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Bound-state transition: an analytical model

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Abstract. By using an accurate dielectric function for a homogeneous paramagnetic electron liquid we attempt a simple analytical treatment of the bound-state (metal–insulator) transition in a system consisting of a single proton immersed in the electron liquid, as a function of global density. The inability of the resulting effective Thomas–Fermi picture to account for the transition is remedied by the inclusion of the appropriate cusp condition that is also introduced in a simple analytical manner. The expected transition from a delocalized state (at high density) to a localized state (at low density) is shown to be the result of the combined action of a minimal number of very general principles such as overall charge neutrality, the compressibility sum rule and the so-called q^4 sum rule, at the simplest analytical level.

1. Introduction

The simplest model that shows the basic physics behind Mott’s metal–insulator transition [1] is a system consisting of a single fixed proton immersed in a continuous paramagnetic electron liquid at zero temperature; the transition is then represented by the formation of a bound (localized) electronic state around the proton as the density is lowered. Electronic screening is crucial in this effect, and even the simplest case of Thomas–Fermi screening has been subjected to extensive numerical work, that yields a critical density not far from the standard textbook value of $r_{s,0} \simeq 2.44$ (that is obtained from the rough analytical estimate $q_0 a_0 \sim 1$, with q_0 the Thomas–Fermi wavevector and a_0 the Bohr radius).

We present here an analytical model that approximately deals with the above problem through sequential improvements of the simple Thomas–Fermi picture. The method consists of an approximate mapping of an accurate analytical form of the dielectric function of the interacting electron liquid onto an *effective* Thomas–Fermi (T.F.) problem, and its subsequent correction with a simple interpolation procedure that respects very general long-range *and* short-range principles and that incorporates the correct low- q and high- q behaviour of static structure factors [8].

Section 2 attempts to account for the transition by focusing on the long-range aspect of screening through an effective Thomas–Fermi approach. A basic inability of this picture to account for the transition is demonstrated and is remedied in section 3, by focusing on the short-range behaviour of response functions (through the q^4 sum rule) and by interpolating analytically between long-range and short-range behaviours. This simple analytical model is shown to lead to a transition to an atomic-like state at a value of density very close to quantum Monte Carlo results.

2. Effective T.F. model

The total effective interaction that an electron feels due to the presence of the proton in the electron liquid is

$$V_{eff}(q) = -\frac{4\pi e^2}{q^2 \epsilon(q)} \quad (1)$$

where $\epsilon(q)$ is the static dielectric function of the electron liquid. The above effective interaction is density dependent and it defines an effective single-particle problem which we will attempt to solve approximately, i.e. to determine the point at which the first bound state may appear as the density is lowered, starting from the high-density metallic phase.

The dielectric function is determined by

$$\epsilon(q) = 1 - \frac{4\pi e^2}{q^2} \chi_{scr}(q) \quad (2)$$

with the response function $\chi_{scr}(q)$ given by

$$\chi_{scr}(q) = \frac{\chi_0(q)}{1 + (4\pi e^2/q^2)\chi_0(q)G(q)} \quad (3)$$

where $\chi_0(q)$ is the noninteracting static response function

$$\chi_0(q) = -\frac{3n}{2E_F} f\left(\frac{q}{2q_F}\right) \quad (4)$$

with f being the Lindhard function [12]

$$f(y) = \frac{1}{2} + \frac{1}{4y}(1 - y^2) \ln \left| \frac{y+1}{y-1} \right|. \quad (5)$$

We begin by using the local field correction $G(q)$ that was proposed by Ichimaru and Utsumi [2], namely

$$G(q) = A \left(\frac{q}{q_F}\right)^4 + B \left(\frac{q}{q_F}\right)^2 + C + \left[A \left(\frac{q}{q_F}\right)^4 + \left(B + \frac{8}{3}A\right) \left(\frac{q}{q_F}\right)^2 - C \right] \left(\frac{4q_F^2 - q^2}{4q_F q} \right) \ln \left| \frac{2q_F + q}{2q_F - q} \right| \quad (6)$$

