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Sampling the Fermi-Dirac Density

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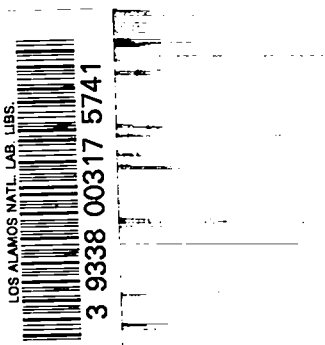
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Sampling the Fermi-Dirac Density

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SAMPLING THE FERMI-DIRAC DENSITY

by

E. D. Cashwell and C. J. Everett

ABSTRACT

A method is given for sampling the nonrelativistic Fermi-Dirac electron energy density for all values of the "degeneracy parameter" η on the range $-\infty < \eta \leq 50$. The efficiency of the various rejection techniques employed is never less than 30%, and drops below 50% only for a short range of η values around $\eta = 2$. The range can certainly be extended beyond $\eta = 50$, the efficiency there being 71%, and decreasing very slowly.

I. THE FERMI-DIRAC DENSITY

The nonrelativistic Fermi-Dirac density for the electron velocity (Ref. 1, p. 333) is given by

$$P(v_x, v_y, v_z) dv_x dv_y dv_z = \frac{2m^3}{nh^3} \Phi(E) dv_x dv_y dv_z, \quad (1)$$

$$\Phi(E) = 1 / \left[\exp\left(\frac{E}{\theta} - \eta\right) + 1 \right], \quad (2)$$

where $m = 9.1096 \times 10^{-28}$ g is the electron mass, n is the number of electrons per cm^3 , $h = 6.6262 \times 10^{-27}$ erg sec is Planck's constant, $E = \frac{1}{2} mv^2$ erg is the electron energy, with $v^2 = v_x^2 + v_y^2 + v_z^2$, and $\theta = kT$ erg is the "temperature," $k = 1.3806 \times 10^{-16}$ erg/°K being the Boltzmann constant. In Eq. (2), η is the "degeneracy parameter," depending on n and θ in such a way as to make

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} P(v_x, v_y, v_z) dv_x dv_y dv_z = 1. \quad (3)$$

If $Q(v, \theta, \phi)$ denotes the corresponding "spherical coordinate density," then $Q(v, \theta, \phi) dv d\theta d\phi = \frac{2m^3}{nh^3} \phi(E) (v^2 \sin \theta) dv d\theta d\phi$, and the speed density is, therefore, given by

$$q(v) dv = \frac{8\pi m^3}{nh^3} \phi(E) v^2 dv, \quad 0 < v < \infty \quad (4)$$

Since $E = \frac{1}{2} mv^2$, we obtain for the energy density

$$f(E) dE = q(v) \frac{dv}{dE} dE = \frac{8 \sqrt{2} \pi m^{3/2}}{nh^3} E^{1/2} \phi(E) dE, \quad 0 < E < \infty \quad (5)$$

Setting $y = E/\theta$, the y density is seen to be

$$p(y) dy = f(E) \frac{dE}{dy} dy = \frac{8 \sqrt{2} \pi m^{3/2} \theta^{3/2}}{nh^3} \cdot \frac{y^{1/2} dy}{e^{y-\eta} + 1} \quad (6)$$

$$\equiv C^{-1} \frac{y^{1/2} dy}{e^{y-\eta} + 1}, \quad 0 < y < \infty \quad (7)$$

From the necessary relation

$$\int_0^\infty p(y) dy = 1,$$

it follows that the n, θ -dependent parameter η must be determined so that

$$I(\eta) \equiv \int_0^\infty \frac{y^{1/2} dy}{e^{y-\eta} + 1} = \frac{h^3}{8 \sqrt{2} \pi m^{3/2}} \cdot \frac{n}{\theta^{3/2}} \equiv C \quad (8)$$

It is easy to verify that $I(\eta)$ and $I'(\eta)$ are positive

for $-\infty < \eta < \infty$, while

$$I(\eta) = \int_0^{\infty} \frac{y^{1/2} e^{-y} dy}{e^{-\eta} + e^{-y}} < \frac{\Gamma(3/2)}{e^{-\eta}} \rightarrow 0 \text{ as } \eta \rightarrow -\infty ,$$

$$I(\eta) > \int_0^{\eta} \frac{y^{1/2} dy}{e^{y-\eta} + 1} > \int_0^{\eta} \frac{y^{1/2} dy}{2} = \frac{\eta^{3/2}}{3} \rightarrow \infty \text{ as } \eta \rightarrow \infty .$$

Thus $I(\eta)$ strictly increases from $I(-\infty) = 0$ to $I(\infty) = \infty$, and for every $C > 0$ in Eq. (8), there is a unique η on $(-\infty, \infty)$ such that $I(\eta) = C$.

