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## Exact solution of one-dimensional self-trapping systems in the mean-field approximation

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**Abstract.** The self-trapping of a light particle in a fluid is solved exactly in one dimension when the interaction between the light particle and fluid molecules is purely repulsive. It is shown that there is always at least one self-trapped state in the system. The uniqueness of the self-trapped state is proved for the ideal gas. In contrast, multiple trapped states are possible in the hard rod gas.

### 1. Introduction

It is well known that in a dense fluid a light particle (electron, positron or positronium, hereafter LP) can be bound in self-trapped states. Experimental measurements of the decay rate of positrons [1] and positronium atoms [2] strongly support the existence of the self-trapped states in a broad region about the critical point of simple fluids. These states can be obtained as a solution of a self-consistent mean-field problem involving the wavefunction for the LP,  $\psi(\mathbf{r})$ , and the density  $\rho(\mathbf{r})$  of the fluid in its vicinity. Moore *et al* [3] proved that, for an ideal gas, the existence of the self-trapped state is determined by the value of a parameter arising from the normalisation condition. This constant becomes larger when either the coupling constant or the average fluid density increases, or the temperature decreases. If this constant is less than a certain minimum, the LP does not have a self-trapped state. Recently, Reese and Miller [4] showed numerically that, for a real physical system, self-trapped states do not exist if the fluid density is too high or too low. In [3] there is also some evidence which suggests that, in 1D systems, the self-trapped state always exists. To our knowledge the exact proof of this problem is still missing.

In this paper we will give an *analytical* proof for the existence of a self-trapped state in *any* 1D system with a repulsive interaction between the LP and fluid molecules. The paper is arranged as follows. Section 2 formally solves the non-linear Schrödinger equation. Section 3 gives the proof of the existence of the self-trapped state in a 1D system. Section 4 addresses the uniqueness of this state in two specific systems, i.e. the ideal gas (IG) and the hard rod gas (HR). It is shown that the trapped state is unique in the IG, whereas multiple solutions are possible in the HR.

### 2. Formal solution to the differential equation

This combined system of LP and dense fluid can be described by the non-linear

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Schrödinger equation

$$-(\hbar^2/2m)\psi''(x) + \psi(x) \int dx' w(x-x')\rho(x') = E\psi(x). \quad (2.1)$$

In equation (2.1),  $\rho(x)$  is the average fluid density and  $w(x-x')$  is the two-body interaction between the LP and a fluid molecule; the interaction is not local. Equation (2.1) is formally no different than the usual Schrödinger equation. The integral  $\int dx' w(x-x')\rho(x')$  represents the average potential energy experienced by the LP at  $x$ . Here, however,  $\rho(x)$  is influenced by the effective interaction of the LP on the fluid. Equation (2.1) can also be derived from either a path integral formulation [4] or a free-energy density functional approach [3]. A common simplification is to assume that  $w$  is short ranged compared with the length scale for variations in  $\psi$ , as it is in many real systems. Here we also adopt this assumption and approximate  $w$  by

$$w(x-x') = g\delta(x-x') \quad (2.2)$$

where

$$g = \int dx w(x) > 0. \quad (2.3)$$

Equation (2.3) simplifies (2.1) to the local form

$$-(\hbar^2/2m)\psi''(x) + g\rho(x)\psi(x) = E\psi(x). \quad (2.4)$$

The fluid density  $\rho(x)$  is, in general, a functional of  $\psi^2(y)$

$$\rho(x) = \tilde{\rho}[\psi^2(y)] \quad (2.5)$$

because  $g\psi^2(x)$  acts like an external potential for the fluid. The explicit dependence of  $\rho$  on  $\psi^2$  is available in very few systems, e.g. the HR gas [5]. Even with the exact solution, the non-local relation [5] still prevents us from solving (2.4) exactly. Following the most popular treatments, we further assume that the local density approximation (LDA) is valid here. The LDA results in a local relation between  $\rho(x)$  and  $\psi^2(x)$

$$g\psi^2(x) = \mu(\rho_0) - \mu(\rho(x)) \quad (2.6)$$

where  $\mu$  is the chemical potential of the fluid and  $\rho_0$  is the fluid density when  $\psi(x) = 0$ . Theoretically we can always invert (2.6) to obtain

$$\rho(x) = \tilde{\rho}(\psi^2(x)) \quad (2.7)$$

at least numerically. Then (2.4) becomes

$$-(\hbar^2/2m)\psi''(x) + g\tilde{\rho}(\psi^2(x))\psi(x) = E\psi(x). \quad (2.8')$$

