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# Density of states in disordered one-dimensional systems

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**Abstract.** The variational approximations to the partition function of a particle interacting with systems of disordered scatterers, presented by Luttinger for uniformly random systems and generalised by the author to systems with arbitrary positional disorder, are used to carry out explicit calculations on one-dimensional model systems. The models consist of uniform random configurations of  $\delta$  functions with a given density which are constrained by a two-particle correlation preventing a closer approach than specified for any pair. The results are used to calculate approximations to the densities of states for such systems with reasonable and interesting results.

## 1. Introduction

Luttinger (1976) proposed a variational method for approximating the partition function, at arbitrary temperature, of a particle interacting with identical scatterers positioned 'randomly,' with uniform probability, with some average density; each scatterer interacts with the particle via a short-ranged potential without bound states. Averages were performed analytically over all 'random configurations' of the same average density. The following year, I was able to generalise that formulation to include arbitrary correlations among the positions of the scatterers in order to allow calculations on arbitrary positionally disordered systems of a given density (Hernandez 1977). Although Luttinger was able to show that the variational estimate became asymptotically exact for high and low temperatures, no systematic program of calculations has been reported to test the method in the intermediate regime and to explore the difficulties of calculations with it for specific systems. Such a program has been initiated and preliminary results are reported herein; the calculations are further used to calculate approximate densities of states.

The model system chosen is the one-dimensional array of repulsive  $\delta$ -function scatterers on which only a short-range correlation is imposed to prevent any pair of scatterers from approaching any closer than some specified distance<sup>†</sup>. It should be noted that this problem, in three dimensions, presents no additional computational problems since the inherent spherical symmetry makes the problem effectively one

<sup>†</sup> In the notation of Hernandez (1977),  $C_2(x, x') = C_2(|x - x'|) = -1$  for  $|x - x'| < d, d/(d' - d)$  for  $d < |x - x'| < d'$  and 0 elsewhere. The limit  $d' \rightarrow \infty$  is taken. It has been assumed that  $C_n = 0, n > 2$ , which is a good approximation for small packing fraction ( $\rho d$ ). However, it results in an unphysical treatment of clusters in which three or more atoms mutually overlap. Work is in progress to include such clusters correctly or to justify, in detail, their neglect.

dimensional for calculational purposes. The main reason for choosing this one-dimensional problem is that the simplest ordered arrays constitute the Kronig-Penney model whose solutions are well known (Merzbacher 1970). Further, by letting the effective diameter ( $d$ ) of the atoms (distance of closest approach) vary from zero to the reciprocal of the average density ( $\rho$ ), the problem under consideration varies from the 'random' case ( $d = 0$ ) to the completely ordered one ( $\rho d = 1$ ). The last statement follows from the fact that if higher density fluctuations than average are forbidden by the impenetrability of the scatterers, then lower density than average fluctuations must likewise be forbidden to maintain the average density. The 'random' case has been solved in general for a particle of arbitrary mass ( $m$ ) and scatterers of arbitrary density ( $\rho$ ) and interaction strength  $u(z) = \gamma\delta(z)$ , by scaling the inverse temperature into a variable  $K = \gamma\rho\beta/a$  where  $\beta = (kT)^{-1}$  and all the physical parameters are effectively contained in  $a = (\hbar^2\rho/2m\gamma)^{1/2}$ . The correlated case has been solved for the case  $a = 1$  and  $\rho d = 0.2$  in order to illustrate the effects of non-randomness.

In addition to calculating the variational approximation to the average partition function asymptotically for high and low temperature, nine other temperatures have been calculated. This information has been used to calculate approximate average densities of states for the particle by inverting an assumed Laplace transform relation between the variational estimate for the partition function and the approximate average density of states; this relationship is known to exist between the actual partition function and the density of states. It cannot be claimed that this approximation to the density of states is at the same level as the variational approximation is to the actual partition function due to the integral nature of the transform; however this seems a reasonable way of proceeding.

