Pairing transition of a one-dimensional classical plasma

1981 J. Phys. A: Math. Gen. 14 3277

(http://iopscience.iop.org/0305-4470/14/12/024)

J. Phys. A: Math. Gen. **14** (1981) 3277–3300. Printed in Great Britain

Pairing transition of a one-dimensional classical plasma

H Schulz

Institut für Theoretische Physik, Universität Hannover, Germany

Received 16 April 1981

Abstract. A classical one-dimensional gas of charges $e_i = \pm 1$ with interaction potential $-\Sigma\, e_i e_j \ln(1+|x_i - x_j|)$ is shown to undergo a transition from a metallic (or plasma) state at high temperature to an insulating (or dielectric) state at low temperature due to the formation of pairs of oppositely charged particles. This transition is the 1D analogue of the pairing transition of a 2D Coulomb plasma. The early method (Baxter 1964) of mapping real gas statistics in 1D to ordinary quantum mechanics is applied, and is demonstrated to work fairly well even when the latter involves an infinite number of degrees of freedom. By variational treatments of this quantum mechanics a first-order phase transition is obtained. At small fugacity z the transition line starts perpendicular to the inverse temperature axis at $\beta = 2$ and turns to the right for large z. An exact relation is derived between the dielectric constant and the effective mass of a Bloch band problem. On the insulator side the dielectric constant is argued to be identical to one. The equivalence of the model gas to a sine-Gordon type theory is also established and soliton solutions of the latter are given. By function space analysis the gas is again found to be metallic at sufficiently large fugacity but arbitrary temperature.

1. Introduction

Two-component classical gases can behave metallically at high temperature and be insulating at low temperature due to the formation of pairs of oppositely 'charged' particles. Basic to this possibility is a logarithmic interaction between the particles at large distance but not the dimension of the space they are moving in. Therefore, the classical two-dimensional Coulomb gas (2DCG) is not the only model which exhibits a pairing transition.

The novel interest in the 2DCG (Hauge and Hemmer 1971) arose with realising its equivalence to the quantum sine-Gordon theory as well as to models of interacting fermions in 1D (Solyom (1979) and references therein), while the interest in the pairing transition of the 2DCG was initiated by Kosterlitz and Thouless (1973), who defined the transition as the sudden change of the dielectric constant from infinity (metal) to finite values (insulator). Then details of the dielectric function for small wavevectors were worked out by Everts and Koch (1977) and Minnhagen *et al* (1978). So far little is known, however, about the shape of the transition line in the fugacity (z) over inverse temperature (β) diagram (Kosterlitz 1974, Ohta and Kawasaki 1978, Saito and Müller–Krumbhaar 1981), or even about the physics near this line. It is then tempting to study the metal–insulator transition in *one* dimension where more powerful techniques are available. To present the corresponding model, henceforth called LG (for 'logarithmic gas'), is one purpose (among two others) of this paper.

0305-4470/81/123277+24$01.50

There is yet another philosophy suggesting the gas model considered here. It starts from the one-dimensional Coulomb plasma (1DCG). In contrast to the 2DCG, this Coulomb gas provides us with an ideal situation in statistical physics, since all quantities of interest can be calculated exactly (Lenard 1961, Edwards and Lenard 1962), including the dielectric constant (Apel *et al* (1979), henceforth referred to as AES). The 1DCG insulates for all values of z and β, but is on the verge of becoming metallic for high density. By weakening the interaction from $|x|$ to $\ln(1+|x|)$ the transition is shifted inside the $z\beta$ plane, and one might ask then if (or how much of) the analysis of AES can be maintained by merely rewriting it to apply to the LG. To answer this question is the second purpose of this paper. The essentials of the AES theory, such as a relation of the dielectric constant to the effective mass of a Bloch band and the function space analysis, are rediscovered for the LG (see §§ 5 and 6, respectively).

The third purpose of this paper is to present a non-trivial example for an early method of Baxter (1964). In one dimension the statistics of a classical real gas (including correlation functions) can be traced back to a one-particle problem of ordinary quantum mechanics. The power of this method is its applicability to an arbitrary interaction potential. Apart from special cases, however, the related quantum problem involves an infinite number of variables. This might be the reason why Baxter's mapping, apparently, has been applied only to models which involve one or two variables. The interaction in these models is a simple power (Kunz 1974, Choquard 1975, Schotte and Truong 1980) or an exponential (Behncke and Schotte 1979) or even has a hard core (Baxter 1965). In contrast, the LG is a 'normal' model. The crucial trick for dealing properly with the infinity of variables is a convenient embedding of the logarithm (see equation (3) of § 2). In § 3 the quantum mechanics of the LG is established. It is also shown there that the many variables can always be associated with harmonic oscillators. Furthermore, the dielectric function is shown to be related to only the ground state wavefunction of the quantum problem.

No exact solution for the LG has been found (although there may be still some chance of this). The main information is obtained from several approximate treatments given in § 4. They strongly suggest a first-order transition of the LG (see also figure 2) occurring at the line shown in figure 1. Obviously, the shape of this line at small fugacity z is in contrast to the 2DCG case, where it forms an oblique angle. This reflects a difference of the two models. In fact, by strictly following the renormalisation procedure of Kosterlitz (1974, Appendix C) vertical trajectories are obtained for the LG as shown in figure 1. Nevertheless, LG and 1DCG have much in common. So, using the

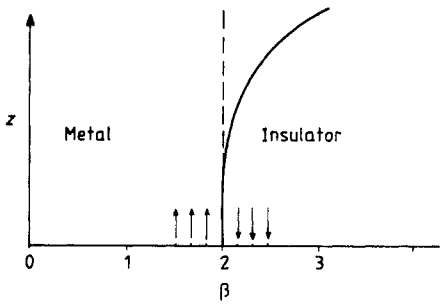

Figure 1. Transition line in a diagram of schematic fugacity against inverse temperature for the LG. The tunnelling catastrophe occurs at the broken line. The arrows refer to flow lines from Kosterlitz renormalisation.

method of Zittartz (1976), the analytical structure of the grand canonical potential ϕ can be worked out as $\phi = az^{\nu} + bz^2 + \ldots (z \to 0)$ where $\nu = 2/(2-\beta)$ and a, b are functions of the temperature. Here the only difference to the 2DCG is a shift (due to dimension) of the critical temperature from $\beta = 4$ to $\beta = 2$. One could also suspect the LG in essence to be the Kondo problem, since the 1D gas version of the latter (Anderson and Yuval 1969, Schotte 1970) differs from the LG only by the requirement of alternating order of the charges. However, the Hamiltonians associated with both gases look rather different (see the end of § 3). Thus, more than similarities should not be expected.

2. The model

Consider a classical system of two kinds of particles in 1D in an interval of length L in contact with a thermal reservoir at temperature β^{-1} and with particle reservoirs at equal chemical potentials. The particles have equal masses and equal but opposite (unit) charges $e_i = \pm 1$ ($i = 1, 2, \ldots, N = N_+ + N_-$) and interact in pairs by $e_i e_j v(x_i - x_j)$ with the soft-core potential

$$v(x) = -\ln(1 + |x|). \tag{1}$$

The grand partition function of this system is given by

$$Z(L, \beta, z) = \sum_{N_+, N_-}^{\infty} \frac{z^N}{N_+! N_-!} \int_0^L \mathrm{d}^N x \, \exp[-\beta(V + V_R)] \tag{2}$$

where $V = \sum_{i<j}^{N} e_i e_j v(x_i - x_j)$, z is the fugacity and V_R is the interaction of the system with the particle reservoirs, which have to be included in cases of long-range forces (Edwards and Lenard 1962). The variables L, β, z, x are dimensionless as a result of choosing proper units (such as some 'real' soft core as the length scale). This model (LG) can be viewed as a system of (soft) charged rods on the xy plane, which are all parallel to the y direction, but only move in the x direction and penetrate each other.

