 1/4$) kinetic energy densities for the interacting ($t(r)$) and noninteracting ($t_s(r)$) systems [17, 20].

FIG. 6:
The radial $\tau_{rr}(r)$ and angular $\tau_{\theta\theta}$ components of the kinetic energy density tensor $\tau_{\mu\nu}$ in the Wigner regime ($k \approx 3.00891 \times 10^{-4}$).

FIG. 7:
The correlation-kinetic field $\mathcal{Z}_{t_c}(\mathbf{r})$ in the Wigner regime ($k \approx 3.00891 \times 10^{-4}$).

TABLE I:

The total E , kinetic T , correlation-kinetic T_c , external E_{ext} , Hartree E_H and electron-interaction E_{ee} energies in atomic units for the low correlation ($k = \frac{1}{4}$) [19, 22] and high correlation ($k \approx 3.00891 \times 10^{-4}$) regimes.

Property	$k = \frac{1}{4}$	$k \approx 3.00891 \times 10^{-4}$
E	2.000000	0.1214235
T	0.664418	0.021158
T_c	0.029173	0.005700
E_{ext}	0.888141	0.047527
E_{ee}	0.447443	0.052739
E_H	1.030250	0.151474
E_{ee}/E	22.4%	43.4%
T/E	33.2%	17.4%
T_c/T	4.4%	26.9%
T_c/E	1.45%	4.5%
$(T_c + E_{ee})/E$	24%	48%
$(E_{ee} - E_H + T_c)/T_s$	-0.871528	-6.018956