## 2. Calculations and results

In one dimension, with Hamiltonians

$$H(p, x) = \frac{p^2}{2m} + \sum_{i=1}^N \gamma\delta(x - X_i)$$

constrained to a length  $L$  with  $N$ ,  $L \rightarrow \infty$  and  $N/L \rightarrow \rho$ , with the  $X_i$ 's positioned with uniform probability except that no pair of them may be closer than some distance  $d$ , the average partition function per unit length has the following variational limit (Hernandez 1977, but changed to one dimension and scaled.  $A[K]$  is to be identified with  $C[\chi]/(\gamma\rho)$ )

$$\frac{\langle Z(\beta) \rangle}{L} \geq \frac{\rho}{(4\pi)^{1/2}a} \frac{\exp(-aKA[K])}{(aK)^{1/2}}$$

where, as previously noted,  $K = \gamma\rho\beta/a$ ,  $a = (\hbar^2\rho/2m\gamma)^{1/2}$  and  $A[K]$  is a functional, desired at its minimum,

$$A[K] = \frac{E_K}{\gamma\rho} + \frac{1}{K} \int_{-\infty}^{\infty} dy \left( 1 - \exp(-\phi(y)^2)(1 + \phi^2(y)) \right. \\ \left. - \frac{1}{2}a[(1 + 2\phi(y)^2)\exp(-\phi(y)^2) - 1] \int_{-\rho(d/a)}^{\rho(d/a)} (1 - \exp[-\phi(y+X)^2]) dX \right),$$

constrained by  $\int_{-\infty}^{\infty} \phi^2(y) dy = K$ , which is extremised to the above expression when the

real function  $\phi(y)$  obeys the nonlinear Schrödinger equation:

$$\frac{\phi''(y)}{\phi(y)} = \left[ \left( 1 - \frac{E_K}{\gamma\rho} \right) - \left( 1 - \exp(-\phi(y)^2) - a \exp(-\phi(y)^2) \int_{-\rho(d/a)}^{\rho(d/a)} (1 - \exp[-\phi(y+X)^2]) dX \right) \right].$$

The minimum of  $A[K]$  occurs when  $\phi(y)$  is even and nodeless.  $E_K/\gamma\rho$  is the eigenvalue of the equation, which must be determined.

It should be noticed that for  $d = 0$  the nonlinear Schrödinger equation has a local potential (due to the contact interaction  $\gamma\delta(z)$ ) and is independent of  $a$ .  $A[K]$  also becomes independent of  $a$  and thus it can be found in general. When  $d \neq 0$  the equation has the more general nonlinear, nonlocal, potential and both  $\phi(y)$  and  $A[K]$  have an explicit dependence on  $a$  and  $\rho d$ .

It may be verified that as  $K \rightarrow \infty$ ,  $E_K/\gamma\rho \rightarrow 0$ , and  $E_K/\gamma\rho \rightarrow 1$  as  $K \rightarrow 0$ . The asymptotic behavior of  $A[K]$  may be obtained variationally as  $K \rightarrow \infty$  and yields the Lifshitz result (for  $\rho d = 0$ ) as obtained by Luttinger (1976):

$$\lim_{K \rightarrow \infty} A[K] = 3(\pi/2K)^{2/3} (1 + \rho d)^{2/3}.$$

As  $K \rightarrow 0$ , the result  $A[K] \rightarrow 1 - \frac{1}{16}K^2(1 - 2\rho d)^2$  is obtained for  $\rho d < \frac{1}{2}$ . This follows from noticing that  $\phi(y)$  must be slowly varying and small everywhere; thus expansion yields  $\phi''/\phi \approx \delta - (1 - 2\rho d)\phi^2$  for  $\delta = 1 - E_K/\gamma\rho$  with solution  $\phi(y) = [2\delta/(1 - 2\rho d)]^{1/2} \operatorname{sech} \delta^{1/2}y$  and  $K = 4\delta^{1/2}/(1 - 2\rho d)$  if  $\rho d < \frac{1}{2}$ . For  $\frac{1}{2} < \rho d < 1$  no solution exists with  $\delta$  small and positive since the effective potential is repulsive. This is reminiscent of the problem that arises in three dimensions in the absence of bound states; this problem will be discussed briefly later and requires further study.

Numerical solutions for the equations have been obtained for integer values of  $K(1-9$  or  $12)$ . The case with  $d = 0$  is simplest. Since  $1 - E_K/\rho d$  varies monotonically from 0 to 1 as  $K$  varies from 0 to  $\infty$ , the equations were solved for various values of the eigenvalue to obtain  $K$  and  $A[K]$ ; high-accuracy interpolation then became possible to obtain the values in table 1.