To deal with the term V_R in (2) (but also for later convenience) one may construct a sequence of models characterised by an interaction $v_\varepsilon(x)$, which converges to $v(x)$, (1), for $\varepsilon \to 0$, but saturates at large x for any finite ε. The most convenient choice is

$$v_\varepsilon(x) = -\ln[1 + (1 - \mathrm{e}^{-\varepsilon|x|})/\varepsilon] = -v_0 + w(x) \tag{3}$$

with $v_0 = \ln(1 + 1/\varepsilon) \to +\infty$ ($\varepsilon \to +0$). The function $w(x)$, given by

$$w(x) = -\ln(1 - \lambda^2 \, \mathrm{e}^{-\varepsilon|x|}), \tag{4}$$

is that part of (3) which can be Fourier transformed:

$$w(q) = \int \mathrm{d}x \, \mathrm{e}^{\mathrm{i}qx} w(x) = \frac{2}{\varepsilon} \sum_k \frac{\lambda^{2k}}{k^2 + q^2/\varepsilon^2}. \tag{5}$$

The notation $\lambda^2 = 1/(1+\varepsilon)$ is often used in the following, and, if not specified, sums or products over k run from 1 to ∞. For later use note that

$$w_0(q) = \lim_{\varepsilon \to 0} w(q) = \frac{2}{q} \int_0^{\infty} \mathrm{d}t \frac{\mathrm{e}^{-qt}}{1 + t^2} = \frac{\pi}{q}[1 + \mathrm{O}(q \ln q)] \tag{6}$$

and

$$w_0(q) = (2/q^2)[1 + \mathrm{O}(1/q)]. \tag{7}$$

Only the long-range part $-v_0$ of (3) needs to be included in V_R if, in the following, the thermodynamic limit $L \to \infty$ is performed first and $\varepsilon \to 0$ afterwards. Considering system plus reservoir as electrically neutral, we have

$$V_R = v_0(N_+ - N_-)^2. \tag{8}$$

Obviously, in the limit $\varepsilon \to 0$ the exponential $\exp(-\beta V_R)$ in (2) enforces neutrality of the system itself. As the derivation shows, strict neutrality results for *any* confinement interaction, since it is possible in general to embed the latter by functions of the form (3). The known strict neutrality of the 1DCG (Edwards and Lenard 1962) serves us with one more example. Furthermore, it is permitted to include only part of V_R in (2) without changing the physics of the model system at hand. Including half of V_R, using (3) and $2\sum_{i<j}^{N} e_i e_j = (N_+ - N_-)^2 - N$, the sequence Z_ε converging to (2) can be written as

$$Z_\varepsilon = \sum_{N_+,N_-}^{\infty} \frac{z_0^N}{N_+!N_-!} \int_0^L \mathrm{d}^N x \, \mathrm{e}^{-\beta \bar{V}} \tag{9}$$

with $z_0 = z \exp(-\frac{1}{2}\beta v_0)$ and $\bar{V} = \sum_{i<j}^{N} e_i e_j w(x_i - x_j)$, which is the convenient starting point for all further analysis of the LG.

The interaction (1) is not the Coulomb interaction of 1D electrodynamics. It is necessary, therefore, to give the terms 'metal' or 'insulator' a precise meaning. Let a weak external potential V_{ex} induce the changes $\pm\chi_\pm V_{ex}$ in the (Fourier transformed) particle densities. Then the induced potential is given by

$$V_{in} = w(\chi_+ + \chi_-)V_{ex} = -bV_{ex}. \tag{10}$$

If, in the long-wavelength limit $q \to 0$, the system is able fully to compensate the external potential, i.e. if $b_{q=0} = 1$, the system is called a metal. If not, i.e. if $0 \leq b_0 < 1$, it is called an insulator. Equivalently, one may consider the 'dielectric function' $\epsilon_q = 1/(1 - b_q)$ to decide whether the system is metallic ($\epsilon_0 = \infty$) or insulating ($1 \leq \epsilon_0 < \infty$). It should be noted that there are also other possibilities of defining the transition, which are not considered here. For example, one could associate an additional 'electrodynamic' charge with the particles, interpret (1) as the net interaction between them and then compare the induced 'electrodynamic' potential with V_{ex}.

Linear response calculation relates the functions χ_α, $\alpha = \pm 1$, in (10) to the density correlation functions,

$$\chi_\alpha = -\beta(n + f_{\alpha\alpha}(q) - f_{\alpha\,-\alpha}(q)), \tag{11}$$

where $f_{\alpha\alpha'}(q)$ is the Fourier transform of

$$f_{\alpha\alpha'}(x - x') = Z_\varepsilon^{-1} \sum_{N_+,N_-}^{\infty} \frac{z_0^N}{N_+!N_-!} N_{\alpha'}(N_\alpha - \delta_{\alpha\alpha'}) \int_0^L \mathrm{d}^{N-2} x \, \mathrm{e}^{-\beta \bar{V}}, \tag{12}$$

and $n = \langle N_+ \rangle / L = \langle N_- \rangle / L$ is the particle density of one species. Now (10) reads

$$b_q = 1 - 1/\epsilon_q = w(q) 2\beta(n + f_q) \tag{13}$$

where $f = \frac{1}{2}(f_{++} + f_{--} - f_{+-} - f_{-+})$. Note that the fluctuation term

$$n_f = n + f_{q=0} = \langle (N_+ - N_-)^2 \rangle / L \tag{14}$$

is non-zero for the interactions $w(x)$, (4). It could be omitted due to the strict neutrality arrived at for $\varepsilon \to 0$. Nevertheless, the term n_f is included in the following to control the consistency of approximations and to maintain the correct physics even for $\varepsilon \neq 0$, i.e. for a class of models other than the LG.

3. Mapping to quantum mechanics

The beauty of Baxter's work (1964) lies in the simplicity and generality of the idea. Its challenge is to exploit the possibility of mapping to treat non-trivial models, which involve an infinite number of degrees of freedom in the related quantum problem. These degrees of freedom, as is now shown, can always be dealt with as harmonic oscillators coupled via a cosine of the sum of variables.

For a two-component 1D real gas the Baxter transformation can be roughly summarised as follows.

(1) Generalise the partition function to the functional $\phi(L;\, G(x))$ obtained from $Z_\varepsilon(L)$, (8), by adding to $\bar{V}$ the potential $\Sigma_{i=1}^{N} e_i G(L-x_i)$. Note that $\phi(L;\, 0) = Z_\varepsilon(L)$ and $\phi(0;\, G(x)) = 1$.

(2) Restrict the functions $G(x)$, $0<x$, to be in the subspace

$$G(x) = c_0 w(x) + c_1 w'(x) + c_2 w''(x) + \dots . \tag{15}$$

Derive for ϕ the 'time-dependent Schrödinger equation' $\partial_L \phi = -\mathcal{H}\phi$, where $\mathcal{H}$ acts on the coefficients c_k of (15) only. The formal solution is $\phi = \mathrm{e}^{-L\mathcal{H}} 1$, or, by a proper similarity transformation in c_k space,

$$\phi = \mathrm{e}^{-A}\, \mathrm{e}^{-LH}\, \mathrm{e}^{A} 1, \qquad H = \mathrm{e}^{A} \mathcal{H}\, \mathrm{e}^{-A}. \tag{16}$$

(3) For the correlation functions $f_{\alpha\alpha'}$, (12), proceed similarly but keep the positions x, x' $(0<x<x')$ fixed when varying L down to zero. The resulting functionals $\varphi_{\alpha\alpha'}$ corresponding to $f_{\alpha\alpha'}$ may be written as

$$\varphi_{\alpha\alpha'} = \phi^{-1}\, \mathrm{e}^{-A} \exp[-(L-x')H] K_{\alpha'} \exp[-(x'-x)H] K_\alpha\, \mathrm{e}^{-xH}\, \mathrm{e}^{A} 1,$$

$$K_\alpha = \mathrm{e}^{A} \mathcal{K}_\alpha\, \mathrm{e}^{-A}. \tag{17}$$

(4) Expand the 'wavefunction' $\mathrm{e}^{A}1$ in eigenfunctions $|n\rangle$ of H, $H|n\rangle = E_n|n\rangle$. Return to the original quantities Z_ε and $f_{\alpha\alpha'}$ by setting all $c_k = 0$ and perform the thermodynamic limit.

The results are

$$Z_\varepsilon = \exp(-LE_0) \tag{18}$$

and

$$f_{\alpha\alpha'} = \sum_n \exp(-\alpha_n |x|) \langle 0|K_{\alpha'}|n\rangle \langle n|K_\alpha|0\rangle, \tag{19}$$

where E_0 is the ground state energy of H and $\alpha_n = E_n - E_0$.

In steps (2) and (3) the operators $\mathcal{H}$ and $\mathcal{K}_\alpha$ are also obtained:

$$\mathcal{H} = -\mathcal{K}_+ - \mathcal{K}_- - D, \qquad \mathcal{K}_\pm = z_0\, \mathrm{e}^{\mp \beta G(0)}\, \mathrm{e}^{\pm \partial}, \tag{20}$$

where D and ∂ are operators acting in the c space such that

$$DG(x) = G'(x), \tag{21}$$

$$\partial G(x) = w(x). \tag{22}$$

No explicit use has been made so far of the special representation (15). In fact, there is a much more convenient representation that is obtained from (15) by first expanding the interaction (4) in powers of $\lambda^2\, \mathrm{e}^{-\varepsilon x}$ and then collecting the terms with equal exponential:

$$G(x) = -\mathrm{i}\beta^{-1} \sum_k y_k\, \mathrm{e}^{-k\varepsilon x}. \tag{23}$$

Then, from (21)

$$D = -\sum_k \varepsilon k y_k \partial_{y_k}, \tag{24}$$

from (22)

$$\partial = \mathrm{i} \sum_k \sigma_k \partial_{y_k} \tag{25}$$

with

$$\sigma_k = \beta \lambda^{2k}/k \tag{26}$$

and from (20)

$$\mathscr{K}_\pm = z \exp\Big(\pm \mathrm{i} \sum_k (y_k + \sigma_k \partial_{y_k})\Big), \tag{27}$$

where $\mathrm{e}^A \mathrm{e}^B = \mathrm{e}^{A+B} \mathrm{e}^{[A,B]/2}$ has been used as well as $\Sigma_k \sigma_k = \beta v_0$. Specifying the similarity transformation mentioned above by

$$\mathrm{e}^A = \prod_k \exp[-(1/4\sigma_k) y_k^2] \exp(-\tfrac{1}{2}\sigma_k \partial_{y_k}^2), \tag{28}$$

the final result of mapping is constituted:

$$K_\pm = z \exp\Big(\pm \mathrm{i} \sum_k y_k\Big), \tag{29}$$

$$H = \varepsilon \sum_k \left(-k\sigma_k \partial_{y_k}^2 + \frac{k}{4\sigma_k} y_k^2 - \frac{k}{2}\right) - 2z \cos\Big(\sum_k y_k\Big), \tag{30}$$

together with the equations (18) and (19).