Following the scaling procedure in 3D systems [3, 4], we perform the following transformations:

$$t = (2m/\hbar^2)^{1/2}x \quad (2.9a)$$

$$\varphi(x) = (\beta g)^{1/2}\psi(x) \quad (2.9b)$$

$$\varepsilon = E/(g\rho_0) \quad (2.9c)$$

$$n(x) = \rho(x)/\rho_0. \quad (2.9d)$$

These transformations change (2.8') to a neat form

$$\varphi''(t) = [n(\varphi^2) - \varepsilon]\varphi(t). \quad (2.8)$$

The construction of the first integral of (2.8) is routine

$$(\varphi')^2 + \left( \varepsilon \varphi^2 - 2 \int_0^\varphi n(x^2)x \, dx \right) = 0 \tag{2.10}$$

where the constant of integration has been determined by the conditions

$$\varphi(\pm\infty) = \varphi'(\pm\infty) = 0. \tag{2.11}$$

There is a simple mechanical analogue for (2.10) [3, 6]. It is equivalent to the energy conservation law for a particle moving in a 1D system at position  $\varphi$  and time  $t$ . The quantity in the large bracket looks like a time-independent potential (figure 1). Equation (2.10) describes a state similar to that in a soliton problem [6], i.e. the particle is moving toward a position it can never reach in finite time. This state requires the potential energy at  $t=0$  to be exactly the same as that at  $t=\infty$ . Consequently, in contrast with 3D systems, there can be at most one self-trapped state for a fixed  $\varepsilon$  [3, 4]. This state also requires a potential well which restricts the possible values of  $\varepsilon$ . We will discuss this in more detail later on.

The normalisation condition

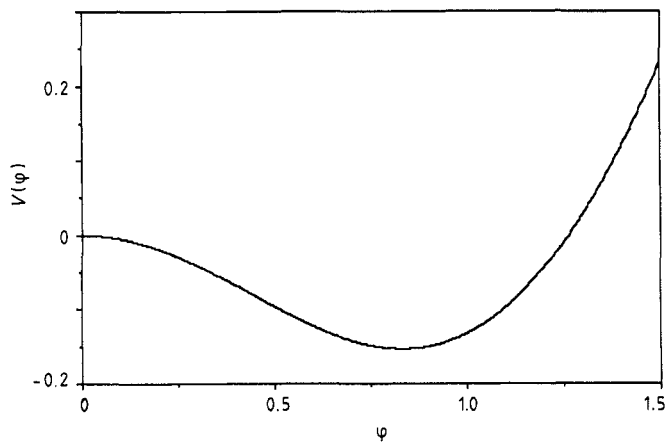
$$\int \psi^2(x) \, dx = 1 \tag{2.12}$$

requires that  $\varphi$  satisfies

$$I(\varepsilon) = \int \varphi^2(t) \, dt = \beta g (2mg\rho_0/\hbar^2)^{1/2} \tag{2.13}$$

according to equations (2.9). For a given equation of state, the dimensionless constant  $\beta g (2mg\rho_0/\hbar^2)^{1/2}$  contains all of the required system parameters. It determines the eigenvalue  $\varepsilon$  and, implicitly, the properties of the trapped state. The integral expressed in (2.13) can be transformed to an integration over  $z \equiv \varphi^2$  by making use of (2.10), the first integral of the non-linear Schrödinger equation. We find

$$I(\varepsilon) = \int_0^{z_0} dz \, z^{1/2} / [f_1(z) - f_2(z)]^{1/2} \tag{2.14}$$



**Figure 1.** The ‘potential energy’  $V(\varphi) \equiv \varepsilon \varphi^2 - 2 \int_0^\varphi n(\varphi^2)\varphi \, d\varphi$  defined in (2.10). The minimum is determined by  $\varepsilon = n(\varphi^2)$ . Therefore  $0 < \varepsilon < 1$ .

where the symmetry of  $\varphi$  about  $t=0$  has been taken into account and  $f_1$  and  $f_2$  are defined by

$$f_1(z) = \int_0^z n(z') dz' \quad f_2(z) = \varepsilon z. \tag{2.15}$$

In (2.14),  $z_0$  is a function of  $\varepsilon$  and is determined by requiring that the kinetic energy ( $\varphi(0)^2$ ) be equal to 0, i.e.

$$f_1(z_0) - f_2(z) = 0. \tag{2.16}$$

This occurs for two values of  $t$ , the turning point and the origin of the classical orbit (see figures 1 and 2). Here we mean the non-trivial value which occurs at the turning point.