Defining an approximation to the density of states  $G(\epsilon)$  by equating the variational approximations of the average partition function to

$$\int_0^\infty \exp(-\beta\epsilon)G(\epsilon) d\epsilon$$

**Table 1.** Random configurations (the accuracy is believed to be at least seven figures).

| $K$ | $A[K]$     |
|-----|------------|
| 1   | 0.8043802  |
| 2   | 0.3304509  |
| 3   | 0.7605926  |
| 4   | 0.81999330 |
| 5   | 0.6871399  |
| 6   | 0.72304317 |
| 7   | 0.8268792  |
| 8   | 0.64702730 |
| 9   | 0.61540568 |

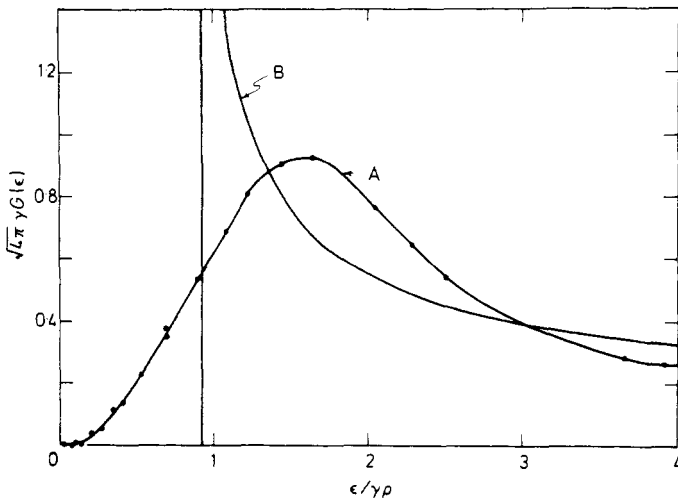
yields

$$\exp(-aKA[K])/K^{1/2} = \int_0^\infty [(4\pi a)^{1/2} \gamma G(\gamma\rho x/a)] \exp(-Kx) dx.$$

The inversion of this Laplace transform was carried out using the  $N$ -(7-12) point methods (Bellman *et al* 1966) which assume it is a smooth function, and use a weighted Legendre polynomial fit to change the equation to a matrix relation. Inversion of the matrix yields the function  $G$  at  $N$  points.

The results of this procedure for  $a = 1$  are shown in figure 1 together with the density of states for part of the lowest energy band of the Kronig-Penney model ( $\delta$  functions of strength  $\gamma$ , at separation  $\rho^{-1}$  with  $a = 1$ ) which lies in the interval  $0.923 \leq \epsilon/\gamma\rho \leq \pi^2$  (Merzbacher 1970). For the region  $\epsilon/\gamma\rho > 4$  the calculation of  $G(\epsilon)$  is quite near its high-energy asymptote:

$$(4\pi)^{1/2} \gamma G(\epsilon) \rightarrow \{\pi[\epsilon/(\gamma\rho) - 1]\}^{-1/2}.$$



**Figure 1.** A, calculated approximation to the average density of states of a particle, of mass  $m$ , in the field of 'random' configurations of  $\delta$ -function scatterers of strength  $\gamma$  and density  $\rho$  for  $\hbar^2\rho/2m\gamma = 1$ . B, low-energy part of the density of states, in the first band, for the Kronig-Penney model of  $\delta$ -functions of strength  $\gamma$  ordered to a density  $\rho$  with  $\hbar^2\rho/2m\gamma = 1$ . The points are calculated, the curve sketched through them; inversion used the 7-9-point methods.

The low-energy asymptote is, as previously noted, given by the Lifshitz result

$$\lim_{\epsilon \rightarrow 0} G(\epsilon) \sim \exp[-(\pi^2 \gamma\rho/\epsilon)^{1/2}].$$

The number of states represented by  $G(\epsilon)$  for  $\epsilon/\gamma\rho < 4$  is equal, within  $\approx 2\%$ , to those represented by its asymptotic value in the interval  $1 < \epsilon/\gamma\rho < 4$ ; at higher energy the curves are essentially the same. As can be seen, the band-gaps and Van Hove singularities of ordered densities of states have disappeared in  $G(\epsilon)$  though a broadened peak remains as well as an asymptotically vanishing 'tail' at low energy. It is noteworthy that the Kronig-Penney model density of states in this figure is not the only