It should be emphasised now that the Hamiltonian (30) depends on the special interaction (1) (or (4)) of the LG only through the coefficients σ_k, (26). In fact, the above way of mapping can be followed for a rather general class of interactions $v(x)$, the only requirement being that $w(x) = v(1/\varepsilon - \mathrm{e}^{-\varepsilon x}/\varepsilon) - v(1/\varepsilon)$ (cf (3) and (4)) can be expanded in powers of $\mathrm{e}^{-\varepsilon x}$ to obtain through (22) and (25) the corresponding coefficients. These coefficients should have normal values as $\varepsilon \to 0$ (do not use exponentials for $v(x)$). To give examples, for (a) $v(x) = -x/(1+x)$, (b) $v(x) = (1+x)^{-1/2} - 1$, (c) $v(x) = 1 - (1+x)^{1/2}$, (d) $v(x) = -x$ $(0 < x)$, the coefficients are (a) $\sigma_k = \beta\varepsilon\lambda^{2k+2}$, (b) $\sigma_k = \beta\varepsilon^{1/2}\lambda^{2k+1}(2k-1)!!/(2k)!!$, (c) $\sigma_k = \beta\varepsilon^{-1/2}\lambda^{2k-1}(2k-3)!!/(2k)!!$ and (d) $\sigma_k = \beta\varepsilon^{-1}\lambda^{2k-2}\delta_{k,1}$, respectively. Changing the potential $v(x)$ smoothly through these four cases, the decrease of σ_k with k becomes more and more pronounced. For the models (a) and (b) there is certainly no confinement and no pairing, while for the 1DCG (d) the insulating behaviour is proven, and model (c) is most probably also an insulator. Thus again: a borderline case must exist. Note that the LG is placed between cases (b) and (c) with regard to both $v(x)$ and σ_k.

To study the dielectric function (13) of the LG only the ground state properties of H really need to be worked out. This has been shown by AES for the 1DCG and can be reformulated for the problem at hand. For the present, the function f_q in (13) still involves the excited states $\psi_n = \langle y_1, y_2, \ldots | n \rangle$ with energies E_n,

$$f_q = -\sum_n \mathscr{F}_n^2 \frac{\alpha_n}{(\alpha_n^2 + q^2)}, \qquad \mathscr{F}_n = 2z \int \psi_n \psi_0 \sin\Big(\sum_k y_k\Big), \tag{31}$$

where (19) has been Fourier transformed, (29) is used, the ψ_n are chosen real and the shorthand notation $\int$ is introduced for the integration over the whole y_k-space. Consider now the inhomogeneous auxiliary problem

$$(H - E_0 + iq)\chi = \psi_0 2z \sin\Big(\sum_k y_k\Big), \tag{32}$$

solve it formally for χ by expansion in the ψ_n and form

$$g_q = 2z \int \psi_0 \chi \sin\Big(\sum_k y_k\Big) \tag{33}$$

to obtain $g_q = \Sigma_n \mathscr{F}_n^2/(\alpha_n + iq)$, i.e.

$$f_q = -\mathrm{Re}\, g_q. \tag{34}$$

By (32)–(34) and (13) the correlation function b_q is traced back to the ground state wavefunction ψ_0. However, the additional problem (32) to be solved is the price for this simplification. To complete (13), the particle density n can be obtained thermodynamically from (18) as

$$n = -\tfrac{1}{2} z \partial_z E_0 \tag{35}$$

and rewritten as

$$n = z \int \psi_0^2 \cos\Big(\sum_k y_k\Big) \tag{36}$$

by differentiating $H\psi_0 = E_0\psi_0$ with respect to z and integrating.

Two different pictures can be drawn about the physics described by the Hamiltonian (30). To start with, H can be viewed classically as an infinite number of masses on springs of increasing spring constant, the sum of elongations of which is coupled (e.g. by pistons) to the angle of a simple pendulum. Clearly this 'machine' has a large but finite number of equilibrium positions, each specified by a set of variables $y_k^{(n)}$, where $n = 0, \pm 1, \pm 2, \ldots, \pm n_0$ refers to the nth potential minimum and n_0 is of order $z\beta/\varepsilon$ in magnitude. From (30) these minimum positions are easily obtained as

$$y_k^{(n)} = (S_n/I)\lambda^{2k}/k^2, \tag{37}$$

where $I = \Sigma_k \lambda^{2k}/k^2$. In (37) the factors S_n are the solutions of

$$\sin S = -S\varepsilon/4z\beta I \tag{38}$$

with $\cos S > 0$. Note that S_n approaches $2\pi n$ for $|n| \ll n_0$, the absolute minimum corresponds to $n = 0$ and the energy separation of adjacent minima is of order $n\varepsilon/\beta$ in magnitude. Everything concerning the LG is in the quantum mechanics of the above machine. For small β (large masses, stiff springs) the ground state wavefunction might be governed by the lowest potential minimum, while tunnelling should dominate at large β (see also § 4.3).

In a second picture only *one* particle is associated with H. After slight scaling

$$y_k = (k\sigma_k)^{1/2} x_k \tag{39}$$

of the variables, the Hamiltonian

$$H = \varepsilon \sum_k (-\partial_{x_k}^2 + \tfrac{1}{4}k^2 x_k^2 - \tfrac{1}{2}k) - 2z \cos\Big(\beta^{1/2} \sum_k \lambda^k x_k\Big) \tag{40}$$

describes a particle in an infinite-dimensional space in an anisotropic oscillator potential, to which a potential of 'corrugated iron' shape is superposed in one special direction. But the equilibrium positions

$$x_k^{(n)} = (S_n/I\beta^{1/2})\lambda^k/k^2 \tag{41}$$

mark another direction (see also § 5). The period of the corrugated iron is governed by β.

Furthermore, H may also be considered as the discrete version of a certain quantum field theory in one space and one time dimension. A familiar formulation of this field theory (for one real field over a finite interval) could be given, but seems to be of no use for practical calculations. Even Bose operators, which would be useful in proving $\langle 0|\exp(-LH)|0\rangle = Z_\varepsilon$ by expansion in powers of z, need not be introduced, since the method of guessing H and verifying it afterwards (Behncke and Schotte 1979) is overcome here by Baxter.

For comparison, it is perhaps worth treating the 1D gas version of the Kondo problem (see the end of the Introduction) by exactly the same procedure as the LG. The result is

$$H_{\text{Kondo}} = H_0 - z\left[\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \exp\left(\mathrm{i}\sum_k y_k\right) + \text{HC}\right] \tag{42}$$

where H_0 equals H at $z = 0$ (multiplied by the unit matrix). The difference between (42) and (30) is obvious.

4. Variational calculations

This section is devoted to various approximations of the ground state of H, (40). Three of them are introduced by selecting a class of trial functions for the variational problem associated with H. A rough approximation philosophy arises already from simple perturbation theory with respect to the cosine term in (40). To first order the ground state energy E_0 is given by

$$E_0^{(1)} = -2z[\varepsilon/(1+\varepsilon)]^{\beta/2} \tag{43}$$

and vanishes for $\varepsilon \to 0$ due to the 'period' of the cosine going to zero. In fact, inserting typical oscillator-spacings x_k in the cosine argument, it diverges with $\varepsilon \to 0$. All ε dependence can be deferred into the perturbation term by changing the energy scale by a factor of $1/\varepsilon$. Then $E_0^{(1)}/\varepsilon$ exhibits a threshold at $\beta = 2$ due to concurrence between the prefactor $1/\varepsilon$ and the cosine period. For $\beta < 2$ the prefactor dominates, and the cosine is no longer a 'weak' perturbation but influences strongly the shape of the wavefunction ψ_0. Thus, a dramatic change of ψ_0 is expected when β decreases through $\beta = 2$. Since ψ_0 determines the correlation function ϵ_q, one may already conjecture that the transition line ends up at $\beta = 2$ for small z.