where the parameters A , B , C are given by

$$A = 0.029$$

$$B = \frac{9}{16}\gamma_0 - \frac{3}{64}[1 - g(0)] - \frac{16}{15}A$$

and

$$C = -\frac{3}{4}\gamma_0 + \frac{9}{16}[1 - g(0)] - \frac{16}{5}A$$

and with γ_0 determined below by [7] the Padé approximants expression [3] for the energy per particle of an electron liquid, given by

$$\begin{aligned} \epsilon(r_s) = a \left\{ \ln \left(\frac{r_s}{r_s + br_s^{1/2} + c} \right) + \frac{2b}{Q} \tan^{-1} \left(\frac{Q}{2r_s^{1/2} + b} \right) \right. \\ \left. - \left(\frac{bx_0}{x_0^2 + bx_0 + c} \right) \left[\ln \left(\frac{(r_s^{1/2} - x_0)^2}{r_s + br_s^{1/2} + c} \right) + \frac{2(b + 2x_0)}{Q} \tan^{-1} \left(\frac{Q}{2r_s^{1/2} + b} \right) \right] \right\} \\ + \frac{3}{5} \left(\frac{9\pi}{4} \right)^{2/3} \frac{1}{r_s^2} - \frac{3}{2\pi} \left(\frac{9\pi}{4} \right)^{1/3} \frac{1}{r_s} \text{ Ryd} \quad (7) \end{aligned}$$

where the constants have the following values: $a = 0.062\ 1814$, $b = 3.727\ 44$, $c = 12.9352$, $Q = (4c - b^2)^{1/2}$ and $x_0 = -0.104\ 98$.

In (6) $g(0)$ is approximately given by

$$g(0) = \frac{1}{8} \left(\frac{z}{I_1(z)} \right)^2$$

where

$$z = 4 \left(\frac{4}{9\pi} \right)^{1/6} \left(\frac{r_s}{\pi} \right)^{1/2}$$

and $I_1(z)$ is the modified Bessel function of the first kind and of the first order; γ_0 is defined by

$$\lim_{q \rightarrow 0} G(q) = \gamma_0 \frac{q^2}{q_F^2} \tag{8}$$

and is determined by the compressibility sum rule

$$\lim_{q \rightarrow 0} \chi_{scr}(q) = -n^2 K \tag{9}$$

where K is the ground-state compressibility

$$K = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_{T=0}$$

of the electron gas and $\chi_{scr}(q)$ is defined by (3).

Combination of the above expressions leads to

$$\frac{K_0}{K} = 1 - \frac{4}{\pi q_F a_0} \gamma_0(r_s) \tag{10}$$

where K_0 is the noninteracting value $K_0 = 3/(2nE_F)$ and K can be determined by using equation (7) in combination with

$$K^{-1} = \frac{1}{12\pi a_0^3 r_s} \frac{\partial}{\partial r_s} \left(\frac{1}{r_s^2} \frac{\partial \epsilon}{\partial r_s} \right). \tag{11}$$

The final result for γ_0 turns out to be

$$\gamma_0(r_s) = \frac{1}{4} - \frac{\pi}{48} \left(\frac{4}{9\pi} \right)^{1/3} \frac{[r_s^{5/2} \{b_0 b_1 R - b_0 r_s^{1/2} (1 + b_1 r_s^{1/2}) S\} - 4b_0 r_s^2 (1 + b_1 r_s^{1/2}) R]}{R^2}$$

where

$$R = r_s + b_1 r_s^{3/2} + b_2 r_s^2 + b_3 r_s^{5/2}$$

and

$$S = 2 + 3b_1 r_s^{1/2} + 4b_2 r_s + 5b_3 r_s^{3/2}$$

with the constants given by $b_0 = 0.062\ 1814$, $b_1 = 9.813\ 79$, $b_2 = 2.822\ 24$ and $b_3 = 0.736\ 411$.

