Secondary infall and the pseudo-phase-space density profiles of cold dark matter haloes

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ABSTRACT

We use N-body simulations to investigate the radial dependence of the density, ρ, and velocity dispersion, σ, in cold dark matter (CDM) haloes. In particular, we explore how closely Q ≡ ρ/σ^2, a surrogate measure of the phase-space density, follows a power law in radius. Our study extends earlier work by considering, in addition to spherically averaged profiles, local Q estimates for individual particles, Q_i; profiles based on the ellipsoidal radius dictated by the triaxial structure of the halo, Q(\rho); and by carefully removing substructures in order to focus on the profile of the smooth halo, Q^s. The resulting Q^s(\rho) profiles follow closely a power law near the centre, but show a clear upturn from this trend near the virial radius, r_200. The location and magnitude of the deviations are in excellent agreement with the predictions from Bertschinger’s spherical secondary-infall similarity solution. In this model, Q ∝ r^{-1.875} in the inner, virialized regions, but departures from a power-law occur near r_200 because of the proximity of this radius to the location of the first shell crossing – the shock radius in the case of a collisional fluid. Particles there have not yet fully virialized, and so Q departs from the inner power-law profile. Our results imply that the power-law nature of Q profiles only applies to the inner regions and cannot be used to predict accurately the structure of CDM haloes beyond their characteristic scale radius.

Key words: methods: numerical – dark matter.

1 INTRODUCTION

The study of the clustering of cold dark matter (CDM) on the scale of individual haloes has progressed dramatically over the past couple of decades due to the advent of powerful simulation techniques and ever faster computers. As a result, a number of basic properties of the structure of CDM haloes are generally agreed upon, even when many of these empirical findings lack a solid theoretical underpinning. One example is the approximately ‘universal’ mass profile of virialized CDM haloes (Navarro, Frenk & White 1996, 1997, hereafter NFW). CDM haloes are also strongly triaxial, with a preference for prolate shapes (see e.g. Frenk et al. 1988; Jing & Suto 2002; Allgood et al. 2006; Hayashi, Navarro & Springel 2007, and references therein), and have plentiful, albeit non-dominant, substructure (Klypin et al. 1999; Moore et al. 1999).

The mass profile of CDM haloes can be well approximated by the simple law proposed by NFW, where the logarithmic slope of the spherically averaged density profile follows the simple relation γ = d log ρ/d log r = -(1 + 3x)/(1 + x), with x = r/r_2 being the radial coordinate expressed in units of a characteristic halo scale radius, r_200. More recent work shows evidence for small but systematic deviations from this simple law and suggests that a third parameter may actually be required to accurately describe the mean mass profiles of CDM haloes (Navarro et al. 2004; Merritt et al. 2005, 2006; Gao et al. 2008; Hayashi & White 2008). These authors argue that the density profile of ΛCDM haloes steepens monotonically with radius, with no sign of converging to a central asymptotic power law. The profiles are more accurately described by the ‘Einasto’ formula for which γ = -2(r/r_2)α, with α being an adjustable ‘shape’ parameter that can be tailored to provide an improved fit to a given halo density profile.

As discussed by Navarro et al. 2010, this not only implies that CDM haloes are not strictly self-similar, but also makes it difficult to predict the asymptotic properties of CDM halo mass.
profiles. For example, the Einasto and NFW formulae predict quite different asymptotic central behaviours: the Einasto profile has a true ‘core’ with a well-defined central density, whereas the central density of the NFW profile diverges like $r^{-1}$. It seems clear from the latest simulation results (see e.g. Navarro et al. 2010; Stadel et al. 2009) that the asymptotic slope is shallower than $-1$, but it is unclear whether the Einasto formula holds all the way to the centre and whether there is truly a well-defined central density for CDM haloes, aside from the ultimate upper bound set by the Tremaine–Gunn phase-space density constraint (Tremaine & Gunn 1979). The gently curving nature of the Einasto profile makes it difficult to extrapolate available simulations in order to predict the central properties of the halo with certainty.

One alternative is suggested by the realization that although the density, $\rho(r)$, and velocity dispersion, $\sigma(r)$, are complex functions of radius, the quantity $Q(r) = \rho/\sigma^2$ follows closely a simple power law, $Q(r) \propto r^{Q}$, with roughly the same exponent, $\chi \sim -1.875$, for all haloes (hereafter TN Taylor & Navarro 2001). $Q(r)$ has the same dimensions as the phase-space density, $\rho$, but it is not a true measure of it (Ascasibar & Binney 2005; Sharma & Steinmetz 2006). We shall therefore refer to $Q$ as a pseudo-phase-space density or as a surrogate measure of phase-space density. Despite this, $Q$ relates two moments of $\rho$ which occur often in equations that describe equilibrium systems, and therefore simple relations between them are extremely useful when constructing dynamical models (see e.g. Austin et al. 2005; Dehnen & McLaughlin 2005; Barnes et al. 2006; Ascasibar, Hoffman & Gottlöber 2007).

The proposal of TN has been confirmed in subsequent numerical work (see e.g. Rasia, Tormen & Moscardini 2004; Dehnen & McLaughlin 2005; Faltenbacher et al. 2007; Vass et al. 2009; Wang & White 2009) and has been used in the literature to motivate dynamical models of dark haloes. One intriguing feature of the TN result is that the exponent of the power-law $Q(r)$ profile is consistent with that found in the similarity solutions of (Bertschinger 1985).

Whether this is a mere coincidence or has a deeper meaning remains unclear. CDM haloes form through a combination of smooth infall and the accretion of smaller progenitors that are subsequently disrupted in the tidal field of the main halo. Bertschinger’s similarity solution, on the other hand, follows the accretion of radial mass shells on to a point-mass perturber in an otherwise unperturbed Einstein–de Sitter universe. The solution assumes spherical symmetry, allows only radial motions and is violently unstable (Vogelsberger et al. 2009). In spite of this, the approximate power-law nature of $Q(r)$ has been confirmed by the latest series of simulations, which resolve CDM haloes with over one billion particles (Navarro et al. 2010).