To confirm the above arguments, consider the first-order correction of ψ_0:

$$\psi_0^{(1)} = \psi_0^{(0)} \frac{2z}{\varepsilon}\left(\frac{\varepsilon}{1+\varepsilon}\right)^{\beta/2} \int_0^\lambda \mathrm{d}r \frac{1}{r}\left[(1-r^2)^{-\beta/2}\cos\left(\beta^{1/2}\sum_k r^k x_k\right) - 1\right] \tag{44}$$

with

$$\psi_0^{(0)} = \prod_k (k/2\pi)^{1/4} \exp(-\tfrac{1}{4}kx_k^2). \tag{45}$$

For completeness, the second-order correction to the energy turns out to be

$$E_0^{(2)} = -\frac{4z^2}{\varepsilon}\left(\frac{\varepsilon}{1+\varepsilon}\right)^{\beta} \int_0^{\lambda} \mathrm{d}r \frac{1}{r}[(1-r^2)^{-\beta/2} + (1-r^2)^{\beta/2} - 2]. \tag{46}$$

It diverges with $\varepsilon \to 0$ for $\beta \leqslant 1$ in agreement with the analytical structure of the grand canonical potential ϕ (cf the Introduction). For $1 < \beta$ (46) leads to

$$\lim_{\varepsilon \to 0} E_0^{(2)} = -2z^2/(\beta - 1) \tag{47}$$

in agreement with the fugacity expansion of ϕ. By the way, the possibility of dealing with quantities like (44) and (46), which would not exist for the LG for all parameters, is one more advantage of the embedding (3) of the interaction potential.

4.1. Harmonic approximation (HA)

This subsection is not yet variational but prepares for the next. The HA amounts to the replacement

$$\cos\left(\sum_k y_k\right) \to 1 - \tfrac{1}{2} \sum_{k,k'} y_k y_{k'}, \tag{48}$$

i.e. to bilinear approximation of the lowest potential minimum. This certainly overstates the role played by the cosine, and the possibility of averaging out its periodic variation is lost. Thus, according to the above philosophy, (48) can only be reasonable for small β. With (48) the potential energy in H, (40), becomes a quadratic form $\boldsymbol{x}V\boldsymbol{x}$, and the matrix $V_{kk'} = \frac{1}{4}\varepsilon k^2 \delta_{kk'} + \beta z \lambda^k \lambda^{k'}$ is easily diagonalised by an orthogonal transformation C_0, $C_0 C_0^{\mathrm{T}} = 1$. Introducing by

$$(C_0^{\mathrm{T}} V C_0)_{rs} = \delta_{rs} \tfrac{1}{4}\varepsilon \tau_{0r}^2 \tag{49}$$

the notation for the diagonal elements, the matrix C_0 is obtained as

$$C_{0kr} = \frac{4\beta z}{\varepsilon} \frac{\lambda^k}{\tau_{0r}^2 - k^2} \gamma_{0r} \tag{50}$$

with $\tau_{0r} = \tau_r(z)$, $\gamma_{0r} = \gamma_r(z)$, where the functions $\tau_r(\zeta)$ (or τ_r for brevity) are the positive solutions of

$$\frac{\varepsilon}{4\beta\zeta} = \sum_k \frac{\lambda^{2k}}{\tau_r^2 - k^2}, \tag{51}$$

while

$$\gamma_r(\zeta) = \frac{\varepsilon}{4\beta\zeta}\left(\sum_k \frac{\lambda^{2k}}{(\tau_r^2 - k^2)^2}\right)^{-1/2}. \tag{52}$$

The ground state wavefunction turns out as

$$\psi_0^{\mathrm{HA}} = \text{constant} \times \exp(-\boldsymbol{x}A\boldsymbol{x}) \tag{53}$$

with

$$A_{rs} = \tfrac{1}{4} \sum_k C_{0rk} \tau_{0k} C_{0sk}. \tag{54}$$

The corresponding energy is given by

$$E_0^{\mathrm{HA}} = -2z + \tfrac{1}{2}\varepsilon \sum_k (\tau_{0k} - k). \tag{55}$$

The results (50)–(55) are much less horrible than they look. So the sum in (55) is easily evaluated (see (A7)) to give

$$E_0^{\mathrm{HA}} = -2z + \frac{1}{2\pi}\int_0^\infty \mathrm{d}q\, \ln[1 + 2\beta z w(q)], \tag{56}$$

and the limit $\varepsilon \to 0$ simply amounts to the replacement $w(q) \to w_0(q)$, (6). At $\varepsilon = 0$ the energy (56) has no expansion in powers of z. Its singular part is $-\beta z \ln(2\pi\beta z)$, which may be interpreted as the leading term towards small βz of the exact grand canonical potential (see the Introduction).

With the input (53) the auxiliary problem (32) can be solved exactly, if also in (32) anharmonic terms are suppressed corresponding to the HA. This amounts to linearisation of the sines in (32) and (33). With variables $\boldsymbol{\xi} = C_0^{\mathrm{T}}\boldsymbol{x}$ and for the function φ defined by $\chi = \psi_0^{\mathrm{HA}}\varphi$, the auxiliary problem then reads

$$(-\varepsilon\Delta + \varepsilon\boldsymbol{\xi}\tau\nabla + \mathrm{i}q)\varphi = 2z\beta^{1/2}\boldsymbol{\gamma}\boldsymbol{\xi}, \tag{57}$$

where τ is the diagonal matrix $\tau_{rs} = \delta_{rs}\tau_{0r}$ and $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots)$. The solution of (57) can be guessed as $\varphi = \boldsymbol{a}\boldsymbol{\xi}$ with $\boldsymbol{a} = 2z\beta^{1/2}(\varepsilon\tau + \mathrm{i}q)^{-1}\boldsymbol{\gamma}$. Since the matrix A, (54), becomes diagonal in the $\boldsymbol{\xi}$ space, the function g_q, (33), is readily evaluated to give

$$g_q = \frac{4\beta z^2}{\varepsilon}\sum_k \frac{\gamma_{0k}^2}{\tau_{0k}}\,\frac{1}{\tau_{0k} + \mathrm{i}q/\varepsilon} \tag{58}$$

and, with (34) and (A2),

$$f_q^{\mathrm{HA}} = -2\beta w(q)/(1 + 2\beta z w(q)). \tag{59}$$

To constitute the dielectric function, (13), the particle density n, (36), has to be 'harmonically approximated' consistently. The correct choice

$$n^{\mathrm{HA}} = z\int \psi_0^2 = z \tag{60}$$

is obtained from the requirement that $n_{\mathrm{f}} = n + f_0$ goes to zero with $\varepsilon \to 0$ (see the end of § 2), where from (59) $f_0 = z/(1 + \varepsilon/4\beta z I)$. Combining (13), (59) and (60), the result is

$$\epsilon_q^{\mathrm{HA}} = 1/(1 - b_q^{\mathrm{HA}}) = 1 + 2\beta z w(q). \tag{61}$$

Turning (by $\varepsilon \to 0$) to the LG and considering the long-wavelength limit (see (6)), it becomes clear that the HA predicts a metal in the whole βz plane—a poor approximation.

4.2. Gaussian approximation (GA)

The ground state wavefunction ψ_0 of H, (40), is gaussian not only for small β, where the HA applies, but also for very large β, when the effect of the cosine oscillations is 'washed out' entirely. Therefore, minimising the energy functional $E = \int \psi H\psi / \int \psi^2$ with a general gaussian trial function centred at the lowest potential minimum,

$$\psi = \text{constant} \times \exp(-\boldsymbol{x}B\boldsymbol{x}), \tag{62}$$

must give basic information about the transition. Without specifying the matrix B, this functional becomes

$$E(B) = \varepsilon \operatorname{Tr}(B - \tfrac{1}{2}K + \tfrac{1}{16}K^2 B^{-1}) - 2z \exp(-\tfrac{1}{8} l B^{-1} l), \tag{63}$$

where $K_{rs} = r\delta_{rs}$ and $l_r = \beta^{1/2}\lambda^r$. Varying independently *all* elements of B, (63) reaches its extrema at

$$B = \tfrac{1}{4} C \tau C^{\mathrm{T}}. \tag{64}$$

The matrix C and the objects τ_r are given by the same equations as C_0 (see (50)) and τ_{0r} except that z must be replaced by an 'effective fugacity' ζ (see (51) and (52)). The values of ζ are the positive solutions of

$$\zeta \, \mathrm{e}^{f} = z, \tag{65}$$

where

$$f = f(\zeta, \beta) = \frac{\beta}{2\pi} \int_0^\infty \mathrm{d}q \, \frac{w(q)}{1 + 2\beta\zeta w(q)}, \tag{66}$$

and (A5) has been used. The derivation of (63) and (64) is straightforward and therefore not given here. The condition (65), however, is easily derived from the energy as a function of ζ,

$$E(\zeta) = -2\zeta f - 2z \, \mathrm{e}^{-f} + 2 \int_0^\zeta \mathrm{d}\zeta' \, f(\zeta', \beta), \tag{67}$$

which is obtained from combining (64) and (66) with (63). It also follows from (67) that a given solution ζ_0 of (65) corresponds to an energy minimum (maximum) if the LHS of (65) has a positive (negative) derivative near ζ_0.