Values of $I(\eta)$ have been tabulated (Ref. 2,3) at intervals of 0.1 for $-4 \leq \eta \leq 20$. Table I below gives an idea of the variation of $I(\eta)$ on this range.

TABLE I
THE FUNCTION $I(\eta)$

η	$I(\eta)$
-4	.016128
-3	.043366
-2	.114588
-1	.290501
0	.678094
1	1.39638
2	2.50246
2.5	3.1966
3	3.97699
4	5.77073
5	7.83797
6	10.1443
7	12.6646
8	15.3805
9	18.2776
10	21.3445
11	24.5718
12	27.9518
13	31.4775
14	35.1430
15	38.9430
16	42.8730
17	46.9286
18	51.1061
19	55.4019
20	59.8128

Outside of these limits the following approximations are recommended (Ref. 3):

$$I(\eta) \cong \frac{\sqrt{\pi}}{2} e^{\eta}, \quad \eta < -4, \quad (9)$$

$$I(\eta) \cong \frac{2}{3} \eta^{3/2}, \quad \eta > 20. \quad (10)$$

One may note that $\frac{\sqrt{\pi}}{2} e^{-4} = .016232$, while $\frac{2}{3} (20)^{3/2} = 59.628$, as compared with the values $I(-4)$ and $I(20)$ in

TABLE I

II. PRELIMINARY DETERMINATION OF C AND η

For a given density n and temperature $\theta = kT$, one first computes the value of

$$C = \frac{h^3}{8 \sqrt{2} \pi m^{3/2}} \cdot \frac{n}{\theta^{3/2}} \cong 1.835 \times 10^{-16} \frac{n}{T^{3/2}}. \quad (11)$$

Guided by the above remarks we then determine the corresponding η as follows:

- (a) If $C < .016128$, η is given by $e^\eta = \frac{2}{\sqrt{\pi}} C$,
- (b) if $.016128 \leq C \leq 59.8128$, η is found from the tables cited (Ref. 2, 3),
- (c) if $C > 59.8128$, then $\eta = (3C/2)^{2/3}$.

For the known values of $C > 0$ and η on $(-\infty, \infty)$ one must now sample the density

$$p(y) = C^{-1} \frac{y^{1/2}}{e^{y-\eta} + 1}, \quad 0 < y < \infty \quad (12)$$

for $y > 0$, and set the energy $E = \theta y$. Due to the curious nature of the function $p(y)$ we are forced to use two different methods depending on the value of η .

III. THE CASE $(-\infty < \eta \leq 5/2)$

For a value of $\eta \leq 5/2$, we write

$$\begin{aligned} p(y) dy &= C^{-1} \Gamma(3/2) e^\eta \cdot \frac{y^{1/2} e^{-y} dy}{\Gamma(3/2)} \cdot \frac{1}{1 + e^{\eta-y}} \\ &\equiv A^{-1} \cdot p_1(y) dy \cdot h(y) \quad , \end{aligned} \quad (13)$$

where $p_1(y)$ is the density

$$p_1(y) = y^{1/2} e^{-y} / \Gamma(3/2), \quad 0 < y < \infty \quad , \quad (14)$$

$h(y)$ is the "acceptance factor"

$$0 < h(y) = 1/(1 + e^{\eta-y}) < 1, \quad 0 < y < \infty \quad , \quad (15)$$

and the efficiency of the corresponding rejection technique is

$$A = 2 C / \sqrt{\pi} e^\eta \quad . \quad (16)$$

Following the usual method (Ref. 4, R 7), we sample $p_1(y)$ for y on $(0, \infty)$, and accept y with probability $h(y)$.

The density $p_1(y)$ is easily sampled (Ref. 4, C 32); a brief indication of the routine follows:

Sampling $y^{\frac{1}{2}} e^{-y}/\Gamma(3/2)$ for y on $(0,\infty)$.