The actual value of the exponent has also received attention. Although most simulations seem consistent with $\chi = -1.875$, best fits often give slightly different values for $\chi$, typically in the range from $-1.85$ to $-2$ (but see Schmidt, Hansen & Macciò 2008 for a differing view). Furthermore, there is an indication that $\chi$ may depend on the main mode of mass accretion (Wang & White 2009) and on the slope of the primordial power spectrum (Knollmann, Power & Knebe 2008). The cited work assumes that $Q(r)$ is a power law and then estimates $\chi$ from simple fits to the spherically averaged $Q$ profiles. If $Q$ profiles deviate slightly but significantly from a power law, it could lead to a spread in the values of $\chi$, depending on, for example, the radial range of the fits or the characteristic mass of the haloes considered.

A further complication is introduced by the presence of substructure. Although not dominant in mass, because of their higher density and lower velocity dispersion, subhaloes typically have much higher values of $Q$ than the surrounding halo (Arad, Dekel & Klypin 2004; Diemand et al. 2008; Vass et al. 2009). Together with the fact that CDM haloes are in general triaxial, this hinders a proper definition of the value of $Q$ at given $r$, especially in the outer regions of a halo, where subhaloes are most abundant (Springel et al. 2008).

We address these issues here using a series of high-resolution cosmological $N$-body simulations of the formation of individual CDM haloes. In particular, we compute local estimates of $Q$ at each particle position, $Q_i$, and contrast the resulting profiles with those obtained using spherically averaged estimates. The use of $Q_i$ allows us to carefully excise substructures and to focus our analysis on the pseudo-phase-space density profile of the smooth main halo.

This paper is organized as follows. Section 2 provides a brief description of our numerical simulations and Section 3 discusses our main findings and compares them with Bertschinger’s similarity solutions. We conclude with a brief discussion of our main findings in Section 4.

2 THE SIMULATIONS
We study the formation of 21 CDM haloes selected from a 100$h^{-1}$ Mpc-box cosmological simulation and resimulated at high resolution in their full cosmological context. We provide below a brief summary of the numerical techniques, including the adopted cosmological parameters, the initial conditions set-up, the simulation code as well as the halo selection criteria and analysis techniques. More detailed information about our resimulation and analysis techniques may be found in previous papers by our group (e.g. Power et al. 2003; Navarro et al. 2004, 2008; Springel et al. 2008).

2.1 Cosmological parameters
All our simulations adopt the currently favoured ΛCDM cosmogony with the following parameters: $\Omega_M = 0.25, \Omega_\Lambda = 1 - \Omega_M = 0.75, \sigma_8 = 0.9, n_s = 1$ and a Hubble constant $H_0 = H(z = 0) = 100 h$ km s$^{-1}$ Mpc$^{-1} = 73$ km s$^{-1}$ Mpc$^{-1}$. These parameters are the same as those adopted for the Millennium Simulation (Springel et al. 2005). Although not strictly consistent with the recent Wilkinson Microwave Anisotropy Probe 7-yr data release (Komatsu et al. 2010), the main relevant difference is a slightly smaller value of $\sigma_8 = 0.801 \pm 0.030$. This is expected to affect mainly the average collapse times and abundance of non-linear structures but not the details of their internal structure, which is the main subject of our analysis.

2.2 Halo selection
The 21 haloes were selected from the same 900$h^3$-particle, 100$h^{-1}$ Mpc-box parent simulation used for the Aquarius Project (Springel et al. 2008). These haloes were subsequently resimulated at higher resolution using the technique described in detail by Power et al. (2003). We avoid haloes that form in the periphery of much larger systems by imposing a mild isolation criterion so that no halo more massive than half the mass of the selected system lies within 1$h^{-1}$ Mpc at $z = 0$. This parent simulation was later also resimulated in its entirety at much higher resolution; this is the Millennium-II Simulation recently analysed by Boylan-Kolchin et al. (2009).
Besides the six Aquarius haloes, which were all selected to have virial masses of the order of $\sim 10^{15} h^{-1} M_{\odot}$, we have resimulated a further set of 15 haloes in order to span the mass range from $\sim 10^{12}$ to a few times $10^{14} h^{-1} M_{\odot}$. These 15 simulations have typically a few million particles within the virial radius at $z = 0$ and are of lower numerical resolution than the level-2 Aquarius haloes. Combining these two data sets allows us to assess the sensitivity of our results to numerical resolution. Table 1 lists the main properties of each halo in our sample.