To study the condition (65) assume $0 < \lim_{\varepsilon \to 0} \zeta$, introduce an upper cut-off $q = 1$ in (66) (cf (7)) and replace $w(q)$ by π/q (cf (6)). Then f is approximated by

$$f = -\tfrac{1}{2}\beta \ln[2\pi\beta\zeta/(1 + 2\pi\beta\zeta)], \tag{68}$$

and (65) takes the form

$$(1 + 2\pi\beta\zeta)\left(\frac{2\pi\beta\zeta}{1 + 2\pi\beta\zeta}\right)^{1-\beta/2} = 2\pi\beta z. \tag{69}$$

For $\beta < 2$ the LHS of (69) is a monotonic increasing function of ζ, and thus (69) has only one solution, which corresponds to a minimum of $E(\zeta)$. The corresponding wavefunction ψ_0 is given by (62). Note that the matrix B equals A, (54), when z is replaced by ζ. This replacement even accounts for the gaussian approximation in the equations (57) to (61), so that

$$\epsilon_q^{\mathrm{GA}} = 2\pi\beta\zeta/q + \mathrm{O}(1). \tag{70}$$

Thus, the LG is metallic for $\beta < 2$ and all z. In passing, note that ζ behaves as $z^{2/(2-\beta)}$ for small z and corresponds to the renormalised mass in the sine-Gordon theory (Luther 1976). Probably, by following Minnhagen *et al* (1978), the metallic behaviour of the LG for $\beta < 2$ can be proved in general. Furthermore, the GA is possibly equivalent to a modified Debye–Hückel theory of the LG (Schulz 1977).

The case $2 < \beta$ is more interesting. There is *no* solution of (69) for z smaller than

$$z_0 = (1/4\pi)(1 - 2/\beta)^{1-\beta/2}. \tag{71}$$

This means that the lowest energy is reached at a border of the ζ interval, which is $\zeta = 0$ here. In fact, it follows from (67) and (66) that the derivative

$$\lim_{\zeta \to 0} \lim_{\varepsilon \to 0} E'(\zeta) = \beta \tag{72}$$

is positive. For $z_0 < z$ (and $2 < \beta$) there are two solutions of (69), one corresponding to a maximum. The whole story is illustrated in figure 2, which shows the function

$$E(\zeta) = \frac{1}{2\pi} \ln(1 + 2\pi\beta\zeta) - 2z\left(\frac{2\pi\beta\zeta}{1 + 2\pi\beta\zeta}\right)^{\beta/2} \tag{73}$$

obtained from (67) with the additional approximation (68). Thus, in GA a *first-order* transition is obtained, and the role of the order parameter is played by

$$2\pi\beta\zeta = \lim_{q \to 0} \lim_{\varepsilon \to 0} q\epsilon_q \tag{74}$$

(cf (70)). Denoting by E_i and E_m the energies at the 'insulator minimum' ($\zeta = 0$) and the 'metal minimum', respectively, the GA predicts $E_i = 0$ and $E_m = E(\zeta_m)$, where ζ_m is the larger of the two solutions of (69). The transition line $z(\beta)$ is then defined by $E_m = E_i$ and can be given in parametrised form,

$$\beta = \frac{2x}{\ln(1+x)}, \qquad z = \frac{1}{4\pi} \ln(1+x) \exp\left(x - x\frac{\ln x}{\ln(1+x)}\right), \tag{75}$$

with $0 < x < \infty$. This function starts at $z = 1/4\pi$, $\beta = 2$, with infinite slope,

$$z = \frac{1}{4\pi}\left[1 + (\tfrac{1}{2}\beta - 1)\ln\left(\frac{1}{\beta - 2}\right) + O(\beta - 2)\right] \tag{76}$$

and increases monotonically. Details like (75) may, of course, strongly depend on the approximation used. However, the above qualitative picture of the transition will no more change in the following.

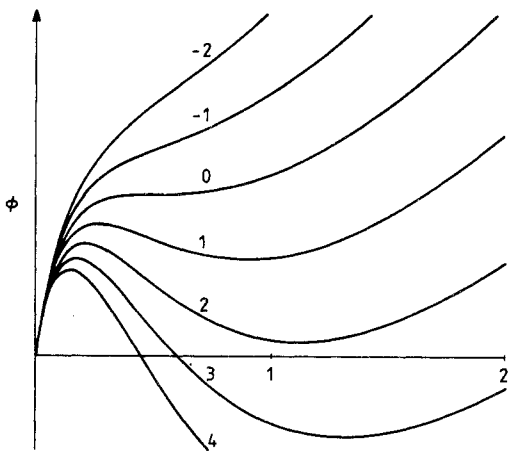

Figure 2. Grand canonical potential $\phi = L\beta^{-1}E(\zeta)$, (73), in gaussian approximation as a function of the order parameter (74) for $\beta = 3$ and seven z-values: $z = z_0(1 + 0.66n)$, $n = -2, -1, 0, 1, 2, 3, 4$.

In the limit of large z and ζ there is no problem in calculating f, ζ_m, E_m directly from (65)–(67), i.e. avoiding the approximation (68). f behaves as $\zeta^{-1/2}$, and the result for E_m is

$$E_m = -2z + \beta^{1/2} z^{1/2} - \tfrac{1}{16}\beta - \mathscr{J} + O(z^{-1/2}) \tag{77}$$

(cf (97)) with

$$\mathscr{J} = \tfrac{1}{2}\int_0^\infty d\zeta\, (\tfrac{1}{4}\beta^{1/2}\zeta^{-1/2} - f(\zeta, \beta)) = \tfrac{1}{4} + \tfrac{1}{24} + \ldots . \tag{78}$$

It remains to discuss the state of the LG corresponding to $\zeta = 0$, or at least to obtain the wavefunction ψ_0 in that case. Note that $\zeta = 0$ violates one of the conditions for the approximation (68) to be valid. In fact, if the function f is evaluated at *non-zero* ε, one more solution

$$\zeta_i = z\left(\frac{\varepsilon}{1+\varepsilon}\right)^{\beta/2} + O(\varepsilon^{\beta-1}) \tag{79}$$

of (65) appears inside the ζ interval $(0, \infty)$ and corresponds to a minimum. Inserting (79) for z into (50) and for ζ into (51) and (52), and performing the limit $\varepsilon \to 0$ only now, τ_k, C_{kr} and B_{kr} approach k, δ_{kr} and $\frac{1}{4}k\delta_{kr}$, respectively. The wavefunction (62) thus goes over to $\psi_0^{(0)}$, indeed, which corresponds to the HA at $z = 0$ and implies $\epsilon_q = 1$ (see (61)). The insulator case is discussed further in § 4.4.

4.3. Tunnelling catastrophe

The ground states considered so far all favour the central lowest potential minimum. The true potential energy, however, has many such valleys of nearly the same form and depth (cf § 3), and it is quite natural to think in terms of tunnelling and relative amounts of probability in adjacent valleys. Since a single gaussian can never form such probability accumulations, the serious question might arise whether the first-order transition of § 4.2 is perhaps an artifact due to impotence of the trial functions. The answer to this question will be *no*. But in tackling the problem a tunnelling phenomenon will be observed, which is special to quantum mechanics with infinitely many degrees of freedom.