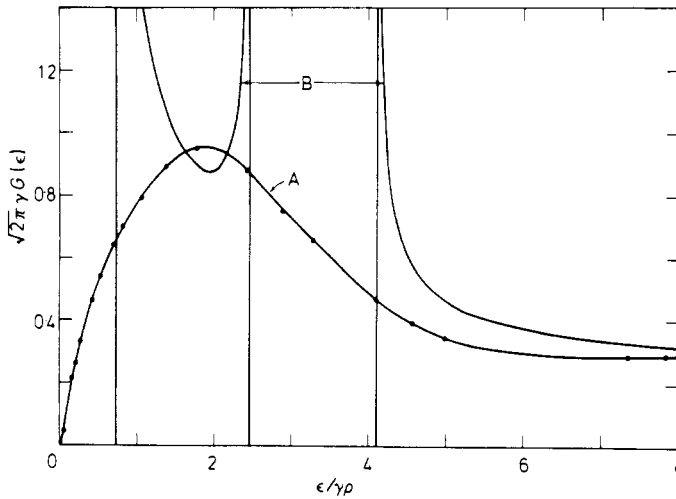
one consistent with the restriction  $a = 1$ ; among other configurations, pairing atoms (superimposing them) at a separation  $2/\rho$  yields a model of the same density (two atoms in  $2/\rho$ ) with the same average potential ( $\gamma\rho$ ) which, of course, is indistinguishable from single atoms of strength  $2\gamma$  at separation  $2/\rho$ . Such a model, naturally, has a different density of states, shown in figure 2 and labelled B (first two bands lie in  $0.740 \leq \epsilon/(\gamma\rho) \leq \frac{1}{4}\pi^2$  and  $4.116 \leq \epsilon/(\gamma\rho) \leq \pi^2$ ). In that figure, the result of the Laplace inversion for averaged 'random' configurations consistent with  $a = \frac{1}{4}$  (note the scale changes relative to figure 1) is also shown. Relative to this curve are its asymptotes

$$\lim_{\epsilon \rightarrow \infty} (2\pi)^{1/2} \gamma G(\epsilon) \rightarrow \left\{ \frac{1}{2}\pi [(\epsilon/\gamma\rho) - 1] \right\}^{-1/2}$$

and

$$\lim_{\epsilon \rightarrow 0} G(\epsilon) \sim \exp[-(\pi^2 \gamma\rho/4\epsilon)^{1/2}],$$

and comments about the area under it, which are comparable with those on figure 1.



**Figure 2.** A, calculated approximation to the average density of states of a particle, of mass  $m$ , in the field of 'random' configurations of  $\delta$ -function scatterers, of strength  $\gamma$  and density  $\rho$  for  $\hbar^2\rho/2m\gamma = \frac{1}{4}$ . B, density of states in the first, and low-energy part of the second, bands for the Kronig-Penney model of  $\delta$  functions of strength  $2\gamma$  ordered to a density  $\frac{1}{2}\rho$  with  $\hbar^2\rho/2m\gamma = 1$  (note:  $(\hbar^2/2m) \times (\text{density}/\text{strength}) = \frac{1}{4}$ ). The points are calculated, the curve sketched through them; inversion used the 7-9-point methods.

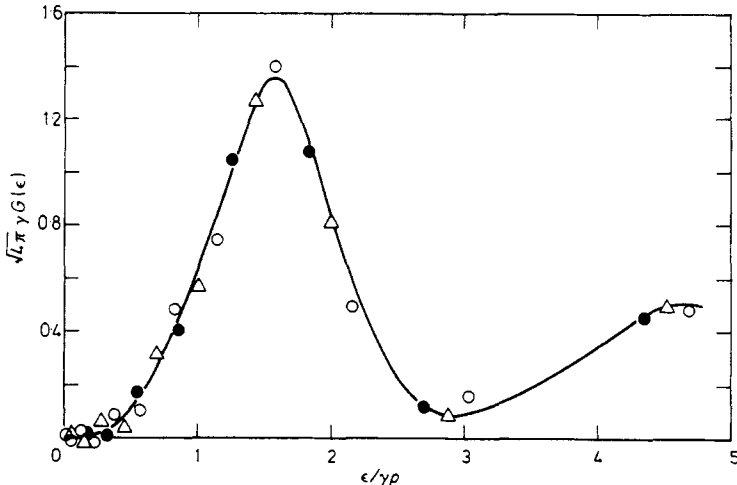
Curves for  $G(\epsilon)$  for any other value of  $a$  are easily obtained from the information in table 1 and the inversion procedure noted (Bellman *et al* 1966).

The 'non-random' case treated,  $a = 1$ ,  $\rho d = 0.2$ , may be expected to show more structure for  $G(\epsilon)$  due to the forbidden configurations. In this case the nonlinear, nonlocal Schrödinger equations were solved iteratively. For a chosen  $K$  and a trial starting function the eigenvalue was determined to an accuracy of  $\sim 10^{-9}$  by outward integration,  $\phi(y)$  was obtained, normalised, and iterated into a new potential in addition to being used to find  $A[K]$ . After about 10 iterations memory was lost of the starting function and the results for  $A[K]$  started oscillating. The subsequent, approximately 20, iterations for  $A[K]$  were averaged and a root-mean-square deviation

found; the results are given in table 2. Calculations were carried out on an IBM 360/155 computer. A run would take about 40 seconds, including compilation; this time was shortened by running groups of calculations with a previously compiled program. Explicit integrations used 'Bode's rule' and the differential equation was integrated implicitly through Taylor expansions including terms up to the fifth derivative; all calculations used double precision. The Laplace inversion was carried out, as before, with the results shown in figure 3. In order to clearly exhibit the second peak,  $K = 1-12$  were calculated. The calculational uncertainties gave rise to maximum uncertainties of  $\pm 0.001$  for the 10-point method,  $\pm 0.005$  for the 11-point method and  $\pm 0.02$  for the 12-point method, in units of the vertical scale of the figure. Clearly the