### Table 1

| Halo   | $\epsilon_G$ (kpc $h^{-1}$) | $r_{\text{conv}}$ (kpc $h^{-1}$) | $r_{200}$ (kpc $h^{-1}$) | $r_{\text{max}}$ (kpc $h^{-1}$) | $V_{\text{max}}$ (km $s^{-1}$) | $M_{200}$ ($10^{10} M_{\odot} h^{-1}$) | $N_{200}$ ($10^9$) | $z_{\text{rel}}$ |
|--------|-----------------------------|-----------------------------------|--------------------------|-------------------------------|-------------------------------|----------------------------------|-----------------|--------------|
| Aq-A-2 | 4.8 x 10^{-2}               | 0.25                              | 179.5                    | 20.5                          | 208.5                         | 134.5                            | 134.5           | –            |
| Aq-B-2 | 4.8 x 10^{-2}               | 0.21                              | 137.0                    | 29.3                          | 157.7                         | 59.8                             | 127.1           | –            |
| Aq-C-2 | 4.8 x 10^{-2}               | 0.248                             | 177.3                    | 23.7                          | 222.4                         | 129.5                            | 126.8           | –            |
| Aq-D-2 | 4.8 x 10^{-2}               | 0.281                             | 177.3                    | 39.5                          | 203.2                         | 129.5                            | 127.0           | –            |
| Aq-E-2 | 4.8 x 10^{-2}               | 0.223                             | 155.0                    | 40.5                          | 179.0                         | 86.5                             | 123.6           | –            |
| Aq-F-2 | 4.8 x 10^{-2}               | 0.209                             | 152.7                    | 31.2                          | 169.1                         | 82.8                             | 167.5           | –            |
| h1     | 0.39                        | 1.090                             | 134.4                    | 44.0                          | 151.9                         | 56.4                             | 2.04             | 0.198        |
| h2     | 0.25                        | 0.852                             | 144.6                    | 35.1                          | 159.9                         | 70.3                             | 4.91             | 0.000        |
| h3     | 0.38                        | 1.063                             | 154.1                    | 33.7                          | 178.6                         | 85.0                             | 2.60             | 0.049        |
| h4     | 0.31                        | 0.899                             | 154.7                    | 30.3                          | 175.8                         | 86.1                             | 4.17             | 0.876        |
| h5     | 0.24                        | 0.797                             | 156.1                    | 32.0                          | 174.8                         | 88.5                             | 6.10             | 0.000        |
| h6     | 0.26                        | 0.829                             | 158.0                    | 47.3                          | 171.6                         | 91.7                             | 6.00             | 0.000        |
| h7     | 0.35                        | 1.001                             | 158.3                    | 37.4                          | 184.8                         | 92.2                             | 3.25             | 0.062        |
| h8     | 0.39                        | 1.148                             | 175.6                    | 39.1                          | 203.5                         | 125.9                            | 3.30             | 0.350        |
| h9     | 0.45                        | 1.351                             | 177.8                    | 45.1                          | 200.2                         | 130.8                            | 2.48             | 0.000        |
| h10    | 0.33                        | 0.944                             | 183.7                    | 21.3                          | 209.2                         | 144.1                            | 4.79             | 0.350        |
| h11    | 1.06                        | 3.239                             | 275.5                    | 188.2                         | 285.6                         | 486.4                            | 1.08             | 0.309        |
| h12    | 1.39                        | 4.006                             | 391.0                    | 114.2                         | 425.6                         | 1389.5                           | 1.26             | 0.140        |
| h13    | 1.61                        | 4.418                             | 396.1                    | 86.9                          | 422.9                         | 1445.2                           | 0.98             | 0.140        |
| h14    | 2.08                        | 6.886                             | 856.0                    | 263.6                         | 888.2                         | 14581.8                          | 2.62             | 0.030        |
| h15    | 3.65                        | 11.595                            | 981.6                    | 444.8                         | 1043.0                        | 21993.1                          | 1.16             | 0.094        |

2.3 The code

All simulations were run with either the publicly available GADGET code (Springel 2005) or its latest version, GADGET-3, which was developed for the Aquarius Project. Softening lengths are chosen according to the ‘optimal’ prescription of Power et al. (2003). Pairwise interactions are fully Newtonian for separations exceeding the spline length-scale $h_i$. Table 1 quotes the equivalent Plummer softening, $\epsilon_G = h_i/2.8$, for each resimulated halo. Throughout the simulations, the softening length is kept fixed in comoving coordinates.

2.4 Analysis

2.4.1 Spherically averaged Q profiles

In order to compute the spherically averaged pseudo-phase-space density profile of each halo, we first identify the halo centre with the location of the particle having the minimum potential energy. Then we compute $Q(r)$ in $N_{\text{bin}}$ spherical shells equally spaced in $\log_{10} r$ in the range $r_{\text{conv}} \leq r \leq r_{200}$. Here $r_{\text{conv}}$ is the convergence radius defined by Power et al. (2003), where circular velocities converge to better than 10 per cent (see also Navarro et al. 2010). For each spherical shell (radial bin), we estimate $Q(r) = \rho / \sigma^3$, where $\rho$ is just the mass of the shell divided by its volume and $\sigma^2$ is twice the specific kinetic energy in the shell. We also compute a ‘radial’ $Q$ estimate, $Q_i(r) = \rho_i / \sigma_i^3$, in an analogous way, although instead of the total kinetic energy we use only the kinetic energy in radial motions to estimate $\sigma_i$.

2.4.2 Local Q profiles

A different estimate of the pseudo-phase-space density may be obtained, for each shell, by considering ‘local’ estimates of $Q$ at the position of each particle. We shall call this $Q_i = \rho_i / \sigma_i^3$ and use $N_{\text{ngb}}$ nearest neighbours in order to compute the local density and velocity dispersion. Density estimates at the location of the $i$th particle are computed as

$$\rho_i = \sum_{j=1}^{N} m_j W((r_{i,j}, h_i),$$

where $r_{i,j} = r_i - r_j$ and $W(r, h)$ is the smoothing kernel often adopted in smoothed particle hydrodynamics simulations:

$$W(r, h) = \frac{8}{\pi h^3} \begin{cases} 1 - 6 \left( \frac{\xi}{h} \right)^2 + 6 \left( \frac{\xi}{h} \right)^3, & 0 \leq \frac{\xi}{h} \leq \frac{1}{2}, \\ 2 \left( 1 - \frac{\xi}{h} \right)^3, & \frac{1}{2} < \frac{\xi}{h} \leq 1, \\ 0, & \frac{\xi}{h} > 1. \end{cases}$$
The smoothing length, $h_i$, of each particle is defined implicitly by the smallest volume that contains $N_{ngb}$ nearest neighbours:

$$h_i = \left( \frac{3}{4\pi N_{ngb}} \right)^{1/3} m_i \rho_i.$$

We use, as default, $N_{ngb} = 48$ for our lower resolution runs and 64 for the level-2 Aquarius haloes.

Given $N_{ngb}$, the local velocity dispersion for particle $i$ is given by

$$\sigma_i^2 = \langle v_i^2 - \bar{v}^2 \rangle,$$

where the unweighted averages are computed over all $N_{ngb}$ neighbours.

### 2.4.3 Relaxation criteria

In order to minimize the effect of transient, rapidly evolving evolutionary stages, such as ongoing mergers, we impose (when explicitly stated) relaxation criteria similar to those introduced by Neto et al. (2007). These include restrictions on the fraction of the virial mass in self-bound substructures, $f_{sub} = M_{sub}(r < r_{200})/M_{200} < 0.07$; on the offset between the centre of mass of the halo and its true centre (as defined by the particle with minimum potential energy), $d_{CM} = |r_{CM} - r_{CM0}|/r_{200} < 0.05$; and on the virial ratio of kinetic to potential energies, $2K/\Phi < 1.3$.