A convenient approach to the above-mentioned purpose is provided by trial functions, which are linear combinations of gaussians each centred at a classical potential minimum $x_k^{(n)}$, (41):

$$\psi = \sum_{n=-\infty}^{\infty} a_n \exp[-(\boldsymbol{x} - \boldsymbol{x}^{(n)})B(\boldsymbol{x} - \boldsymbol{x}^{(n)})]. \tag{80}$$

The matrix B is defined by (64) and depends on the parameter ζ. Thus, the set of variation parameters is made up of ζ and the coefficients a_n. Since the decrease of these coefficients for very large n ($n \sim 1/\varepsilon$) does not interest us here, the approximation $S_n = 2\pi n$ is adopted for simplicity (this explains why the sum (80) is infinite). Again the calculation of the energy functional $E(\zeta, a_n)$ is straightforward (but lengthy) and results in

$$E(\zeta, a_n) = E(\zeta) + F(\zeta, a_n), \tag{81}$$

where $E(\zeta)$ is given by (67) and

$$F(\zeta, a_n) = \sum_{n,m} Q_{nm} a_n a_m \Big/ \sum_{n,m} P_{nm} a_n a_m \tag{82}$$

with

$$P_{nm} = \exp[-(n-m)^2 \ell], \tag{83}$$

$$Q_{nm} = P_{nm}\{nm\varepsilon\pi^2/\beta I - \pi^2\zeta(n-m)^2 + 2z\ \mathrm{e}^{-f}[1-(-1)^{n+m}]\} \tag{84}$$

and

$$\ell = \frac{\pi^2}{2\beta}\left(\frac{4\beta\zeta}{\varepsilon}\right)^2\left(1+\frac{\varepsilon}{4\beta\zeta I}\right)^2 \sum_k \frac{\gamma_k^2}{\tau_k^3}. \tag{85}$$

As (82) shows, the matrix elements P_{nm} represent the overlap integrals $\int \psi_{(n)}\psi_{(m)} / \int \psi_{(n)}^2$, where $\psi_{(n)}$ stands for the nth exponential function in (80). The sum (85) is evaluated in the Appendix. If $\lim_{\varepsilon\to 0}\zeta$ is non-zero,

$$\ell = (2/\beta)\ln(1/\varepsilon) + \mathrm{O}(1) \tag{86}$$

diverges with $\varepsilon \to 0$ independently of ζ. Thus the overlap integrals P_{nm} vanish as $\varepsilon^{2(n-m)^2/\beta}$ in that case. This is a mysterious result (perhaps not to field theorists), since the separation of the potential minima is finite and so are typical x_k-values such as $\Sigma_r C_{kr}\tau_r^{-1/2}$ (from (63) and (64)). The sum over the squares of typical x_k-values, however, diverges for $\varepsilon \to 0$ (see also (A10)). Note that in an infinite-dimensional space the diagonal of a unit cube has infinite length.

The property (86) keeps the following analysis simple. Varying $E(\zeta, a_n)$ with respect to the coefficients a_n, the system of equations

$$\sum_m (Q_{nm} - FP_{nm})a_m = 0 \tag{87}$$

is obtained. Introducing the Fourier transform by

$$a_n = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\varphi\ \mathrm{e}^{\mathrm{i}n\varphi} b(\varphi), \tag{88}$$

this system turns into

$$[-(\varepsilon\pi^2/\beta I)\partial_\varphi U_0 \partial_\varphi + \pi^2\zeta U_1 + 2z\ \mathrm{e}^{-f}U_2]b(\varphi) = U_0 F b(\varphi) \tag{89}$$

where U_0, U_1, U_2 are functions of φ given by

$$\begin{aligned} U_0(\varphi) &= 1 + 2\sum_{n=1}^{\infty} P_{0n}\cos(n\varphi), \\ U_1(\varphi) &= U_0''(\varphi), \\ U_2(\varphi) &= U_0(\varphi) - U_0(\varphi+\pi). \end{aligned} \tag{90}$$

For $\varepsilon \to 0$, and because of (86), these expressions simplify considerably (namely to 1, $-2P_{01}\cos\varphi$, $4P_{01}\cos\varphi$, respectively) and (89) takes the form

$$(-\partial_\varphi^2 - 2\omega\cos\varphi)b(\varphi) = (\beta F/6\varepsilon)b(\varphi), \tag{91}$$

which is Mathieu's equation. But only limiting cases of (91) are relevant here, since due to $P_{01} \sim \varepsilon^{2/\beta}$ the factor

$$\omega = (P_{01}2\beta/3\varepsilon)(\tfrac{1}{4}\pi^2\zeta - z\ \mathrm{e}^{-f}) \tag{92}$$

either vanishes ($\beta < 2$) or diverges ($2 < \beta$). In both cases F goes to zero with an ε power $4/\beta - 1$ or $2/\beta$ for $\beta < 2$ and $2 < \beta$, respectively. Thus, by (81), the value of ζ (if non-zero) is to be determined in the same way as in § 4.2, i.e. from (65).

It is even an easy task to calculate the coefficients a_n from (91). For $\beta < 2$ the function $b(\varphi)$ becomes constant, which means that

$$\lim_{\varepsilon \to 0} a_n = \text{constant} \times \delta_{n,0}. \tag{93}$$

No probability tunnels into the neighbouring valleys! The whole cosine function acts as an anharmonicity. For $2 < \beta$, on the other hand, the function $b(\varphi)$ turns into a delta function at $\varphi = 0$. Consequently, all coefficients become equal. Thus, increasing β through $\beta = 2$, a sudden tunnelling breakthrough occurs, overflowing equally all valleys by the probability which was concentrated at the central minimum before.

Within the approximation introduced by (80) and for $2 < \beta$ the above analysis works if $z > z_0$ (to guarantee the existence of a finite ζ). Therefore another solution of the above variational problem must exist at least for $z < z_0$. Assume ζ to be of order $\varepsilon^{\beta/2}$ in magnitude (cf (79)). Then (86) no longer applies, the overlap integrals P_{0n} remain finite and make U_0, U_1, U_2 non-trivial functions. But now in (89) the terms with U_1 and U_2 may be neglected compared with the first term. The eigenvalue F becomes independent of ζ. Now, varying (81) with respect to ζ, *again* the condition (65) is obtained. Hence ζ is given by (79), which is consistent with the assumption. Correspondingly, the wavefunction (80) is made up of functions $\psi_n = \psi_0^{(0)}(\boldsymbol{x} - \boldsymbol{x}^{(n)})$. It is thus widespread over all valleys, no matter how many coefficients a_n contribute.

To summarise, the whole picture of the metal–insulator transition of § 4.2 is reproduced here with the only exception that (for $2 < \beta$) the sharply peaked gaussians in the metallic range are nearly periodically repeated now. It is highly probable that the auxiliary problem continues to give $\epsilon_q \sim 1/q$ in that range. Remaining doubts are overcome in § 6.

It should be emphasised that the tunnelling catastrophe occurs at the vertical line $\beta = 2$ and hence *differs* from the metal–insulator transition line (figure 1). Moreover, as is shown in § 5, the tunnelling breakthrough phenomenon is special to the embedding (3). It takes place gradually for these models ($\varepsilon \neq 0$).

4.4. *Mathieu approximation (MA)*

The approximations considered so far have rather subordinated the insulating state. The energy E_i^{GA} at the insulator minimum tends to zero as $\varepsilon \to 0$ in contrast to the perturbation correction (47). Also, the wavefunction ($\psi_0^{(0)}$ in GA) corresponding to E_i should vary nearly periodically over the potential valleys such that $\psi_0^{(0)}$ only plays the role of an envelope function. The trial function

$$\psi = \varphi\Big(\beta^{1/2} \sum_k \lambda^k x_k\Big) \psi_0^{(0)} \tag{94}$$

points in this direction. The function φ is to be determined variationally, and the approximation is in the restricted dependence of φ on only the cosine argument. The calculation of the energy functional makes use of the variables v_k of § 5 (see (101)). The resulting equation for φ and E_i is

$$(-\beta \partial_{v_1}^2 + v_0^{-1} v_1 \partial_{v_1} - 2z \cos v_1)\varphi(v_1) = E_i \varphi(v_1), \tag{95}$$

to be solved for the ground state. Since the factor v_0^{-1}, (4), vanishes with $\varepsilon \to 0$, once more Mathieu's equation is obtained. For small z the energy is

$$E_i^{\mathrm{MA}} = -2z^2/\beta + \mathrm{O}(z^4) \tag{96}$$

and is to be compared with the exact second-order correction (47) of the energy. Both expressions agree in the limit $\beta \to \infty$, which fact is well understood physically. For large β, i.e. low temperature, the mean distance of two paired particles becomes so small that $v(x)$ may be approximated by $-|x|$. The LG then must obtain the properties of the 1DCG, for which system Mathieu's equation is exact. Most probably, for $\beta \to \infty$ (95) is correct even to higher orders in z. As a speculation, consider z going to infinity at some fixed value of β (perhaps not even large). Then (95) gives

$$E_i^{\mathrm{MA}} = -2z + \beta^{1/2} z^{1/2} - \tfrac{1}{16}\beta + \mathrm{O}(z^{-1/2}) \tag{97}$$

which exceeds E_{m}, (77), just by a constant. This is in accord with the general qualitative picture of § 4.2 predicting a metallic state at sufficiently large density for any temperature.

The calculation of the dielectric function in MA can be traced back to the exact analysis of AES on the 1DCG. With (94) the integrals $\mathscr{F}_n$, (31), at first take the form

$$\mathscr{F}_n = 2z \int \mathrm{d}v_1 \, \varphi_n \varphi_0 \sin v_1 \int' \psi_0^{(0)2}, \tag{98}$$

where $\int'$ integrates over $v_2, v_3, \ldots$. But for $\varepsilon \to 0$ the unwanted factor

$$\int' \psi_0^{(0)2} = \text{constant} \times \exp(-v_1^2/2\beta v_0) \tag{99}$$

becomes independent of v_1 and can be omitted. From AES (note that their integrals $\mathscr{J}_\nu$ are related to $\mathscr{F}_n$ by $\mathscr{F}_\nu = \alpha_\nu \mathscr{J}_\nu$) it follows that $f_q + n = q^2(1 - 1/\epsilon_q^{\mathrm{1DCG}})$, where $\epsilon_0^{\mathrm{1DCG}}$ is finite and larger than 1, since the 1DCG insulates. Therefore (13) takes the form

$$b_q^{\mathrm{MA}} = 2\pi\beta q(1 - 1/\epsilon_0^{\mathrm{1DCG}}) + \mathrm{O}(q^3) \tag{100}$$

corresponding to a total insulator with $\epsilon_0 = 1$.