1. Generate random numbers, r_1, r_2 on $(0,1)$.
2. Is $S \equiv r_1^2 + r_2^2 \leq 1$? Yes (advance to (3)), No (return to (1)).
3. Set $\mu_i = -\frac{\log S}{S} \cdot r_i^2, i = 1,2$.
4. Generate next random number r .
5. Set $y = -\log r + \mu_i$.

(Two samples of y are obtained, which may be used successively.)

The efficiency A in Eq. (16), based on the values of $C = I(\eta)$ in TABLE I, are listed for various values of $\eta \leq 3$ in TABLE II. Note that, for the recommended approximation $e^\eta = 2 C/\sqrt{\pi}$ ($\eta < -4$), the efficiency A appears to be 1, although, of course, there may be some rejection.

In principle, the above method applies for all η . We have drawn the line at $\eta = 5/2$ simply because the method of the next part is relatively easy to apply for $\eta > 5/2$, as will appear. If enough trouble were taken in finding the minimum h in part IV, the η dividing line could be pushed to the left, with a resulting increase in efficiency.

IV. THE CASE ($\eta > 5/2$).

We first note that the function

$$p(y) = C^{-1} \frac{y^{\frac{1}{2}}}{e^{y-\eta} + 1}$$

TABLE II
EFFICIENCY A

η	A
-4	.99
-3	.98
-2	.96
-1	.89
0	.77
1	.58
2	.38
2.5	.30
3	.22

is decreasing for $y > \eta$, provided η exceeds 1. For, an easy computation shows that the inequality $p'(y) < 0$ follows from the relation $(2y - 1)e^{y-\eta} > (2\eta - 1)e^0 > 1$.

If we define

$$A_1 = \int_0^\eta p(y) dy, A_2 = 1 - A_1, (17)$$

we may sample $A_1^{-1} p(y) dy$ on $(0, \eta)$ with probability A_1 , and $A_2^{-1} p(y) dy$ on (η, ∞) with probability A_2 (Ref. 4, C 3).

(a) The first of these is simple, for we may write

$$A_1^{-1} p(y) dy = A_1^{-1} C^{-1} ((2/3) \eta^{3/2}) (e^{-\eta} + 1)^{-1} \cdot \frac{y^{1/2} dy}{(2/3) \eta^{3/2}} \cdot \frac{e^{-\eta} + 1}{e^{y-\eta} + 1} \quad (18)$$

Thus we easily sample the density $y^{1/2}/((2/3) \eta^{3/2})$ for $y = \eta r^{2/3}$ on $(0, \eta)$, accepting y with probability $(e^{-\eta} + 1)/(e^{y-\eta} + 1) < 1$, the efficiency of the technique being

$$\epsilon_1 = 3 A_1 C (e^{-\eta} + 1) / 2 \eta^{3/2} \quad (19)$$

This certainly exceeds $\frac{1}{2}$. For,

$$A_1 = \int_0^{\eta} C^{-1} \frac{y^{1/2} dy}{e^{y-\eta} + 1} > C^{-1} \frac{((2/3) \eta^{3/2})}{2} = \frac{C^{-1} \eta^{3/2}}{3} \quad .$$

Thus $3 A_1 C > \eta^{3/2}$ and $\epsilon_1 > \frac{1}{2}$ (for any $\eta > 0$).

Note that the value of A_1 is irrelevant for the rejection technique, except insofar as it enters into the efficiency ϵ_1 . However, A_1 is required for the probabilities in Eq. (17).

It is clear that

$$A_1 = B/C \quad , \quad (20)$$

$$\text{where } B \equiv \int_0^{\eta} \frac{y^{1/2} dy}{e^{y-\eta} + 1} \quad . \quad (21)$$

Hence the value of B as well as C is required for each $\eta \geq 5/2$ which arises. These values are listed for $\eta = 3, 4, \dots, 50$ in TABLE III, and were obtained by numerical integration using Simpson's rule. It may be helpful to include the following routine.

Simpson's method for $B = \int_0^\eta \frac{y^{\frac{1}{2}} dy}{e^{y-\eta} + 1}$, $\eta = 3, 4, \dots, 50$.