In practice, when a halo does not satisfy the relaxation criteria at $z = 0$ we track its main progenitor back in time until we find the first snapshot when it does. This typically occurs at redshifts less than $\sim 0.2$, but in one case we had to go back in time until $z \sim 0.8$ in order to find a suitably ‘relaxed’ configuration. In what follows, we shall consider relaxed configurations only for the lower resolution haloes but take the $z = 0$ configuration for the Aquarius haloes. As we show below, the results are similar in the two cases, which means that our conclusions are not particularly sensitive to our requirement of dynamical equilibrium.

The properties of each halo in our sample at $z = 0$ are listed in Table 1 (the virial mass, $M_{200}$; the virial radius, $r_{200}$; the number of particles ($N_{200}$) within $r_{200}$; the gravitational softening, $\epsilon_G$; and the convergence radius, $r_{conv}$. The peak of the circular velocity curve is also specified by $v_{max}$ and $V_{max}$.

### 3 PSEUDO-PHASE-SPACE DENSITY PROFILES

#### 3.1 Spherically averaged $Q$ profiles

Fig. 1 shows the spherically averaged $Q(r)$ profiles for all haloes in our sample, together with residuals from various best fits. The left-hand and right-hand panels correspond to $Q(r)$ and $Q_i(r)$, respectively. The plotted profiles extend from the convergence radius, $r_{conv}$, to the virial radius, $r_{200}$. The middle panels show residuals from best fits to the region inside $r_{200}$ with an $r^{-1.875}$ power law. All profiles are normalized to the scale radius, $r_{200}$, and vertically according to the power-law best fit. The bottom panels show residuals from fits to the $r_{conv} < r < r_{200}$ profile with a power law with a free-floating exponent, $Q \propto r^\chi$.

A few things are worth noting in this figure. The first is how closely both the $Q(r)$ and $Q_i(r)$ profiles follow simple power laws, from the innermost resolved radius out to $r_{200}$. In the case of $Q(r)$, even when the exponent of the fit is fixed at $\chi = -1.875$, which means that a single free parameter (the vertical normalization) is allowed, residuals from best fits do not exceed $\sim 30$ per cent.

![Figure 1](https://example.com/fig1.png)

**Figure 1.** Spherically averaged pseudo-phase-space density profiles for the 21 dark matter haloes in our sample. The six level-2 Aquarius haloes are shown at $z = 0$ (red dot–dashed lines) and the other 15 (solid blue) are shown at the most recent redshift when they pass the dynamical relaxation criteria (Section 2.4.3). The left-hand panels correspond to $Q(r) \equiv \rho/\sigma^3$; the right-hand panels correspond to the ‘radial’ $Q_i(r) \equiv \rho/\sigma_i^3$. Radii are scaled to the scale radius, $r_{200}$, of each halo. The middle panels show residuals from the best $r^{-1.875}$ power-law fit to the $r_{conv} < r < r_{200}$ portion of the profiles. These best fits are also used to choose the vertical normalization of each profile in the top panels, so as to minimize the halo-to-halo scatter in the inner profiles. The bottom panels are analogous to the middle ones, but for power-law fits over the whole range $r_{conv} < r < r_{200}$, with a free-floating exponent, $r^\chi$. Values of $\chi$ and $\chi_i$ for each halo are listed in Table 2.
anywhere within the virial radius. This power-law behaviour holds for roughly three decades in $r$ and six decades in $Q$.

Although the best-fitting $\chi$ differs from $-1.875$ (see Table 2 for actual values), the residuals decrease only very slightly when allowing $\chi$ to float freely. Defining a figure-of-merit function as

$$
\psi^2 = \frac{1}{N_{\text{bins}}} \sum_{i=1}^{N_{\text{bins}}} (\ln Q - \ln Q_{\text{bin}})^2, \tag{4}
$$

we find that $\psi$, averaged over all haloes and fitted over the range $r_{\text{conv}} < r < r_{200}$, varies only from $\langle \psi \rangle = 0.102$ when fixing $\chi = -1.875$ to $\langle \psi \rangle = 0.085$ when allowing $\chi$ to be a free parameter.

The ‘tilt’ in the $Q_t$ residuals shown in the middle-right panel of Fig. 1 indicates that the $\chi_t$ exponent that fits best the $Q_t(r)$ profiles is slightly more negative than $-1.875$. Overall, however, $Q_t(r)$ may also be approximated with a power law with $\chi_t \approx 1.92$, as may be seen in the bottom-right panel of the same figure. The average $\psi$ for power-law fits with variable $\chi_t$ is 0.142, which means that $Q_t(r)$ deviates more than $Q(r)$ from a simple power law, but only slightly so.

The reason why $Q_t(r)$ deviates more from a simple power law than $Q(r)$ may be traced to the complex behaviour of the anisotropy parameter, $\beta(r) = 1 - \sigma_r^2/2\sigma_t^2$, shown for each of our haloes in Fig. 2. All haloes in our sample are almost isotropic near the centre, radially anisotropic further out, but nearly isotropic again close to the virial radius. Because of this complex radial behaviour, $Q_t(r)$ and $Q_r(r)$ cannot both be simultaneously well fitted by a power law with the same exponent.

Although power laws provide excellent fits to the pseudo-phase-space density profiles, further scrutiny of the middle and bottom panels of Fig. 1 reveals a well-defined trend in the residuals of most haloes, which tend to ‘curve up’ slightly but significantly in