To understand the result (100) physically, consider all particles grouped in pairs responding to an external force only by forming finite dipoles. The potential of each dipole vanishes at large distance due to the 'weak' logarithmic interaction. Consequently, the induced potential V_{in} (cf (10)) has no contribution at zero wavevector. Thus (100) reflects the non-Coulomb nature of the LG. In a 2D electrodynamics a 1D dielectric does not contribute to the macroscopic polarisation. As a conjecture, $\epsilon_0 = 1$ is true in the whole insulator region (see also the end of § 5).

5. Bloch problem

In this section a lattice periodic problem H_{B} is derived by a slight modification of the Hamiltonian H. This modification is shown to give another sequence of models converging to the LG 'from below'. The effective mass m^* of the lowest band of this Bloch problem is then related to ϵ_0 in analogy to the 1DCG treatment by AES.

There is an easy direction in the problem H marked by the classical potential minima $x_k^{(n)}$, (41). The probability flowed in this direction after the tunnelling breakthrough and developed a nearly periodic distribution. The step mentioned above is

from nearly to strict periodicity. The first task is to introduce new variables v_k as linear combinations of x_k such that the classical minima lie on the v_1 axis, $v_k^{(n)} = v_1^{(n)}\delta_{k,1}$, *and* all other variables $v_2, v_3, \ldots$ span the hyperspace in which the cosine in (40) remains constant. In the x_k space the easy direction and this hyperspace form an oblique angle. They become orthogonal, however, by scaling the variables x_k by a factor of k. The transformation is therefore given by

$$v_r = I^{1/2}\beta^{1/2}\sum_k D_{rk}kx_k, \tag{101}$$

where D is an orthogonal transformation, $DD^{\mathrm{T}} = 1$, with

$$D_{1k} = I^{-1/2}\lambda^k/k. \tag{102}$$

Note that the above requirements are fulfilled with $v_1^{(n)} = S_n$. The transformation (101) still allows for an arbitrary rotation in the hyperspace. Using this freedom to make the Hamiltonian diagonal in the 'side variables' $v_2, v_3, \ldots$, the matrix D becomes

$$D_{rk} = D_{1k}(\delta_{r,1} + d_r c_r/(k^2 - c_r^2)), \tag{103}$$

where the numbers c_r are the non-negative solutions of

$$I = \sum_k \lambda^{2k}/(k^2 - c_r^2), \tag{104}$$

while

$$d_r = I^{1/2}\left(\sum_k \lambda^{2k}/(k^2 - c_r^2)^2\right)^{-1/2}. \tag{105}$$

The Hamiltonian (40) transforms into

$$H = -\beta\partial_{v_1}^2 + v_1^2\varepsilon/4\beta I - \varepsilon/2 - 2z\cos v_1 - 2\beta\varepsilon I\sum_k{}' c_k d_k \partial_{v_k}\partial_{v_1}$$

$$+ \varepsilon\sum_k{}'(-\beta I c_k^2\partial_{v_k}^2 + v_k^2/4\beta I - k/2), \tag{106}$$

where primed sums exclude $k = 1$.

The discrete translational symmetry in the v_1 direction is broken by only the second term of (106). Note also the factor ε of this term. Thus, the Bloch problem

$$H_{\mathrm{B}} = -\beta\partial_{v_1}^2 - 2z\cos v_1 - 2\beta\varepsilon I\sum_k{}' c_k d_k \partial_{v_k}\partial_{v_1} + \varepsilon\sum_k{}'(-\beta I c_k^2\partial_{v_k}^2 + v_k^2/4\beta I - c_k/2) \tag{107}$$

perhaps represents an alternative description of the physics of the LG. The proof of this conjecture goes through § 3 in the backward direction. The aim is to rewrite H_{B} in a form comparable with (30) such that the underlying interaction can be merely read off. If H_{B} is re-expressed by the variables x_k, in addition to (40) a binnear term appears and requires a further diagonalisation. These two steps are equivalent to introducing the following variables u_k:

$$\begin{aligned} u_1 &= v_1 - \sum_k{}' v_k d_k/c_k, \\ u_r &= v_r d_r/c_r \qquad (r \geq 2). \end{aligned} \tag{108}$$

Using (108), (A12) and the notation $I_0 = \Sigma_k \lambda^{2k}/k^4$ H_B goes over into

$$H_B = -\varepsilon\beta(I^2/I_0)\partial_{u_1}^2 + u_1^2\varepsilon I_0\eta^2/4\beta I^2 + \varepsilon \sum_k{}' (-\beta I d_k^2 \partial_{u_k}^2 + u_k^2 c_k^2/4\beta I d_k^2 - c_k/2) - 2z \cos\left(\sum_k u_k\right) \tag{109}$$

and indeed attains the structure of (30). The second term (in which $\eta \to 0$) is added arbitrarily for convenience in the next step. In fact, the Hamiltonian (30) turns into (109) if one replaces $y_k \to u_k$, $\sigma_1 \to \beta I^2/I_0\eta$, $\sigma_k \to \beta I d_k^2/c_k$ ($k \geq 2$) and $k \to \eta$ for $k = 1$, $k \to c_k$ for $k \geq 2$. Denoting the result of these replacements in $w(x) = \beta^{-1} \Sigma_k \sigma_k \, e^{-k\varepsilon x}$ by $w_B(x)$ and performing the limit $\eta \to 0$, the modified interaction $v_{B\varepsilon}(x) = w_B(x) - w_B(0)$ is obtained as

$$v_{B\varepsilon}(x) = -x\varepsilon I^2/I_0 + I \sum_k{}' [\exp(-\varepsilon c_k x) - 1] d_k^2/c_k. \tag{110}$$

To discuss the function (110) note that $v'_{B\varepsilon}(0) = -1$ and realise that for ε going to zero finite contributions to the sum in (110) can only arise from k values of order $1/\varepsilon$ or larger. For such large k, (104) and (105) give $c_k \sim k$ and $d_k \sim \lambda^k I^{-1/2}$ leading to $-\ln[1 + (1/\varepsilon)(1 - e^{-\varepsilon x})]$ for the second term in (110). Consequently for $\varepsilon \to 0$ $v_{B\varepsilon}(x)$ turns into $v(x) = -\ln(1+x)$. This completes the proof. Due to its linear term, $v_{B\varepsilon}(x)$ represents an embedding of the true interaction $v(x)$ from *below*. It should be noted that the periodic Hamiltonian H_B can be used instead of H for all values of β and z. The calculations of § 4 could have been performed using H_B. No doubt, the same results would have been obtained except for the tunnelling catastrophe.

The Bloch problem H_B, (107), differs from Mathieu's equation 'only' via the coupling to the side variable oscillators. This analogy of the LG to the 1DCG is followed next in deriving a relation between the dielectric constant and the effective mass of the lowest band. For the 1DCG this relation is $\epsilon_0 = 2m^*$(AES). Using the variables v_k and the shorthand notation $h = H_B - E_0$, the auxiliary problem (32) reads

$$(h + iq)\chi = \psi_0 2z \sin v_1. \tag{111}$$

As a first advantage of H_B, the solution of (111) for $q = 0$ can be given explicitly:

$$\chi_{q=0} = -\partial_{v_1}\psi_0, \tag{112}$$

which is easily verified by differentiating $h\psi_0 = 0$ with respect to v_1. Using (112) in (33) and (34) and partial integrating,

$$f_{q=0} = -2z \int \psi_0 \chi_{q=0} \sin v_1 = n \tag{113}$$

is obtained (cf (36)). Thus, the fluctuation term n_f, (14), is zero, as is expected for interactions embedding $v(x)$ from below. Using (112), (113) and combining (13), (33), (34) and (111) one obtains

$$b_q = 2\beta w(q) q \int \psi_0 \partial_{v_1} \bar{\chi} \tag{114}$$

with the function $\bar{\chi}$ to be determined from

$$(h^2 + q^2)\bar{\chi} = -q\psi_0 2z \sin v_1. \tag{115}$$

Furthermore, the solution of (115) can be written as

$$\bar{\chi} = \alpha\Big(\bar{\vartheta} - \vartheta + \sum_k p_k v_k \psi_0\Big) \tag{116}$$

if the functions ϑ and $\bar{\vartheta}$ obey

$$h\vartheta = -2\beta d\psi_0 \tag{117}$$

and

$$(h^2+q^2)\bar{\vartheta} = q^2\vartheta, \tag{118}$$

where $d = \partial_{v_1} + \varepsilon I \sum_k' c_k d_k \partial_{v_k}$. In (116)

$$p_k = c_k d_k/(c_k^2 + q^2/\varepsilon^2), \tag{119}$$

while

$$\alpha = (q/2\beta)\Big(1 - \varepsilon I \sum_k' p_k c_k d_k\Big)^{-1} \tag{120}$$

is evaluated in the Appendix (see (A14)). Simplifications are possible now towards $\varepsilon \to 0$ and small q: α turns into $1/\beta q w(q)$ and the function $\bar{\vartheta}$ is expected to contain one factor of q more than ϑ and is therefore omitted (compare (118) with (115); this step is somewhat delicate, since no rigorous proof is available). It follows that

$$b_{q=0} = 2\int \psi_0 \partial_{v_1} \vartheta. \tag{121}$$

This expression can be related to m^* as follows.