The dielectric function is then determined by equation (2) with $\chi_{scr}(q)$ given above by equation (3). The effective interaction (1) is therefore written approximately in closed form. We show how $V_{eff}(q)$ varies for two different values of r_s in figure 1 where it is also compared with the Thomas–Fermi (T.F.) potential

$$-\frac{4\pi e^2}{q^2 + q_0^2}$$

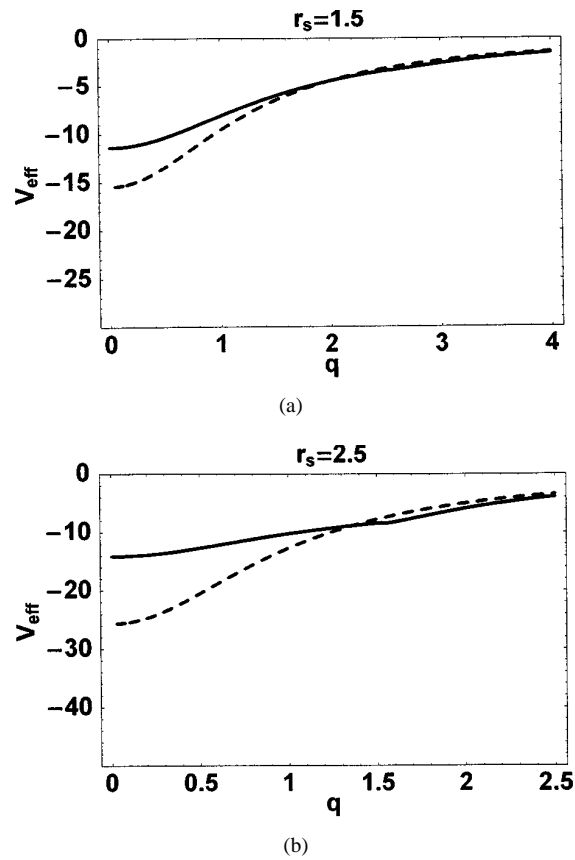


Figure 1. The effective T.F. potential (solid curve) in atomic units (corresponding to setting 1 Ryd = $a_0 = 1$), compared to the standard T.F. potential (dashed curve) at different densities, (a) for $r_s = 1.5$ and (b) for $r_s = 2.5$ where a non-T.F. deviation around $q = 2q_F$ is apparent.

at the same densities. The Thomas–Fermi wavevector is given by

$$q_0^2 = 4\pi e^2 \frac{3n}{2E_F}$$

or, equivalently,

$$q_0 a_0 = \left(\frac{4}{\pi}\right)^{1/2} \left(\frac{9\pi}{4}\right)^{1/6} \frac{1}{r_s^{1/2}}$$

with a_0 the Bohr radius. Note from figure 1(a) that at high densities the potential (1) has approximately the form of a T.F. potential with a renormalized T.F. wavevector q_0^{eff} , which is always higher than the actual q_0 at the same density (see also figure 2). This means that the metal–insulator transition in the electron gas with correlations included is expected to occur at a density lower than the simple Mott value associated with a Yukawa (T.F.) potential. In other words, screening is stronger in the presence of electron–electron correlations, and the transition to a bound state is therefore more difficult to produce; we will actually see that the simplest effective T.F. picture of this section is unable by itself to lead to this transition. It should be noted however that around $r_s \sim 1.6$ the form of V_{eff} starts deviating locally from a T.F. shape in the vicinity of $q = 2q_F$. This gives an opposite trend since the deviation,

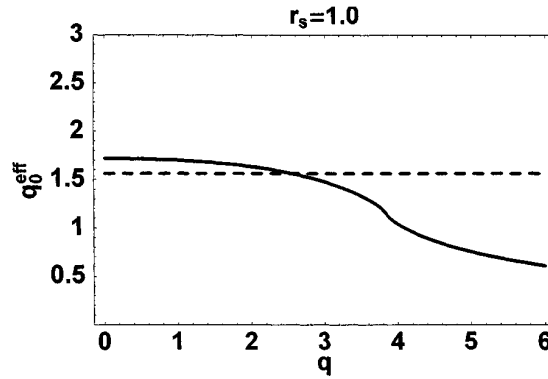


Figure 2. The effective T.F. wavevector q_0^{eff} as a function of wavevector q for $r_s = 1.0$ (always in units $a_0 = 1$), compared with the standard T.F. wavevector for the same density (dashed line).

being always negative, helps the formation of a bound state compared to the simple effective T.F. form (see for example figure 1(b)). (This effect however will turn out to be smaller than the opposite $q = 0$ effect; in the next section we will show that it is the inclusion of the $q \rightarrow \infty$ behaviour that leads to a transition.)