In section 3 we will prove

$$\lim_{\varepsilon \rightarrow 1} I(\varepsilon) = 0 \tag{2.17a}$$

$$\lim_{\varepsilon \rightarrow 0} I(\varepsilon) = \infty. \tag{2.17b}$$

This means that for any  $\rho_0, T, m$  and  $g$  we can find at least one  $\varepsilon$  which satisfies (2.14). The corresponding  $\psi_\varepsilon(x)$  then satisfies conditions (2.11) and is a self-trapped state.

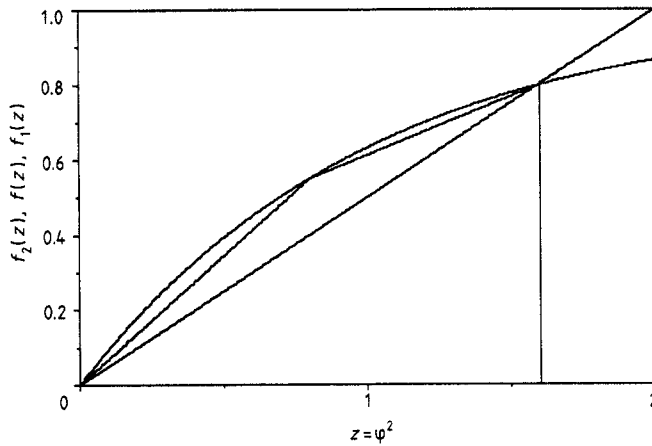


Figure 2. The graphical solution for  $z_0$ , which is indicated by the vertical line. The three curves are, from bottom:  $f_2(z), f(z)$  and  $f_1(z)$ . The function  $f(z)$  is as defined in (3.4).

### 3. Proof for the existence of the self-trapped state

In this section we present our main result; namely that the 1D system always has at least one self-trapped state if the interaction is repulsive. We first list some basic properties of  $f_1(z)$  and  $f_2(z)$ .

- (a)  $f_1(z), f_2(z) \geq 0$ .
- (b)  $n(z) \leq 1$  and so  $f_1(z) < z$ .
- (c)  $f_1(z) \rightarrow \text{constant} (z \rightarrow \infty)$ .
- (d)  $f_1'(0) = n(0) = 1$ .
- (e)  $f_1''(z) = n'(z) < 0$ .

Properties (b), (c) and (d) are a consequence of the repulsive interaction. Property (c) further assumes that when  $z$  goes to infinity  $n(z)$  goes to zero faster than  $1/z$ . This assumption is usually satisfied because large  $z$  is the low-density (ideal gas) limit where  $n(z) \approx \exp(-z)$ .

Usually (2.16) for  $z_0$  must be solved graphically (numerically) (figure 2). Some general behaviour, which is helpful in the later calculations, can be derived from the properties (a)-(e).

(f) As mentioned above, for any positive  $\epsilon$  there is a trivial root  $z=0$  which corresponds to  $t = \infty$ . If  $0 < \epsilon < 1$  there is a non-trivial root  $z_0$  which provides another point where the kinetic energy is equal to zero. To get localised states we require  $0 < \epsilon < 1$ .

- (g)  $z_0(\epsilon \rightarrow 0) \rightarrow \infty$ .
- (h)  $z_0(\epsilon \rightarrow 1) \rightarrow 0$ .

