$$\rho c^{s}(r) = \frac{1}{2\pi} \int_{0}^{\infty} dq \, q J_{0}(qr) \left[\frac{4}{q^{2}} - \frac{1}{\exp(q^{2}/4) - 1} \right]$$
(4)

[this is equivalent to Eq. (14) of Ref. 3, by an integration by parts]. The asymptotic behavior of $c^s(r)$ is governed by the four poles of its Fourier transform [defined by Eq. (4)] which are closest to the real axis, i.e., at $q^2 = \pm 8i\pi$. Keeping only the contributions of these poles gives

$$\rho c^{s}(r) \approx -\frac{1}{2\pi} \int_{0}^{\infty} dq \, q J_{0}(qr) \left[\frac{4}{q^{2} + 8i\pi} - \frac{4}{q^{2} - 8i\pi} \right]$$

$$= -(4/\pi) \ker(8^{1/2} \pi^{1/2} r), \tag{5}$$

where ker is a Bessel function⁴ of known asymptotic behavior:

$$\rho c^{s}(r) \underset{r \to \infty}{\sim} - (2/\pi)^{3/4} r^{-1/2} \times \exp(-2\pi^{1/2} r) \cos[2\pi^{1/2} r + (\pi/8)]. \tag{6}$$

Thus, it is seen, on this model, that c(r) behaves asymptotically as $-\beta v(r)$ and that the remainder $c^s(r)$ is indeed short ranged and, more explicitly, has the exponential decay [Eq. (6)].

A second remark is about the asymptotic behavior of the "bridge function" B(r), which is defined by

$$B(r) = \ln[1 + h(r)] - h(r) + c^{s}(r). \tag{7}$$

Since, here h(r) is the Gaussian $-\exp(-r^2)$, the bridge function B(r) has the same asymptotic behavior [Eq. (6)]

as $c^s(r)$. Therefore, B(r) has an exponential decay, which is slower than the Gaussian decay of h(r). This is in contradiction with a common belief that B(r) has a faster decay. Of course, our observation might be a pathology of the present model at the special value $\Gamma = 2$.

It is amusing to note that, if we express B(r) as an infinite sum of graphs built with h bonds, f since f is a Gaussian, every given graph can be explicitly computed and gives a Gaussian result. For instance,

Therefore, the exponential decay of B(r) results from the infinite summation of Gaussians of increasing ranges.

ERRATA

Erratum: The thermodynamics of ammonium scheelites. III. An analysis of the heat capacity and related data of deuterated ammonium perrhenate ND_4ReO_4 [J. Chem. Phys. 85, 5963 (1986)]

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Equation (3) contains a misplaced bracket at C_{11} plus an incorrect $2C_{13}\alpha_1\alpha_3$ term. It should read $c_p - c_\epsilon = VT\{2(c_{11} + c_{12})\alpha_1^2 + 4c_{13}\alpha_1\alpha_3 + c_{33}\alpha_3^2\}$.

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