Let us for the moment ignore this deviation around $2q_F$ and approximate (1) with the simple T.F. form. The renormalized q_0^{eff} is a function of q and is defined with the help of (1), (2), (3) and (6) by

$$V_{eff}(q) = -\frac{4\pi e^2}{q^2 + q_0^{eff2}}. \quad (12)$$

The resulting form of $q_0^{eff}(q)$ for a particular density is shown in figure 2. It is important to have in mind that this description of the high-density metallic phase in terms of an effective T.F. potential can be acceptable only under the proviso that

$$2q_F \geq q_0^{eff}. \quad (13)$$

This is a consequence of the physical definition of screening, i.e. of the requirement that the effective screening length $1/q_0^{eff}$ must be longer than the mean distance between particles. In particular, we expect that any description in terms of a T.F. problem will break down when

$$2q_F \simeq q_0^{eff} \quad (14)$$

i.e. when the screening length is equal to the period of the Friedel oscillations [4]. An interesting result of the analysis of this section is that the density where (14) is satisfied is close to the density where the Mott transition occurs according to Monte Carlo results [5], and the effective T.F. picture approaches very close to the transition at exactly this point. (For the exact T.F. problem, equation (13) is always satisfied for $r_s \leq 6$.)

Note also that (13) is indeed progressively better satisfied as $r_s \rightarrow 0$, and as a consequence at high densities $q_0^{eff}(q)$ is insensitive to q (and hence closer to a constant as in the standard T.F. problem) for a higher range of q -values (from 0 to $2q_F$). As a first estimate then, let us use $q_0^{eff}(q=0)$ as the quantity independent of q taken to play the role of the effective T.F. wavevector, since this value is far from the region of the highest rate of decrease which is around $q \sim 2q_F$ (see the dip in figure 2). So we can approximately use $q_0^{eff}(0)$ to determine the point of the transition to a bound state in the corresponding T.F. potential, but we should have in mind that the value of $q_0^{eff}(q)$ for $q = 0$ is the highest, at least for high enough densities

(see figure 2), and our use of the $q = 0$ value is therefore an exaggeration. With this in mind we plot $q_0^{eff}(0)$ as a function of r_s in figure 3; we observe that $q_0^{eff}(0) \rightarrow q_0$ as $r_s \rightarrow 0$, as expected. Also, for high densities, q_0^{eff} decreases with r_s which is in accordance with the fact that screening becomes weaker as we lower the density. However, we observe a minimum at

$$r_{s0} \simeq 2.6 \quad (15)$$

and beyond that an increase which must be unphysical for the behaviour of screening with density for a uniform system. It is interesting to note that the minimum is indeed located close to the point where

$$2q_F \simeq q_0^{eff}(0) \quad (16)$$

holds and that the unphysical increase is indeed in the region

$$2q_F < q_0^{eff}(0) \quad (17)$$

where the effective T.F. description is not physically meaningful.

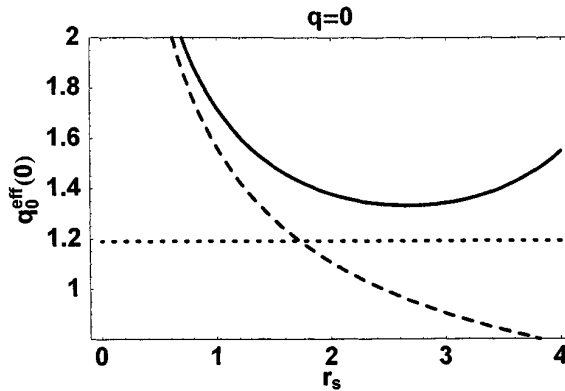


Figure 3. The effective T.F. wavevector at $q = 0$ as a function of r_s (solid curve) that shows the correct limiting behaviour at high density, being the same as that of the standard T.F. wavevector q_0 (dashed curve); the dotted horizontal line shows the value of $1/0.83991$ ($a_0 = 1$).