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
Halo & $\chi$ & $\chi_t$ & $\chi$ & $\chi$ & $\chi$ & $\chi$ \\
& ($r_{\text{conv}} < r < r_{200}$) & ($r_{\text{conv}} < r < r_{200}$) & ($r_{\text{conv}} < r < r_{200}$) & ($r_{\text{conv}} < r < r_{200}$) & ($r_{\text{conv}} < r < r_{200}$) & ($r_{\text{conv}} < r < r_{200}$) \\
\hline
Aq-A-2 & $-1.917$ & $-1.967$ & $-1.873$ & $-1.955$ & $-1.910$ & $-1.821$ \\
Aq-B-2 & $-1.868$ & $-1.938$ & $-1.832$ & $-1.872$ & $-1.914$ & $-1.808$ \\
Aq-C-2 & $-1.948$ & $-2.010$ & $-1.883$ & $-1.948$ & $-1.932$ & $-1.823$ \\
Aq-D-2 & $-1.862$ & $-1.942$ & $-1.831$ & $-1.901$ & $-1.939$ & $-1.804$ \\
Aq-E-2 & $-1.912$ & $-1.947$ & $-1.894$ & $-1.902$ & $-1.863$ & $-1.853$ \\
Aq-F-2 & $-1.911$ & $-1.980$ & $-1.885$ & $-1.954$ & $-1.965$ & $-1.823$ \\
\hline
\multirow{5}{*}{h} & $-1.826$ & $-1.847$ & $-1.858$ & $-1.813$ & $-1.798$ & $-1.792$ \\
h1 & $-1.862$ & $-1.920$ & $-1.811$ & $-1.908$ & $-1.828$ & $-1.696$ \\
h2 & $-1.993$ & $-2.076$ & $-1.864$ & $-1.903$ & $-1.967$ & $-1.800$ \\
h3 & $-1.895$ & $-1.942$ & $-1.863$ & $-1.943$ & $-1.879$ & $-1.766$ \\
h4 & $-1.916$ & $-1.999$ & $-1.872$ & $-1.938$ & $-1.887$ & $-1.771$ \\
h5 & $-1.898$ & $-2.010$ & $-1.863$ & $-1.908$ & $-1.856$ & $-1.801$ \\
h6 & $-1.960$ & $-1.918$ & $-1.940$ & $-1.957$ & $-1.878$ & $-1.863$ \\
h7 & $-1.864$ & $-1.951$ & $-1.808$ & $-1.916$ & $-1.871$ & $-1.727$ \\
h8 & $-1.869$ & $-1.953$ & $-1.858$ & $-1.926$ & $-1.846$ & $-1.792$ \\
h9 & $-1.975$ & $-2.042$ & $-1.871$ & $-1.991$ & $-1.972$ & $-1.754$ \\
h10 & $-1.896$ & $-2.008$ & $-1.843$ & $-1.845$ & $-1.903$ & $-1.756$ \\
h11 & $-1.879$ & $-1.949$ & $-1.875$ & $-2.023$ & $-1.864$ & $-1.758$ \\
h12 & $-1.843$ & $-1.955$ & $-1.847$ & $-1.882$ & $-1.768$ & $-1.724$ \\
h13 & $-1.810$ & $-1.902$ & $-1.817$ & $-1.886$ & $-1.801$ & $-1.732$ \\
h14 & $-1.847$ & $-1.966$ & $-1.835$ & $-1.919$ & $-1.765$ & $-1.648$ \\
\hline
\hline
\end{tabular}
\caption{Values of the exponent $\chi$ obtained from $r'$ fits to various $Q$ profiles, as indicated in the legend. $\chi_t$ refers to fits to the ‘radial’ $Q_t$ profiles. The average $\chi$ for all haloes is listed in the next-to-last row, together with its standard deviation. The average figure of merit for all haloes, $\langle \psi_{\text{min}} \rangle$, is listed in the last row of the table.}
\end{table}
the outer regions and, to a lesser extent, in the innermost regions as well. The latter deviations are best appreciated in the Aquarius haloes, which have much better resolution than the rest.

These results seem to apply both to the Aquarius haloes and to the dynamically relaxed halo sample, which suggests that our conclusions are not crucially dependent on the adoption of the particular relaxation criteria we used to select the sample. The above-noted trend in the residuals means that the exponent, $\chi$, derived from $r^\chi$ power-law fits will depend on the radial range adopted for the fit.

Given the desirable properties of a simple power law, it is worth investigating whether the deviations from a simple $r^\chi$ behaviour might be due to the presence of substructure or to the aspherical nature of halo structure. We explore these possibilities next.

### 3.2 Local $Q$ profiles

Fig. 3 shows $Q_i$, the local estimate of $Q$ at the location of each particle in the halo, as a function of the distance from the halo centre. Because substructures are overdense and have lower velocity dispersion than their immediate surroundings, they show up prominently in this plot as particles with very high $Q_i$ at a given radius. This is confirmed by the colour coding adopted in the figure: particles in dark blue are those associated by the substructure-finder SUBFIND (Springel et al. 2001) to self-bound subhaloes that survive within the main halo. Clearly, because their pseudo-phase-space density is so distinct from the main halo, substructures have the potential to bias estimates of $Q(r)$, especially in the outer regions, where subhaloes are more prevalent.

Although it would be simple enough to remove the self-bound structures from $Q(r)$ profiles, the cyan dots in Fig. 3 illustrate a second, related problem. These are particles that SUBFIND associates with the main halo, but which clearly have deviant $Q_i$ values relative to the surrounding average. As discussed, for example, by Maciejewski et al. (2009), these are particles recently stripped from substructures; although now unbound to any subhalo, they have yet to phase mix fully with the underlying main halo.

Fig. 4 shows the $Q_i$ distribution of all particles in the thin spherical shell near the virial radius of the halo shown in Fig. 3. Substructures identified by SUBFIND are shown in blue and the main SUBFIND halo in cyan. Various thin lines illustrate the effect of varying the number of neighbours in the $\rho_i$ and $\sigma_i$ estimates, as labelled in the legend. As discussed in the text, a simple cut $Q_i < Q_{\text{cut}}$ identifies unequivocally all well-mixed particles in the main halo; $Q_{\text{cut}}$ is shown by the vertical dotted line. Down-pointing arrows indicate the median of the distribution of each set of particles. Because there are few particles in the high-$Q_i$ tail, the median $Q_i$ of the main SUBFIND halo and that of particles with $Q_i < Q_{\text{cut}}$ are nearly identical. We adopt the latter as the characteristic pseudo-phase-space density of the smooth halo at each radius.