**Table 2.**  $a = 1, \rho d = 0.2$ . The RMS deviation (from the average) is less than  $2 \times 10^{-8}$ .

| $K$ | $A[K]$     |
|-----|------------|
| 01  | 0.99241195 |
| 02  | 0.96918059 |
| 03  | 0.93199346 |
| 04  | 0.88696243 |
| 05  | 0.84038418 |
| 06  | 0.79586683 |
| 07  | 0.75484659 |
| 08  | 0.71763756 |
| 09  | 0.68407228 |
| 10  | 0.65381019 |
| 11  | 0.62647318 |
| 12  | 0.60170095 |



**Figure 3.** Calculated approximation to the average density of states of a particle, of mass  $m$ , in the field of configurations of  $\delta$ -function scatterers of strength  $\gamma$  and average density  $\rho$ , for  $\hbar^2 \rho / 2m\gamma = 1$ , which are 'random' except that no pair of scatterers can be closer than a distance  $d = 0.2/\rho$ . The points are calculated with a larger uncertainty than those of the previous figures (see text); the curve is sketched through them. Inversion used the 10-12-point methods and different symbols are used for each result: open circles,  $N = 12$ ; open triangles,  $N = 11$ ; closed circles,  $N = 10$ .

desire to use as many points as possible in order to improve the inversion procedure must be compromised with the calculational uncertainty achievable to yield reasonable uncertainties in the inversion. A small modulation can be observed between alternate points in each inversion; it has been averaged in sketching a line in the figure. Thus the dip and second peak in the calculated  $G(\epsilon)$  are real and reminiscent of the gap between the first and second bands in ordered configurations with two atoms per unit cell and unit cell dimension of  $2/\rho$ ; the peak, of reinforcements of second band extrema, broadened. These remarks are somewhat speculative but, for example, three superimposed atoms, i.e. a strength  $3\gamma$ , at separation  $3/\rho$  with  $\hbar^2\rho/2m\gamma = 1$ , have a second band in the interval  $2.424 \leq \epsilon/\gamma\rho \leq 4.386$ , completely astride the second gap in the KP result of figure 2; however, this is a forbidden configuration. Other authors have found gaps or pseudogaps in systems in which the atoms are not allowed to approach too closely (Makinson and Roberts 1960, Edwards 1961, Beeby and Edwards 1963, for example). Interpretation and further calculations of this type need to be extended.

### 3. Comments

We have been hesitant to extend the calculations to  $\rho d \rightarrow 1$  for two reasons. First, the inversion procedure would tend to filter out sharp structure (Bellman *et al* 1966) which might be expected near the ordered case,  $\rho d = 1$ , though it is not clear what this variational method will yield. Also, the lack, at present, of analytic guidance on the high-energy, low-temperature, asymptote for  $\rho d > \frac{1}{2}$  is a problem as mentioned previously. Further work is in progress.

As to three-dimensional calculations, for the 'random'  $\delta$ -function case, calculations are no more difficult than in one dimension and related results have been reported (Hernandez 1975, Moore *et al* 1978). There is a problem: analytically it can be shown that the present variational method, which is essentially a mean field theory, yields an approximation to the partition function which, although continuous, has a cusp at a specified temperature (a function of the strength and density of the potentials)—a stability transition between 'unbound' particles and 'bound' ones. This feature must be an artefact of the mean field approach. Since a cusp in the actual partition function would indicate a phase transition, this is hard to accept for scatterers fixed in place, even though the system is averaged. This cusp or stability change has been used as a signal of the electron mobility collapse in helium gas, in reasonable agreement with experimental measurements (Hernandez 1975). In nature, atoms may move, but not in the model being used. It would be interesting to see if beyond the mean field theory there are fluctuations which smooth the cusp; this also is a problem for the future.

In summary, preliminary calculations based on the variational approximation to the average partition function of a particle interacting with a positionally disordered system of scatterers give apparently reasonable and interesting results which should be pursued further to show the limitations and successes of this method.

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