1. $1/100 \rightarrow d$.
2. $e^d \rightarrow E$.
3. $3 \rightarrow \eta$.
4. $N = 100 \eta$.
5. $0 \rightarrow y_0$.
6. $e^{-\eta} \rightarrow E_0$.
7. $0 \rightarrow Z_0$.
8. $0 \rightarrow n$.
9. $y_{n+1} = y_n + d$.
10. $E_{n+1} = E_n E$.
11. $Z_{n+1} = y_{n+1}^{\frac{1}{2}} / (1 + E_{n+1})$.
12. $n + 1 \rightarrow n$.
13. Is $n < N$? Yes (return to (9)), No (advance to (14)).
14. $B_\eta = \frac{d}{3} [Z_0 + Z_N + 4(Z_1 + Z_3 + \dots + Z_{N-1}) + 2(Z_2 + Z_4 + \dots + Z_{N-2})]$.
15. Is $\eta < 50$? Yes ($\eta + 1 \rightarrow \eta$, return to (4)), No (advance to (16)).
16. Print B_3, B_4, \dots, B_{50} .

(b) To sample the second density (and this is the whole difficulty) we write

$$A_2^{-1} p(y) dy = A_2^{-1} C^{-1} e^\eta \Gamma_\eta H \cdot \frac{ye^{-y} dy}{\Gamma_\eta} \cdot \frac{H^{-1}}{y^{\frac{1}{2}}(1 + e^{\eta-y})}, \quad (22)$$

where

$$H = \max 1/[y^{\frac{1}{2}}(1 + e^{\eta-y})] \text{ for } \eta < y < \infty, \quad (23)$$

$$\Gamma_\eta = \int_\eta^\infty ye^{-y} dy = (\eta + 1) e^{-\eta}. \quad (24)$$

Hence, if we determine

$$h = \min [y^{\frac{1}{2}}(1 + e^{\eta-y})] \text{ for } \eta < y < \infty, \quad (25)$$

the density (22) becomes

$$A_2^{-1} C^{-1} (\eta + 1) h^{-1} \cdot \frac{y e^{-y}}{\Gamma_\eta} \cdot \frac{h}{y^{\frac{1}{2}} (1 + e^{\eta-y})} \quad (26)$$

We propose to sample ye^{-y}/Γ_η for y on (η, ∞) , accepting y with probability

$$h/[y^{\frac{1}{2}}(1 + e^{\eta-y})] < 1 \quad , \quad (27)$$

the efficiency of the technique being now

$$\epsilon_2 = A_2 C h/(\eta + 1) \quad . \quad (28)$$

Recalling that $A_2 = 1 - A_1$ and $A_1 = B/C$, this becomes

$$\epsilon_2 = (C - B) h/(\eta + 1) \quad , \quad (29)$$

where B is defined by Eq. (21), and tabulated in TABLE III.

Thus the minimum value h in Eq. (25) is required not only for evaluating the efficiency ϵ_2 , but also for the acceptance probability (27). We next turn to the determination of h .

For the function

$$h(y) = y^{\frac{1}{2}} (1 + e^{\eta-y}), \quad y \geq \eta \quad , \quad (30)$$

one may show that $h(\eta) = 2\eta^{\frac{1}{2}}$, $h(\infty) = \infty$, with

$$h'(y) = [1 - (2y - 1) e^{\eta-y}]/2y^{\frac{1}{2}} \quad . \quad (31)$$

Thus $h'(\eta) < 0$, $h'(\infty) = 0$, and the minimum of $h(y)$ occurs at some $y_0 > \eta$. We therefore require the unique $y_0 > \eta$ for which $h'(y) = 0$, that is to say, for which

$$g(y) \equiv (2y - 1) e^{\eta-y} - 1 = 0. \quad (32)$$

Now $g(\eta) = (2\eta - 1)^{-1} > 0$ since $\eta > 1$, and $g(\infty) = -1$. However, it can be shown that $g(y)$ is decreasing on (η, ∞) only if $\eta > 3/2$, and is concave up only if $\eta > 5/2$. Hence, Newton's method for the zero y_0 of $g(y)$, with an initial $y = \eta$, is safe only if $\eta > 5/2$, and this has dictated our requirement $\eta > 5/2$ in the present method. The values of h for $\eta = 3, 4, \dots, 50$ are listed in TABLE III, together with the corresponding efficiencies ϵ_2 .