By using (a)-(h), (2.17b) can be proved immediately:

$$\begin{aligned}
 I(\epsilon) &= \int_0^{z_0} dz z^{1/2} / [f_1(z) - \epsilon z]^{1/2} \\
 &> \int_0^{z_0} dz z^{1/2} / [(1 - \epsilon)z]^{1/2} \quad (\text{property (b)}) \\
 &= z_0 / (1 - \epsilon)^{1/2} \\
 &> z_0 \rightarrow \infty \quad (\epsilon \rightarrow 0).
 \end{aligned}
 \tag{3.1}$$

The proof of equation (2.17a) is far more involved. To set it up, first we write down the explicit expressions for  $\epsilon(z_0)$ ,  $\epsilon'(z_0)$  and  $\epsilon''(z_0)$  where, as usual, the single prime and the double prime represent the first and second derivatives with respect to  $z_0$ ; when  $z_0$  approaches zero the corresponding limits for  $\epsilon(z_0)$  and its derivatives may be obtained as follows:

$$\epsilon(z_0) = f_1(z_0) / z_0 \rightarrow n(z_0) \rightarrow 1 \tag{3.2a}$$

$$\epsilon'(z_0) = n(z_0) / z_0 - f_1(z_0) / z_0^2 \rightarrow n'(0) / 2 < 0 \tag{3.2b}$$

$$z_0 \epsilon''(z_0) = n'(z_0) - 2\epsilon'(z_0) \rightarrow 0. \tag{3.2c}$$

Next we construct a function  $f(z)$  which satisfies

$$f_2(z) < f(z) < f_1(z) \quad 0 < z < z_0. \tag{3.3}$$

The choice is certainly not unique. For reasons which will become clear, we choose (figure 2)

$$f(z) = \begin{cases} f_1(z_0/2)(2z/z_0) & 0 < z < z_0/2 \\ a + bz & z_0/2 < z < z_0 \end{cases} \tag{3.4}$$

where

$$a = 2f_1(z_0/2) - f_1(z_0) \tag{3.5a}$$

$$b = [f_1(z_0) - f_1(z_0/2)](2/z_0). \tag{3.5b}$$

In terms of (3.4) and (3.5) we can get an explicit inequality for  $I(\varepsilon)$ :

$$I(\varepsilon) < \int_0^{z_0} dz z^{1/2} / [f(z) - \varepsilon z]^{1/2} = C_1 + C_2 \quad (3.6)$$

where

$$C_1 = \{(z_0^3/8) / [f_1(z_0/2) - f_1(z_0)/2]\}^{1/2} \quad (3.7a)$$

$$C_2 < \{z_0^3 / [f_1(z_0/2) - f_1(z_0)/2]\}^{1/2} = 8^{1/2} C_1 \quad (3.7b)$$

correspond to the integrals in each region specified in (3.4), respectively. Now we take the limit  $z_0 \rightarrow 0$  in (3.7) to demonstrate that both  $C_1$  and  $C_2$  go to zero. Using l'Hospital's theorem and (3.2) repeatedly, the calculation is straightforward, and we just give the final results:

$$\lim C_1 = \lim[-6z_0/n'(0)]^{1/2} = 0 \quad (3.8a)$$

$$\lim C_2 \leq \lim(8^{1/2} C_1) = 0. \quad (3.8b)$$

From the obvious fact that  $I(\varepsilon)$  is a continuous function of  $\varepsilon$  we arrive at the conclusion. *In any 1D system with a repulsive interaction between the LP and fluid molecules there always exists at least one self-trapped state.* This result is different from 3D systems for both the IG [3] and real fluids [4].

#### 4. The discussion of uniqueness

In § 3 we proved that  $I(\varepsilon)$  has the limits  $\infty$  and 0 corresponding to the limits 0 and 1 for  $\varepsilon$ . We have not been able to determine the condition on the equation of state or, equivalently,  $\tilde{\rho}(\psi^2)$ , which distinguishes whether or not the intersection of the horizontal line  $\beta g(2mg\rho_0/\hbar^2)^{1/2}$  and  $I(\varepsilon)$  is unique. If it is, there is a single trapped state. Below we give an example for each possibility. Because  $z_0$  is an implicit function of  $\varepsilon$ , working with  $I(z_0)$  will be more convenient. The question revolves about whether or not  $I'(z_0)$  is positive definite. If it is simply positive, and  $I'(z_0)$  vanishes on a set of positive measure, then degeneracy will occur. To proceed further, it is convenient to introduce the variable  $y = z/z_0$ .  $I(z_0)$  then takes the form

$$I(z_0) = z_0^{3/2} \int_0^1 dy y^{1/2} / [f_1(yz_0) - f_1(z_0)y]^{1/2}. \quad (4.1)$$

The derivative with respect to  $z_0$  is now given by

$$I'(z_0) = (z_0^{1/2}/2) \int_0^1 dy y^{1/2} / [f_1(yz_0) - f_1(z_0)y]^{1/2} \\ \times \{3f_1(z_0y) - 3f_1(z_0)y - z_0yn(z_0y) + z_0yn(z_0)\}. \quad (4.2)$$

The explicit evaluation of (4.2) for a specific equation of state is difficult and may not be possible. In the rest of this section we will use (4.2) to analyse two special cases, the ideal gas and the hard rod gas.