Therefore, constraining to within the region $r_s \leq r_{s0}$, we now try to determine a possible transition to a bound state by solving the corresponding T.F. problem. It is known from an accurate numerical analysis [6] that the first zero-energy bound state for a Yukawa potential (for $Z = 1$) appears at a screening length

$$1/q_{0c} = 0.83991 a_0. \quad (18)$$

This gives the result that the Mott transition for an exact T.F. problem (i.e. for $q_0 = 0.815q_F r_s^{1/2}$) will occur at $\bar{r}_s = 1.724$ (the point of intersection of the two dashed curves in figure 3) which would be the usual textbook value $\bar{r}_s = 2.44$ had we used the standard but rough estimate $1/q_{0c} \sim a_0$ for the transition instead of (18). For the effective T.F. problem, equation (18) would give the condition that the curve $q_0^{eff}(r_s)$ intersects with the curve $1/(0.83991 a_0)$ at the transition point. We see from figure 3 that the fact that we ignored the q -variation of $q_0^{eff}(q)$ had the consequence that the two curves do not intersect (but they approach each other at the minimum $r_s = r_{s0}$). As noted earlier, the point $r_{s0} \sim 2.6$ of the closest approach between the two curves is about the point of the transition found from a Monte Carlo analysis [5] of the problem of a single proton in an electron gas. However, the basic inability of the

effective T.F. picture to account for the transition has been clearly demonstrated, and this will be remedied in the next section.

An improvement of the above T.F. picture would certainly consist of accounting for all the non-T.F. deviations for high q , and especially the features of $\epsilon(q)$ around $2q_F$ that become more and more pronounced as the density is lowered. However, we will see next that simply imposing general constraints on the short-range behaviour of the response functions, and in particular the so-called q^4 sum rule (equivalent to the well-known cusp condition), leads to a transition from monotonic behaviour (pertaining to an extended state) to oscillatory behaviour (pertaining to a localized state). This provides evidence that the imposition of the right short-range behaviour is the important physical element that, if combined with the effective T.F. long-range behaviour of this section, leads to the expected transition. (Note that the $2q_F$ feature is a higher-order effect, and its inclusion would provide a more accurate location for the transition density but at the same time destroy the simplicity of the model presented in the next section.)

3. Interpolation procedure

Instead of addressing further the energetics of an effective one-particle problem, we now focus on a particularly simple (and approximate) description of the electronic density induced by a single fixed proton. The model reveals a particular type of change in the form of the one-particle density at some point as we lower the density starting from the infinitely dense phase. The description is based on a minimal number of very general constraints valid for Coulomb systems, such as overall charge neutrality, the compressibility sum rule and the appropriate cusp condition. We will see as a result that this combination of long-range and short-range sum rules is sufficient to give a qualitative prediction for the expected transition, that manifests itself as a change of behaviour in the induced one-particle density.

Let us then consider a proton fixed at \vec{r}_0 and denote by $\rho_e(\vec{r})$ the number density of electrons induced by the presence of the proton. We will work with the Fourier transform $\rho_e(\vec{q})$ which is dimensionless:

$$\rho_e(\vec{r}) = \int \frac{d^3q}{(2\pi)^3} e^{i\vec{q}\cdot\vec{r}} \rho_e(\vec{q}). \quad (19)$$

Let us look at the low- q behaviour of $\rho_e(\vec{q})$: the induced charge density around the proton (taken as isotropic) is

$$\rho_c(q) = \chi_{scr}(q) \frac{4\pi e}{Vq^2\epsilon(q)} \quad (20)$$

where $e > 0$. If we focus on the $q \rightarrow 0$ limit we may first take the response and dielectric functions of Thomas–Fermi theory, namely

$$\chi_{scr}(q) = -\frac{Vq_0^2}{4\pi} \quad (21)$$

and

$$\epsilon(q) = 1 + \frac{q_0^2}{q^2} \quad (22)$$

where the T.F. wavevector is given by

$$q_0^2 = \frac{4}{\pi} \left(\frac{9\pi}{4} \right)^{1/3} \frac{1}{r_s a_0^2}. \quad (23)$$

Hence

$$\lim_{q \rightarrow 0} \rho_c(q) = \frac{-eq_0^2}{q^2 + q_0^2} \quad (24)$$

so the induced number density of electrons is

$$\lim_{q \rightarrow 0} \rho_e(q) = \frac{q_0^2}{q^2 + q_0^2} = \frac{1}{1 + q^2/q_0^2}. \tag{25}$$