**Figure 3.** ‘Local’ estimates of the pseudo-phase-space density, $Q_i$, as a function of distance from the halo centre for all halo particles in one of our simulations. Different colours correspond to various particle subsamples. (i) Blue denotes particles in self-bound substructures, as identified by SUBFIND. (ii) Cyan indicates particles not bound to any substructure but with higher than average $Q_i$ for their location in the halo. These are particles in recently stripped tidal streams which, although assigned to the main halo by SUBFIND, have yet to phase mix within the main halo (Maciejewski et al. 2009). (iii) Red dots indicate particles with $Q_i < Q_{\text{cut}}(r)$, which we define as belonging to the relaxed main halo (see Fig. 4). Also plotted are the spherically averaged $Q(r)$ profile (solid blue line) and the best-fitting $r^{-1.875}$ power law (dashed line). Vertical and horizontal bands show, respectively, the particles selected for Figs 4 and 5.

**Figure 4.** Distribution of local phase-space densities, $Q_i$, for particles in the thin (shaded) spherical shell near the virial radius of the halo shown in Fig. 3. Substructures identified by SUBFIND are shown in blue and the main SUBFIND halo in cyan. Various thin lines illustrate the effect of varying the number of neighbours in the $\rho_i$ and $\sigma_i$ estimates, as labelled in the legend. As discussed in the text, a simple cut $Q_i < Q_{\text{cut}}$ identifies unequivocally all well-mixed particles in the main halo; $Q_{\text{cut}}$ is shown by the vertical dotted line. Down-pointing arrows indicate the median of the distribution of each set of particles. Because there are few particles in the high-$Q_i$ tail, the median $Q_i$ of the main SUBFIND halo and that of particles with $Q_i < Q_{\text{cut}}$ are nearly identical. We adopt the latter as the characteristic pseudo-phase-space density of the smooth halo at each radius.
in the high-$Q$ tail, the median $Q$ of the main SUBFIND halo and that of particles with $Q < Q_{\text{cut}}$ are nearly identical.

We therefore adopt the simple $Q < Q_{\text{cut}}$ prescription to define the main ‘smooth’ halo. Once $Q_{\text{cut}}$ is chosen at some radius, we may use the approximate power-law behaviour of $Q$ to scale it to any other radius by $Q_{\text{cut}}(r) \propto r^{-1.875}$. Particles shown in red in Fig. 3 are those assigned to the smooth halo by this criterion. At each radius, we shall adopt the median $Q_i$ of these particles in order to construct the pseudo-phase-space density profile of the main smooth halo. We shall refer to this profile as $Q'_i(r)$.

We note that this definition is insensitive to the number of nearest neighbours ($N_{\text{neigh}}$) adopted to compute $Q_i$: the various lines in Fig. 4 illustrate the results for $N_{\text{neigh}} = 48$ particles (our default value) as well as for 1000 (long-dashed), 500 (dotted) and 100 (dot–dashed) particles.

### 3.3 Correction for triaxiality

Dark haloes are not spherically symmetric. Because of this, a shell of particles at a constant distance from the halo centre will have a wide $Q$ distribution, even if one subtracts substructure as specified in the previous subsection. Iso-$Q$ surfaces track fairly well the isodensity contours of the main halo and follow closely three-dimensional ellipsoidal surfaces. Fig. 5 shows three orthogonal projections of particles with similar values of $Q_i$, selected from those falling in the horizontal band highlighted in Fig. 3. Only particles in the smooth main halo are plotted here. The original particle positions (in red) in a thin slice perpendicular to the line of sight are seen to trace a nearly prolate ellipsoid, which for convenience has been rotated so that its principal axes coincide with the coordinate axes of the projection.

Given that the ‘iso-$Q$’ surfaces are well approximated by ellipsoids, we may use the eigenvalues of the diagonalized inertia tensor to compute an elliptical radius, $r'$, for each $Q_i$, to define an ‘ellipsoidal’ $Q'_i(r')$ profile that may be contrasted directly with $Q'_i(r)$. In practice, we slice the smooth main halo in narrow bins in $Q_i$; compute the axis lengths $a, b$ and $c$; and use them to reassign an ellipsoidal radius $r'$ to each particle in the smooth main halo. We compute $r'$ as

$$r'^2 = \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2},$$

(5)

after normalizing $a, b$ and $c$ so that $abc = 1$ for all shells. This choice preserves the typical distance to the halo centre of particles in a given $Q$ shell. The result of the procedure is illustrated in Fig. 5, where the green dots are the same particles as those shown in red, but the coordinate axes are now $x' = x/a, y' = y/b$ and $z' = z/c$.

The green dots in Fig. 6 delineate the $Q'_i(r')$ profile for the smooth main halo. The lines in Fig. 6 show the variations in the pseudo-phase-space density profile induced by the various alternative ways of estimating distances and $Q$ that we have discussed so far.

Although the profiles change appreciably, they all show the same upturn in the outer regions, relative to a simple $r^{-1.875}$ power-law fit, noted when discussing the spherically averaged $Q(r)$ profiles.

![Figure 5. Orthogonal projections of particles in a shell of roughly constant pseudo-phase-space density (i.e. those in the horizontal shaded band in Fig. 3, excluding substructures). For clarity, we plot in each panel only particles in a thin slice perpendicular to the viewing axis. Red points show the original positions; these delineate a nearly prolate ellipsoid, which has been rotated so that its principal axes coincide with the coordinate axes of the plot. Green points show the projected particle positions after correcting for triaxiality by the method outlined in the text.](https://academic.oup.com/mnras/article-abstract/406/1/137/1069429)

![Figure 6. Local pseudo-phase-space density as a function of radius for the same halo shown in Fig. 3. Coloured dots are as in Fig. 3. Red and green dots indicate smooth main halo particles before and after correcting for the halo shape, respectively. The solid curve is the spherically averaged profile and is compared with the curves tracing the median $Q_i$ for (i) all particles (blue dot–dashed), (ii) all particles in the smooth main halo (red dashed) and (iii) smooth main halo particles corrected for triaxiality (dashed). The dotted line shows a power law, $r^{-1.875}$.)](https://academic.oup.com/mnras/article-abstract/406/1/137/1069429)
(Section 3.1). The upturn is indeed more pronounced when using local-$Q$ estimates, because (i) local densities are sensitive to inhomogeneities and are therefore higher than the spherical average and (ii) local $\sigma$ estimates are lower than the spherical average, since they do not include the bulk motion of subhaloes and recently stripped material. Interestingly, Fig. 6 shows that after correcting for triaxiality, the spherically averaged profile is indistinguishable from the $Q_i(r)$ profile. We conclude that the upturn is not caused by the presence of substructures in the outer regions nor by departures from spherical symmetry. We discuss the interpretation of this robust feature of the $Q$ profiles next.