The zero y_0 and associated minimum h of $h(y)$ were computed by the following routine.

Newton's method for $h = \min_{(\eta, \infty)} [y^{\frac{1}{2}}(1 + e^{\eta-y})]$, $\eta = 3, 4, \dots, 50$.

1. $3 \rightarrow \eta$.
2. $\eta \rightarrow y$.
3. $y' = y + \frac{(2y - 1)e^{\eta-y} - 1}{(2y - 3)e^{\eta-y}}$.
4. Is $y' - y < .001$? No ($y' \rightarrow y$, return to (3)), Yes (advance to (5)).
5. $h_\eta = (y')^{\frac{1}{2}}(1 + e^{\eta-y'})$.
6. Is $\eta < 50$? Yes ($\eta + 1 \rightarrow \eta$, return to (2)), No (advance to (7)).
7. Print h_3, h_4, \dots, h_{50} .

It only remains to indicate how the "tail end" of the Γ -density ye^{-y}/Γ_η , $\eta < y < \infty$, is to be sampled for $y > \eta$. For this, we employ the ingenious method of Carey and Drijard (Ref. 5), which in our case may be formulated by the following routine.

1. Set $P = e^{-\eta}$, $A = e^{-\eta}(1 + \eta)$, $B = 1/(1 + \eta)$.
2. Generate random numbers ρ_1, ρ_2 on $(0,1)$.
3. Is $\rho_1 \leq B$? Yes (advance to (4)), No (advance to (5)).
4. Set $r_1 = A\rho_1$, $r_2 = \rho_2$ (advance to (6)).
5. Set $r_1 = P \exp[(1 + \eta)\rho_1 - 1]$, $r_2 = \rho_2 P/r_1$ (advance to (6)).
6. Set $y = -\log r_1 r_2$.

The justification of this is based on the remarks below.

(a) To sample the density $ye^{-y}/\Gamma(2)$ on its full range $(0, \infty)$ (Ref. 4, C 22), one generates random numbers r_1, r_2 and sets

$$y = -\log r_1 r_2,$$

where (r_1, r_2) may be thought of as a point uniformly distributed in the unit square.

TABLE III

DATA FOR CASE $\eta > 5/2$

η	C	B	h	ϵ_2	A_1	η	C	B	h	ϵ_2	A_1
3	3.97699	2.56919	2.539	.89	.646	27	93.5307	90.0099	5.691	.72	.962
4	5.77073	4.19987	2.834	.89	.728	28	98.7747	95.1863	5.786	.72	.964
5	7.83797	6.11994	2.967	.85	.781	29	104.113	100.458	5.851	.71	.965
6	10.1443	8.29047	3.157	.84	.817	30	109.545	105.825	5.941	.71	.966
7	12.6646	10.6854	3.336	.83	.844	31	115.067	111.283	6.027	.71	.967
8	15.3805	13.2830	3.488	.81	.864	32	120.680	116.833	6.115	.71	.968
9	18.2776	16.0682	3.656	.81	.879	33	126.380	122.471	6.212	.71	.969
10	21.3445	19.0287	3.809	.80	.892	34	132.168	128.198	6.274	.71	.970
11	24.5718	22.1544	3.956	.80	.902	35	138.042	134.012	6.356	.71	.971
12	27.9518	25.4368	4.072	.79	.910	36	144.000	139.911	6.438	.71	.972
13	31.4775	28.8685	4.225	.79	.917	37	150.041	145.894	6.519	.71	.972
14	35.1430	32.4434	4.315	.78	.923	38	156.165	151.960	6.598	.71	.973
15	38.4430	36.1558	4.440	.77	.928	39	162.370	158.108	6.678	.71	.974
16	42.8730	40.0008	4.557	.77	.933	40	168.655	164.337	6.757	.71	.974
17	46.9286	43.9739	4.676	.77	.937	41	175.019	170.646	6.836	.71	.975
18	51.1061	48.0711	4.792	.77	.941	42	181.461	177.033	6.910	.71	.976
19	55.4019	52.2887	4.887	.76	.944	43	187.980	183.498	6.988	.71	.976
20	59.8128	56.6233	5.012	.76	.947	44	194.575	190.040	7.049	.71	.977
21	64.1561	61.0719	5.121	.72	.952	45	201.246	196.658	7.124	.71	.977
22	68.7928	65.6317	5.196	.71	.954	46	207.991	203.352	7.195	.71	.978
23	73.5361	70.2998	5.316	.72	.956	47	214.811	210.119	7.269	.71	.978
24	78.3837	75.0740	5.401	.72	.958	48	221.703	216.960	7.342	.71	.979
25	83.3333	79.9518	5.500	.72	.959	49	228.667	223.874	7.415	.71	.979
26	88.3830	84.9311	5.599	.72	.961	50	235.702	230.860	7.483	.71	.979