##### 4.1. Ideal gas

The  $n$ - $z$  relation for the IG is simply

$$n(z) = \exp(-z) \quad (4.3)$$

and

$$f_1(z) = 1 - \exp(-z). \tag{4.4}$$

In the following we will show that the quantity in the curly bracket of (4.2) is positive, proving that here the trapped state is unique. Define this quantity as a function  $F(z_0, y)$ :

$$F(z_0, y) = 3(1 - y) - 3[\exp(-z_0 y) - y \exp(-z_0)] - y z_0 [\exp(-z_0 y) - \exp(-z_0)]. \tag{4.5}$$

It is easy to see that

$$F(z_0, 0) = F(z_0, 1) = 0. \tag{4.6}$$

If  $F(z_0, y)$  has the same sign in  $(0, 1)$  then  $I'(z_0)$  has the same sign for all  $z_0$ , and  $I(z_0)$  is monotonic. Thus the sufficiency condition for  $I(z_0)$  to be monotonic is that  $\partial F/\partial y = F_y(z_0, y)$  has only one root in  $(0, 1)$ . It turns out that this is not too difficult to prove for the 1G.  $F_y(z_0, y) = 0$  is equivalent to

$$(2z_0 + z_0^2 y) / [3 - 3 \exp(-z_0) \exp(-z_0 y)] = \exp(z_0 y). \tag{4.7}$$

It is easy to show that the left-hand side of (4.7) is greater than one when  $y = 0$  and therefore (4.7) has one and only one root. Moreover, for any  $z_0 > 0$ , simple computation shows

$$F_y(z_0, 0) = 2z_0 - 3 + 3 \exp(-z_0) + z_0 \exp(-z_0) > 0. \tag{4.8}$$

Noticing that all other quantities in the integrand of (4.2) are positive, we immediately get

$$I'(z_0) > 0. \tag{4.9}$$

The numerical result of  $I(\epsilon)$  for the 1G is shown in figure 3. It is obvious that there is exactly one trapped state.

#### 4.2. Hard rod

The exact local thermodynamics of the HR is given by Percus [5]. As mentioned earlier, it is one of the few fluids where this is known exactly. Within the LDA it takes the form

$$\varphi^2(t) \equiv z(t) = P(1) - P(n(t)) + \ln[P(1)/P(n(t))] \tag{4.10}$$

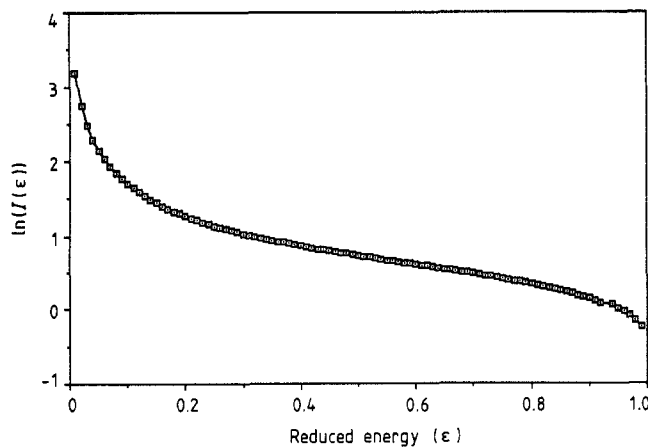


Figure 3. The normalisation  $I(\epsilon)$  for the ideal gas using a logarithmic scale.



where  $P(n) = a\rho_0 n / (1 - a\rho_0 n)$  and  $a$  is the length of an individual HR. Here the integral of  $f_1(z)$  cannot be carried out directly as for the 1G. After the transformation  $n = n(z)$ ,  $f_1(z)$  changes to

$$\begin{aligned} f_1(z) &\equiv \tilde{f}_1(n) \\ &= \int_1^n dn' n' (dz/dn') \\ &= [P(1) - P(n(z))]/a\rho_0. \end{aligned} \tag{4.11}$$