Indeed we can check that the above form explicitly satisfies charge neutrality, namely

$$\rho_e(q = 0) = \int d^3r \rho_e(\vec{r}) = 1 \tag{26}$$

as expected, since the total induced electronic charge around \vec{r}_0 must be equal to the charge of a single proton. Also by Fourier transformation we obtain

$$\rho_e(r) = \frac{q_0^2}{4\pi} \frac{e^{-q_0 r}}{r} \tag{27}$$

i.e. the standard Thomas–Fermi density.

Expression (25) is of course a special case of the more general form

$$\rho_e(q) = \frac{(q_0^2/q^2) f(q/2q_F)}{1 + (q_0^2/q^2) f(q/2q_F)(1 - G(q))} \tag{28}$$

(which is a better approximation for all q for linear response, and is of course equivalent to equation (3)), since the local field correction satisfies (8); that is,

$$\lim_{q \rightarrow 0} G(q) = \lim_{q \rightarrow 0} \gamma_0(r_s) \frac{q^2}{q_F^2} = 0 \tag{29}$$

and the Lindhard function (5) also satisfies

$$\lim_{q \rightarrow 0} f(q/2q_F) = 1. \tag{30}$$

By including the $q \rightarrow 0$ limit of the local field $G(q)$ in (25) we can therefore make an improvement by imposing the compressibility sum rule (9) which finally gives a rewriting of equation (10) in the form

$$\frac{K_0}{K} = 1 - \gamma_0(r_s) \frac{q_0^2}{q_F^2}. \tag{31}$$

So the low- q behaviour of $\rho_e(q)$ is

$$\rho_e(q) = \frac{q_0^2}{q^2 + q_0^2(1 - \gamma_0 q^2/q_F^2)} = \frac{q_0^2}{q_0^2 + q^2(1 - \gamma_0 q_0^2/q_F^2)} = \frac{1}{1 + (q^2/q_0^2) K_0/K}. \tag{32}$$

This is an especially compact form that generalizes the Thomas–Fermi result (25), and that actually incorporates all the physics of the previous section.

Equation (32) has now the correct low- q behaviour (for a charged system) but *not* the right high- q behaviour. In this limit $\rho_e(q)$ should be proportional to $1/q^4$ because of the e–p cusp condition [9–11], namely

$$\left. \frac{\partial \rho_{ep}(r)}{\partial r} \right|_{r=0} = -\frac{2}{a_0} \rho_{ep}(r = 0) \tag{33}$$

which in q -space reads (with N/V the global density of the electron liquid)

$$\frac{N}{V} + \int \frac{d^3q}{(2\pi)^3} \rho_e(q) = \frac{a_0}{16\pi} \lim_{q \rightarrow \infty} q^4 \rho_e(q) \tag{34}$$

showing that the high- q behaviour of $\rho_e(q)$ has to be of the form

$$\lim_{q \rightarrow \infty} \rho_e(q) = \frac{\lambda^4}{q^4} \tag{35}$$

with λ a wavevector to be determined (as a function of density) by (34).

Combining (35) with (32), we are finally led to the interpolation

$$\rho_e(q) = \left(1 + \frac{q^2}{q_0^2} \frac{K_0}{K} + \frac{q^4}{\lambda^4}\right)^{-1} \quad (36)$$

for *all* q . This is constrained to have the right low- and high- q limits and we expect it to give correct qualitative trends for intermediate values of q as well. The q^4 -correction approximates nonlinear effects (for electrons very close to the proton) that are not included in any linear response (or, more generally, in any perturbational) argument [11].

To determine $\lambda(r_s)$ we now impose the cusp condition (34). Using the final form (36) for $\rho_e(q)$, the integration can be carried out analytically, the result being

$$\int \frac{d^3q}{(2\pi)^3} \rho_e(q) = \frac{1}{4\pi} \frac{\lambda^3 q_0^2 \sqrt{K/K_0}}{\sqrt{\lambda^2 + 2q_0^2 K/K_0}}. \quad (37)$$

The cusp theorem leads therefore to

$$(\lambda a_0)^4 - 2(\lambda a_0)^3 \left(2 / \left[1 + \frac{\lambda^2}{2q_0^2} \frac{K_0}{K}\right]\right)^{1/2} - \frac{12}{r_s^3} = 0 \quad (38)$$

which is an equation that $\lambda(r_s)$ is required to satisfy.