### 3.4 Numerical convergence

Before considering the meaning of the departures of $Q$ profiles from simple power laws, we should check explicitly that our conclusions are not affected by the numerical resolution of the simulations. We show this in Fig. 7, where we compare the $Q(r)$ and $Q_i(r)$ profiles of one of the Aquarius haloes at four different resolutions. The highest, Aq-A-2, has more than 100 million particles within the virial radius and the lowest, Aq-A-5, about 600 thousand. The non-Aquarius haloes in the series analysed in this paper have numerical resolution comparable to Aq-A-4. Fig. 7 shows convincingly that our results are unlikely to be adversely affected by numerical resolution. Both the spherically averaged and the local pseudo-phase-space density profiles are very well reproduced at all radii, down to the innermost resolved radius, $r_{\text{com}}$, of each run.

### 3.5 Comparison with Bertschinger’s similarity solution

The local pseudo-phase-space density profiles for the smooth main halo of all our systems are shown in Fig. 8. The profiles are shown as a function of the elliptical radius (equation 5), scaled to the scale radius of each halo, $r_{\text{e}}$. All profiles have been normalized vertically so that they coincide at $r' = r_{\text{e}}$. The dotted line shows a $Q \propto r^{-1.875}$ power law, also normalized at $r_{\text{e}}$. The bottom panel shows residuals relative to the $r^{-1.875}$ power law.

Fig. 8 shows the main result of our analysis. The pseudo-phase-space density profiles of our simulated haloes clearly deviate from a simple power law in the outer regions. This deviation is actually predicted by the secondary-infall similarity solution of Bertschinger (1985). Indeed, in the similarity solution the $Q \propto r^{-1.875}$ behaviour occurs only asymptotically in the inner regions of the halo. In the outer regions and, more precisely, near the location of the ‘shock radius’, $r_{\text{shock}}$ (for collisional fluids), or, equivalently, of the first infall caustic (for collisionless fluids), the pseudo-phase-space density profile (or the entropy profile in the case of a collisional fluid) shows a clear upturn from the inner asymptotic power-law behaviour.

The reason for this upturn is that the fluid is not fully virialized near $r_{\text{shock}}$, since this radius marks the transition between mass shells that are infalling for the first time and those that have already crossed (or shocked) material that collapsed earlier. For example, in the case of collisionless fluids, a mass shell must cross the centre and complete roughly two to three full oscillations before settling on to a periodic orbit of constant apocentre. In the case of a collisional fluid, a newly shocked shell drifts inwards from the radius at which it was shocked before reaching hydrostatic equilibrium (see fig. 4 of Bertschinger 1985). As a result, $Q(r)$ (or the ‘entropy’ in the case of a collisional fluid) shows a characteristic upturn at $r_{\text{shock}}$ like the one shown in Fig. 8.

As discussed by White et al. (1993), the first caustic/shock, which occurs at about a third of the current turnaround radius, lies close to the virial radius, as defined here. Given that our haloes have concentrations, $c = r_{200}/r_{\text{e}}$, of the order of 7–10 (Neto et al. 2007), we would then expect the upturn in the $Q$ profiles to occur roughly at $\sim 7–10 r_{\text{e}}$.

The dashed black curves in Fig. 8 show the similarity solution, assuming $r_{\text{shock}} = 8 r_{\text{e}}$, and normalized vertically at $r = r_{\text{e}}$ to coincide with the simulated halo profiles. It is clear from Fig. 8 that the similarity solution is in excellent agreement with the $Q$ profiles.
Although the outer upturn may be robust, the fact that the exponent of the inner power law is consistent with Bertschinger’s solution ($\chi \sim -1.875$) is somewhat surprising. As shown by (Fillmore & Goldreich 1984), the non-linear structure of haloes formed through self-similar secondary infall depends on the scaling index that characterizes the mass dependence of the initial perturbation, $\delta M/M \propto M^{-\epsilon}$. In the case of Bertschinger’s solution $\epsilon = 1$, but this is a poor approximation to the typical overdensity that seeds the collapse of galaxy-sized $\Lambda$CDM haloes. The agreement between Bertschinger’s $Q(r)$ and the simulated profiles is therefore a non-trivial result whose significance remains unclear.

The presence of an upturn in the $Q(r)$ profiles casts doubts on work that attempts to construct dynamical equilibrium models of CDM haloes by assuming that the power-law behaviour of $Q$ profiles applies to all radii (see e.g. Austin et al. 2005; Dehnen & McLaughlin 2005). The $r'$ behaviour seems to hold only in the inner regions, and our results caution against fitting power laws to $Q(r)$ over a radial range that extends outside the scale radius, $r_{200}$. It is worth mentioning, however, that the approximate power-law behaviour of the $Q(r)$ profiles over the range $r < r_{200}$ may still be used to constrain the inner mass profile of CDM haloes, if such an asymptotic power law exists.

Because the radius where the upturn becomes noticeable marks the transition to the region where virial equilibrium no longer holds, this radius, expressed as a fraction of the virial radius, may vary systematically with halo mass, collapse time or cosmological parameters. Indeed, the virial radius definition we adopt here does not depend on the formation history of each object, but the boundary of the region where virial equilibrium might hold. For example, the shock radius of an early collapsing halo that has accreted little mass in the recent past might occur farther away (in units of $r_{200}$) than that of another system of similar mass that has assembled a considerable fraction of its present-day mass more recently.

It may be worth checking whether the trends of $\chi$ with the power spectrum and mode of assembly noted in the literature (see e.g. Knollmann et al. 2008; Wang & White 2009) might be explained in this way.