Also, in terms of  $n$ ,  $F(z_0, y)$  now takes the form

$$\begin{aligned} \tilde{F}(\eta, n) &= (3/a\rho_0)[P(1) - P(n)] - (3/a\rho_0)[z(n)/z(\eta)][P(1) - P(\eta)] \\ &\quad - (n - \eta)z(n) \end{aligned} \tag{4.12}$$

where  $\eta = n(z_0)$  is determined by

$$[P(1) - P(\eta)](1/a\rho_0 - \varepsilon) = \varepsilon \ln[P(1)/P(\eta)]. \tag{4.13}$$

We have not been able to *analytically* determine whether trapped states are unique for the HR. We are able to show that the sufficiency condition is no longer satisfied, indicating the possibility of multiple states, as we approach the high-density limit, i.e.

$$1 - a\rho_0 \ll 1. \tag{4.14}$$

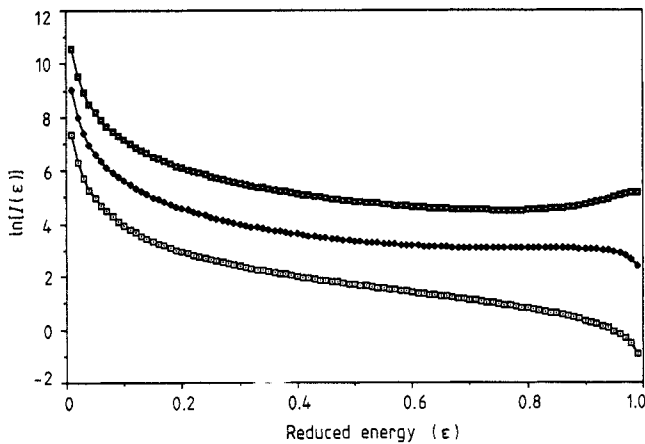
One can then find that  $P(1) \gg P(n)$  if  $n$  is not too close to 1. With the further assumption that  $\varepsilon$  is not close to zero, i.e.  $\eta$  is not too close to one, we have

$$z(n) \approx z(\eta) \approx P(1) \tag{4.15}$$

for such a value of  $n$ . Consequently, (4.12) is a finite negative number

$$F(\eta, n) \approx -(n - \eta)P(1) < 0. \tag{4.16}$$

Figure 4 shows the numerical result for  $a\rho_0 = 0.01, 0.8142$  and  $0.96$ . It appears that  $\rho_c = 0.8142/a$  plays the role of a ‘critical’ density. When  $\rho < \rho_c$ , the HR fluid is similar



**Figure 4.** The normalisations  $I(\varepsilon)$  for the hard rod gas using a logarithmic scale. Curves are shown for three values of  $a\rho_0$ : 0.01 ( $\square$ ), 0.8142 ( $\bullet$ ) and 0.96 ( $\blacksquare$ ). The top curve ( $a\rho_0 = 0.96$ ), has a peak near  $\varepsilon = 0.98$ . The middle curve  $a\rho_0 = 0.8142$  corresponds to a ‘critical’ density and there is a saddle point around  $\varepsilon = 0.8$ .

to the ideal gas and has a unique trapped state. When  $\rho > \rho_c$ , a bifurcation occurs and multiple trapped states appear in a certain parameter region. This result is not too surprising. In the high-density limit,  $a\rho_0 = 1$ , the interaction becomes a periodic delta potential (Dirac comb). In this case the LP cannot alter the local fluid density and the spectrum has a band structure. We have not observed additional bifurcations (local extrema of  $I(\varepsilon)$ ) for larger values of  $a\rho_0$ .

In the next section we calculate the free energy and discuss the stability of the trapped states in the HR. The discussion naturally includes the case of the IG, which is the low-density limit of the HR, i.e.  $a\rho_0 = 0$ .