We have solved (38) numerically for λ for various values of r_s and we plot the results in figure 4. The form of $\rho_e(r)$ for our interpolation scheme is given by Fourier transformation of (36) and can actually be calculated analytically, the final result being

$$\rho_e(r) = \frac{\lambda^2}{4\pi} \frac{1}{\sqrt{[\lambda^4/(4q_0^4)]K_0^2/K^2 - 1}} \frac{\exp[-\lambda r \sqrt{\{1 + [\lambda^2/(2q_0^2)]K_0/K\}/2}]}{r} \times \sinh\left[\lambda r \sqrt{\frac{[\lambda^2/(2q_0^2)]K_0/K - 1}{2}}\right]. \quad (39)$$

(As a consistency check we can use this form and the real-space form of the cusp theorem (33) to derive an equation for $\lambda(r_s)$; the result is again (38)).

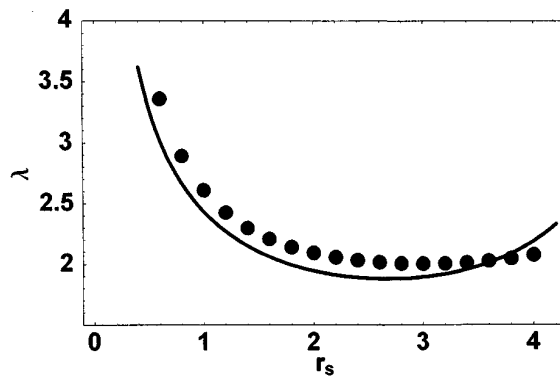


Figure 4. Values of the cusp parameter λ (points) as a function of the density parameter r_s , determined from the cusp theorem (in units $a_0 = 1$). The solid curve is the function $q_0\sqrt{2K/K_0}$; when this is smaller than λ , the behaviour of $\rho_e(r)$ is monotonic (delocalized state); otherwise it is oscillatory (localized state).

It is interesting to note from (39) that, depending on the sign of the second quantity in the square root, $\rho_e(r)$ displays two quite distinct types of behaviour depending on a comparison between the curves

$$\lambda(r_s) \quad \text{and} \quad \sqrt{2}q_0\sqrt{\frac{K}{K_0}}(r_s).$$

We observe a crossing from monotonic to oscillatory behaviour at some value $r_{s,0} \sim 3.5$ (see figure 4), i.e. for $r_s > r_{s,0}$ expression (39) becomes oscillatory; i.e.,

$$\rho_e(r) = \frac{\lambda^2}{4\pi} \frac{1}{\sqrt{1 - [\lambda^4/(4q_0^4)]K_0^2/K^2}} \frac{\exp[-\lambda r \sqrt{\{1 + [\lambda^2/(2q_0^2)]K_0/K\}/2}]}{r} \times \sin \left[\lambda r \sqrt{\frac{1 - [\lambda^2/(2q_0^2)]K_0/K}{2}} \right] \quad (40)$$

where λ is still given by (38).

The imposition, therefore, of the right long- and short-range behaviours seems to lead by itself to a qualitative change of behaviour from one typical of an extended state to one typical of a localized state. It is also interesting that at about the same point we have a minimum in λ (around the hydrogenic value $\lambda = 2/a_0$ as can be shown [8] from the structure factor $S_{ep}(q)$ for a many-body state of hydrogen atoms in the low-density limit and with the definition $\lambda^4 = \lim_{q \rightarrow \infty} q^4 S_{ep}(q)$). This gives further evidence that the qualitative change of behaviour observed can be related to the formation of a bound state between an electron and the fixed proton.

We should note that, in spite of the approximate and very simple form of (36), this value of $r_{s,0}$ agrees well with the value of 3.5 found for the transition from delocalized to localized behaviour as determined by hypernetted-chain variational calculations [13], which explicitly enforce the cusp condition.