Finally, we note that our highest resolution haloes (those from the Aquarius project) also present evidence of departures from a simple power-law $Q$ profile near the innermost resolved radius. At the moment, it is unclear whether this indicates that the power-law behaviour of $Q(r)$ is just an approximation that breaks down inside some characteristic radius or whether estimates of $Q(r)$ at those radii might be affected by numerical uncertainties. For example, it is easy to demonstrate that an isotropic halo whose mass profile follows strictly an Einasto law cannot have a power-law $Q(r)$ that extends all the way to the centre (see e.g. Ma, Chang & Zhang 2009). The radial dependence of these $Q(r)$ profiles might be more accurately represented by an Einasto-like form where the power-law index changes gradually but smoothly with radius. We plan to address this and other pertinent issues in forthcoming work.

4 SUMMARY

We have used a set of 21 high-resolution cosmological N-body simulations to investigate the pseudo-phase-space density profiles, $Q(r) = \rho/\sigma^3$, of CDM haloes. In particular, we concentrate our analysis on the radial dependence of $Q$ for particles in the smooth main halo component, after carefully removing substructures and correcting for the halo shape.

Our main result is that although $Q(r)$ is remarkably well approximated by a power law, a slight but systematic upturn from the power-law profile is clearly seen in the outer regions of all our simulated haloes. Both the exponent of the power law and the upturn in the outer regions are consistent with the secondary-infall similarity solutions derived by Bertschinger (1985). In these solutions, the power-law inner region corresponds to the virialized region of the halo, whereas the upturn in the outer regions coincides with the location of the shock/first caustic of the system or, roughly speaking, with the virial boundary of a halo. Although Bertschinger’s solution is just one particular secondary-infall similarity solution valid in the simple case of a point-mass perturber in an Einstein–de Sitter universe, the upturn in $Q$ marking the virial boundary of the system is expected to be a general feature of such solutions.

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REFERENCES

Allgood B., Flores R. A., Primack J. R., Kravtsov A. V., Wechsler R. H., Faltenbacher A., Bullock J. S., 2006, MNRAS, 367, 1781
Arad I., Dekel A., Klypin A., 2004, MNRAS, 353, 15
Ascasibar Y., Binney J., 2005, MNRAS, 356, 872
Ascasibar Y., Hoffman Y., Gottlöber S., 2007, MNRAS, 376, 393
Austin C. G., Williams L. L. R., Barnes E. I., Babul A., Dalcanton J. J., 2005, ApJ, 634, 756
Barnes E. I., Williams L. L. R., Babul A., Dalcanton J. J., 2006, ApJ, 643, 797
Bertschinger E., 1985, ApJS, 58, 39
Boylan-Kolchin M., Springel V., White S. D. M., Jenkins A., Lemson G., 2009, MNRAS, 398, 1150
Dehnen W., McLaughlin D. E., 2005, MNRAS, 363, 1057
Diemand J., Kuhlen M., Madau P., Zemp M., Moore B., Potter D., Stadel J., 2008, Nat, 454, 735
Faltenbacher A., Hoffman Y., Gottlöber S., Yepes G., 2007, MNRAS, 376, 1327
Fillmore J. A., Goldreich P., 1984, ApJL, 281, 1
Frenk C. S., White S. D. M., Davis M., Efstathiou G., 1988, ApJ, 327, 507
Gao L., Navarro J. F., Cole S., Frenk C. S., White S. D. M., Springel V., Jenkins A., Neto A. F., 2008, MNRAS, 387, 536
Hansen S. H., Moore B., 2006, New Astron., 11, 333
Hayashi E., White S. D. M., 2008, MNRAS, 388, 2
Hayashi E., Navarro J. F., Springel V., 2007, MNRAS, 377, 50
Jing Y. P., Suto Y., 2002, ApJ, 574, 538
Klypin A., Kravtsov A. V., Valenzuela O., Prada F., 1999, ApJ, 522, 82
Knollmann S. R., Power C., Knebe A., 2008, MNRAS, 385, 545
Komatsu E. et al., 2010, preprint (arXiv:1001.4538)
Ma C.-P., Chang P., Zhang J., 2009, preprint (arXiv:0907.3144)
Maciejewski M., Colombi S., Springel V., Alard C., Bouchet F. R., 2009, MNRAS, 396, 1329
Merritt D., Navarro J. F., Ludlow A., Jenkins A., 2005, ApJ, 624, L85
Merritt D., Graham A. W., Moore B., Diemand J., Terzić B., 2006, AJ, 132, 2685
Moore B., Quinn T., Governato F., Stadel J., Lake G., 1999, MNRAS, 310, 1147
Navarro J. F., Frenk C. S., White S. D. M., 1996, ApJ, 462, 563 (NFW)
Navarro J. F., Frenk C. S., White S. D. M., 1997, ApJ, 490, 493 (NFW)
Navarro J. F. et al., 2004, MNRAS, 349, 1039
Navarro J. F. et al., 2010, MNRAS, 402, 21
Neto A. F. et al., 2007, MNRAS, 381, 1450
Power C., Navarro J. F., Jenkins A., Frenk C. S., White S. D. M., Springel V., Stadel J., Quinn T., 2003, MNRAS, 338, 14
Rasia E., Tormen G., Moscardini L., 2004, MNRAS, 351, 237
Schmidt K. B., Hansen S. H., Macciò A. V., 2008, ApJ, 689, L33
Sharma S., Steinmetz M., 2006, MNRAS, 373, 1293
Springel V., 2005, MNRAS, 364, 1105
Springel V., White S. D. M., Tormen G., Kauffmann G., 2001, MNRAS, 328, 726
Springel V. et al., 2005, Nat, 435, 629
Springel V. et al., 2008, MNRAS, 391, 1685
Stadel J., Potter D., Moore B., Diemand J., Madau P., Zemp M., Kuhlen M., Quilis V., 2009, MNRAS, 389, 21
Taylor J. E., Navarro J. F., 2001, ApJ, 563, 483 (TN)
Tremaine S., Gunn J. E., 1979, Phys. Rev. Lett., 42, 407
Vass I. M., Valluri M., Kravtsov A. V., Kazantzidis S., 2009, MNRAS, 395, 1225
Vogelsberger M., White S. D. M., Mohayaee R., Springel V., 2009, MNRAS, 400, 2174
Wang J., White S. D. M., 2009, MNRAS, 396, 709
White S. D. M., Navarro J. F., Evrard A. E., Frenk C. S., 1993, Nat, 366, 429

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