### 5. Stability of the trapped states

When multiple trapped states appear, the calculation of the free energy can distinguish which is the global minimum. In [3] a canonical ensemble was employed to discuss the stability of the three-dimensional ideal gas with respect to fluctuations in the local temperature or density. Because the density and wavefunction are coupled, fluctuations in density produce corresponding fluctuations in the energy eigenvalue of the trapped state. To investigate the stability of the trapped state with respect to energy fluctuations, Moore *et al* [3] defined the specific heat of the trapped state as follows:

$$\begin{aligned} C_V &= \rho_0 g (d\varepsilon/dT)_{N,V} \\ &= \rho_0 g [d\varepsilon/dI(\varepsilon)] [dI(\varepsilon)/dT]_{N,V} \\ &= -[\rho_0 g I(\varepsilon)/T] (dI(\varepsilon)/d\varepsilon)^{-1}. \end{aligned} \tag{5.1}$$

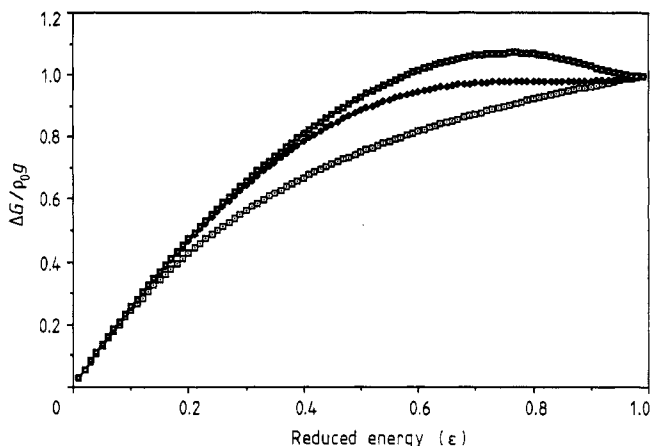
Clearly, when  $I(\varepsilon)$  has positive slope the specific heat is negative and the state is unstable. They also found that the slope of  $I(\varepsilon)$  has the opposite sign to the slope of  $\Delta F(\varepsilon)/\rho_0 g$  everywhere. Here  $\Delta F$  is the free energy difference between the actual free energy and that for a uniform system lacking an LP.

Their proof is not completely rigorous in handling the thermodynamic limit. This point is discussed in more detail by Reese and Miller [4] where it is shown that the canonical ensemble is equivalent to the grand canonical ensemble at the thermodynamic limit. Within LDA, the HR gas has the same energy as an IG, i.e.  $\varepsilon$ , but has a different free energy. Therefore (5.1) is also true for the HR. From figure 4 we conclude immediately that the trapped state with the intermediate value of  $\varepsilon$  has a negative specific heat and hence is unstable. Because the free energy is obviously unbounded from above (consider the delta wavefunction which is the limit of the localised state) this state can only be a local maximum.

With regard to the other two states, we have to distinguish between them numerically. Because our wavefunction is defined in the infinite space (see (2.11)) we use the grand canonical ensemble directly. The Gibbs free energy is defined by

$$\begin{aligned} \frac{\Delta G}{\rho_0 g} &= \left( \Delta F - \int dz \mu_0 (\rho - \rho_0) \right) \frac{1}{\rho_0 g} \\ &= \frac{1}{I(\varepsilon)} \int dt \left\{ \frac{[P(1) - P(n)]}{a\rho_0} - n \left[ P(1) - P(n) + \ln \left( \frac{P(1)}{P(n)} \right) \right] \right\} \end{aligned} \tag{5.2}$$

where  $P$  is defined in (4.10). The numerical result is given in figure 5. Clearly the state corresponding to the smallest value of  $\varepsilon$  has the lower free energy and is the



**Figure 5.** The scaled free energy  $\Delta G/\rho_0 g$  for the hard rod gas. The valleys (peaks) in figure 4 correspond to peaks (valleys) here.

global minimum. The other is a local minimum, i.e. it is metastable. Although we cannot prove that the slopes of  $I(\varepsilon)$  and  $\Delta F$  have opposite sign, plots of the free energy against  $\varepsilon$  for the HR show exactly the same behaviour. The reason for this is far from clear to us. In contrast with 3D systems, metastable states do not always exist here; they only appear in a very narrow range of density ( $\rho_0 > \rho_c$ ). Therefore, for the low-density HR system, which includes the 1G as the limit  $a\rho_0 = 0$ , the trapped state is always stable.

In principle, the classification of the multiple trapped states can be carried out by calculating the second-order variation to the free energy. Unfortunately, neither we nor Moore *et al* [3] have been able to do this. The constraint introduced by the normalisation condition makes the problem especially thorny.

### Acknowledgment

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