Questions concerning the thermodynamics of this transition obviously fall outside the above simple zero-temperature response argument. However, it is interesting to note one final point concerning the energetics involved: as a further check we can use (36) to determine the electron-proton interaction energy $\Delta(r_s)$, which is given in the linear response regime by [7]

$$\Delta = - \int_0^1 d\tilde{\lambda} \frac{1}{V} \sum_{q \neq 0} \left(\frac{4\pi e^2}{q^2} \right) \langle \rho_e(q) \rangle_{\tilde{\lambda}} S_{pp}(q) \quad (41)$$

where now $\tilde{\lambda}$ denotes the electron-proton coupling constant, to distinguish it from the cusp parameter λ . (In our case of a single proton, $S_{pp}(q) = 1$.) Since for linear response the quantity $\langle \rho_e(q) \rangle_{\tilde{\lambda}}$ has an explicit linear dependence on $\tilde{\lambda}$, an integration of (41) can be carried out exactly, now using an interpolation of the form

$$\langle \rho_e(q) \rangle_{\tilde{\lambda}} = \tilde{\lambda} / \left(1 + \frac{q^2 K_0}{q_0^2 K} + \frac{q^4}{\lambda^4} \right)$$

and it finally gives the result

$$\Delta = - \frac{e^2}{\pi} \int_0^\infty \frac{dq}{1 + (q^2/q_0^2)K_0/K + q^4/\lambda^4} = \frac{-\lambda a_0 q_0 \sqrt{K/K_0}}{\sqrt{\lambda^2 + 2q_0^2 K/K_0}} \text{Ryd.} \quad (42)$$

This is to be contrasted with the result

$$\Delta = -q_0 a_0 \sqrt{\frac{K}{K_0}} \text{Ryd}$$

that would have been obtained for the effective T.F. model of section 2 (corresponding to $\lambda \rightarrow \infty$), and is shown in figure 5 to be of order -1 Ryd, as expected for a hydrogen atom. It is therefore interesting to note that the mere inclusion of the cusp condition has had a rather large effect on the energetics of the problem, and it has actually corrected quite substantially the value of the interaction energy and brought it to the value expected for a hydrogen-like state.

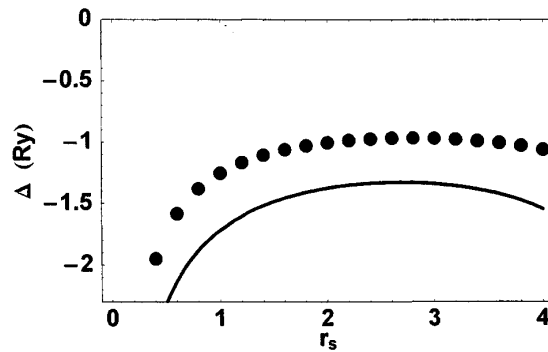


Figure 5. Simple analytical models for the electron–proton interaction energy $\Delta(r_s)$ in the case of a single proton ($S_{pp}(q) = 1$): for an effective Thomas–Fermi model that includes the compressibility sum rule (solid curve) of section 2, and finally including the cusp condition (points).

4. Conclusions

We discussed in this paper a simple analytical model of the bound-state transition. Although we began with an effective T.F. model in linear response theory, we finally corrected with the additional imposition of the known nonlinear short-range behaviour with the use of an interpolation form for the induced electron density. The importance of an accurate treatment of the short-range behaviour to the very existence of the transition should not be a surprise, as the correct short-range behaviour is obviously more crucial for a localized state than it is for an extended state. Because of the simplicity of the model the precise location of $r_{s,0}$ cannot be taken as quantitatively correct. To go beyond our approximations, an inclusion of the $2q_F$ feature of the dielectric function would be the first correction to consider. However, this or other corrections would destroy the analytical simplicity of the model, while apparently not affecting the resulting critical density much. The particular merit of the argument given above lies in the manner in which it is capable of incorporating some quite general properties of charged quantum systems. Their combination in a simple analytical manner leads straightforwardly to a transition to a localized state with declining density, the location of which is expected *a priori* to be given only qualitatively, but in fact is quite close to the actual value.

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