(b) But for the tail end density, one requires only such points for which $y > \eta$, i.e., for which

$$r_1 r_2 < e^{-\eta} \equiv P \quad .$$

One could, of course, throw points (r_1, r_2) uniformly in the unit square, and reject those lying above the hyperbola $r_1 r_2 = P$, but the efficiency would be poor.

(c) The above (nonrejection) device is valid since the two transformations in (4) and (5) both have Jacobian $e^{-\eta}(1 + \eta)$, independent of ρ_1, ρ_2 , and so transform the two rectangular areas of the full ρ_1, ρ_2 unit square determined by the line $\rho_1 = B$ in a uniform way into the required two areas of the r_1, r_2 unit square; the first a rectangle of base $e^{-\eta}$ and height 1, of area $e^{-\eta}$, and the second lying directly below the hyperbola $r_1 r_2 = e^{-\eta}$, with base $1 - e^{-\eta}$, and area $\eta e^{-\eta}$.

V. VALUE OF $I(\eta)$ FOR $\eta \leq 0$

For arbitrary $n > 0$, and $A \equiv e^{\eta} \leq 1$, one may write

$$\begin{aligned} J(\eta) &\equiv \int_0^{\infty} \frac{y^{n-1} dy}{e^{y-\eta} + 1} = \int_0^{\infty} \frac{y^{n-1} (Ae^{-y}) dy}{1 + (Ae^{-y})} \\ &= \sum_{j=1}^{\infty} (-1)^{j+1} \int_0^{\infty} y^{n-1} (Ae^{-y})^j dy \\ &= \sum_{j=1}^{\infty} \frac{(-1)^{j+1} A^j}{j^n} \int_0^{\infty} (jy)^{n-1} e^{-jy} d(jy) \\ &= \left(\sum_{j=1}^{\infty} (-1)^{j+1} \frac{A^j}{j^n} \right) \int_0^{\infty} x^{n-1} e^{-x} dx \equiv \bar{\zeta}(A, n) \Gamma(n) \quad . \end{aligned}$$

For $n = 3/2$, this gives in our case

$$I(\eta) = \bar{\zeta}(A, 3/2) \Gamma(3/2) = \frac{\sqrt{\pi}}{2} \bar{\zeta}(e^{\eta}, 3/2),$$

determining η implicitly in terms of $I(\eta)$.

In particular, this shows that

$$I(0) = \frac{\sqrt{\pi}}{2} \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j^{3/2}} = \frac{\sqrt{\pi}}{2} \left(1 - \frac{1}{\sqrt{2}}\right) \zeta(3/2) = .678094,$$

where ζ is the Riemann zeta-function (cf. TABLE I).

In fact, a method (Ref. 4, R 8) for sampling $p(\dot{y})$ can be based on the above relations when $\eta < 0$, but the routine of Part III seems simpler and does not restrict η to negative values.

VI. THE MARGINAL DENSITY OF v_x

It is remarkable that, by introducing polar coordinates r, θ for v_y, v_z , the marginal density of v_x on $(-\infty, \infty)$ may be obtained in the explicit form (Ref. 1, p. 334)

$$\begin{aligned} P_1(v_x) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} P(v_x, v_y, v_z) dv_y dv_z \\ &= \frac{4\pi m^2 \theta}{nh^3} \text{log} \left[1 + \exp\left(\eta - \frac{mv_x^2}{2\theta}\right) \right]. \end{aligned}$$

For $u = (m/2\theta)^{1/2} v_x$, we then have the u -density

$$d(u) = (2C)^{-1} \text{log}(1 + e^{\eta} e^{-u^2}),$$

which seems a more well-behaved function than $p(x)$, and would, of course, serve our purpose. However, none of our attempts to sample $d(u)$ have proved feasible.

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