The eigenfunctions of H_B are Bloch functions with respect to v_1. The corresponding energies $E_{\kappa\nu}$ might build up a very complicated band structure due to the many side oscillators. The index ν is certainly discrete, however, and the effective mass m^* of the lowest band may be defined by $E_{\kappa 0} = \kappa^2/2m^* + O(\kappa^4)$. Rewriting the eigenvalue equation into one for the Bloch factors u_{k0}, expanding the latter as

$$u_{k0} = \psi_0 - i\kappa\vartheta + \kappa^2\eta + \ldots, \tag{122}$$

and collecting terms of order κ and κ^2 separately, the two equations (117) and

$$h\eta = (1/2m^* - \beta)\psi_0 + 2\beta\, d\vartheta \tag{123}$$

are obtained. Multiplying (117) and (123) by $\psi_0 v_r$ and ψ_0, respectively, and integrating gives

$$2\int \psi_0(d_r\partial_{v_1} + c_r\partial_{v_r})\vartheta = d_r \qquad (r \geq 2) \tag{124}$$

and

$$\beta - 1/2m^* = 2\beta\int \psi_0\, d\vartheta. \tag{125}$$

Using (124) to eliminate the ∂_{v_r} terms in (125) and remembering (A12), the matrix element (121) is obtained as

$$b_{q=0} = 1 - I_0/2m^*\beta\varepsilon I^2. \tag{126}$$

Correspondingly,

$$\epsilon_{q=0} = 2m^* \beta \varepsilon I^2 / I_0 \tag{127}$$

is the desired formula.

The relation (127) is claimed to be exact. It implies that m^* is large at least of order $1/\varepsilon$, since always $\epsilon_0 \geqslant 1$ holds true from physical grounds. This extreme tight binding is apparently an effect of the side oscillators. To verify this, consider H_B to zeroth order, i.e. for $z = 0$. As is physically clear, this case gives a lower bound $m^*_{(0)}$ for m^*. The wavefunctions turn out as

$$\psi^{(0)}_{\kappa 0} = \exp\left(i\kappa v_1 - i\kappa \sum_r{}' v_r d_r / c_r \right) \prod_k{}' \text{(oscillator ground states)}, \tag{128}$$

and the energies $E^{(0)}_{\kappa 0}$ form a parabolic band with effective mass

$$m^*_{(0)} = I_0 / 2\beta \varepsilon I^2 \tag{129}$$

giving $\epsilon_0 = 1$ as expected. To second order

$$m^*/m^*_{(0)} = 1 + \text{constant} \times z^2 \varepsilon^{\beta - 2} \tag{130}$$

either diverges ($\beta < 2$) or remains 1 ($2 < \beta$), in agreement with the results of § 4. Especially, (130) confirms the conclusion drawn from the MA that the LG can only make $\epsilon_0 = \infty$ or $\epsilon_0 = 1$.

6. Solitons

The correlation function ϵ_q can be represented and analysed as a functional integral in full analogy to the function space analysis of AES on the 1DCG. Their functional had minima at the soliton solutions of the static sine-Gordon equation, which in turn is derived from Mathieu's equation. Correspondingly, viewing H_B as a generalised Mathieu problem, the LG might be related to a sine-Gordon type theory as well. Soliton solutions also exist and are given here.

Consider the Bloch Hamiltonian H_B classical, turn to the Lagrangian, change to imaginary time ($t \to i\tau$, $v_r(t) = \phi(r, \tau)$), integrate over τ and take the exponential function of this action (called $-\bar{H}$) to obtain the functional for the thermodynamics of the LG (Kogut 1979). The result is

$$\bar{H} = \int d\tau \left(\frac{1}{4\beta I \varepsilon} \sum_{r,s} T_{rs} \phi'(r, \tau) \phi'(s, \tau) + \frac{\varepsilon}{4\beta I} \sum_r{}' \phi^2(r, \tau) - 2z \cos \phi(1, \tau) + 2z \right), \tag{131}$$

where

$$T_{rs} = \sum_k D_{rk} k^{-2} D_{sk}, \tag{132}$$

and the primes denote derivatives with respect to τ. Note that proper embedding of the interaction, Baxter mapping and the above steps form a concise way to the functional integral formulation of the statistics of a given 1D classical gas. By analogy to AES it is not hard to guess the expression for the correlation function,

$$b_q = 2\beta w(q) 2z^2 \int d\tau \, (1 - \cos q\tau) \langle \sin \phi(1, \tau) \sin \phi(1, 0) \rangle, \tag{133}$$

and to verify it afterwards by discretising the τ axis, constructing the transfer operator (Gupta and Sutherland 1976) and arriving finally at (13) with (34) and (33). The average in (133) is defined as

$$\langle \ldots \rangle = \int \mathscr{D}\phi \, \mathrm{e}^{-\bar{H}} \ldots \Big/ \int \mathscr{D}\phi \, \mathrm{e}^{-\bar{H}}, \tag{134}$$

where $\int \mathscr{D}\phi$ denotes the product $\int \mathscr{D}\phi(1, \tau) \int \mathscr{D}\phi(2, \tau) \ldots$ of functional integrals. To make easy use of this formulation, $\bar{H}$ should develop sharp minima in the function space such that gaussian evaluation of (133) represents a good approximation. The extrema of $\bar{H}$ are the solutions of

$$\sum_s T_{rs}\phi''(s, \tau) = \delta_{r,1} 4\beta z \varepsilon I \sin \phi(1, \tau) + (1 - \delta_{r,1})\varepsilon^2 \phi(r, \tau). \tag{135}$$

Besides the trivial solutions $\phi(r, \tau) = \nu\pi\delta_{r,1}$ of (135) (corresponding to minima at zero energy for even numbered ν) soliton solutions with the property

$$\phi(r, \mp\infty) = (\nu'' + \tfrac{1}{2}\nu' \mp \tfrac{1}{2}\nu')\pi\delta_{r,1} \tag{136}$$

are expected to exist (ν' and ν'' even numbered, $\nu' \neq 0$) and to give the energy $\bar{H}$ a finite value. To work them out the saw tooth approximation

$$\sin\phi \to \phi - \pi \sum_{\nu=-N}^{N+1} \operatorname{sgn}(\phi + \pi - 2\pi\nu) \qquad (N \to \infty) \tag{137}$$

is used as a minor modification of (135), which does not influence the gross qualitative features of the above field theory. Then, using the techniques of Horovitz *et al* (1977) and Koch (1980), who solved similar problems, the single soliton solution ($\nu'' = 0$, $\nu' = 2$; centred arbitrarily at $\tau = 0$ by $\phi(r, 0) = \pi\delta_{r,0}$) is obtained as

$$\phi_{\mathrm{sol}}(r, \tau) = \delta_{r,1} 2\pi\theta(\tau) - \frac{\tau}{|\tau|} \sum_k w_{kr} j_k \exp(-t_k \varepsilon |\tau|) \tag{138}$$

where

$$w_{kr} = \delta_{r,1} + 4\beta z I d_r c_r / \varepsilon (t_k^2 - c_r^2),$$

$$j_k = 4\pi\beta z \Gamma_k^2 / \varepsilon t_k^2,$$

$$\Gamma_k = \gamma_k(\zeta = zE), \qquad t_k = \tau_k(\zeta = zE),$$

with $E = 1 - \varepsilon/4\beta z I$. In verifying (138) note that $w_{k1} = 1$ and $\Sigma_k j_k = \pi$ (see (A4)).

At first sight the soliton (138) has quite reasonable properties. So the derivative at its centre,

$$\phi'(1, 0) = 4\pi\beta z \sum_k \Gamma_k^2 / t_k, \tag{139}$$

has a finite value against $\varepsilon \to 0$ (see (A5)). However, the energy of the soliton (138) derives from (131) as

$$E_{\mathrm{sol}} = \mathscr{E}(\zeta = zE) \tag{140}$$

(cf (85), (86)) and diverges logarithmically with $\varepsilon \to 0$. Accordingly, the soliton density

$$\langle N_{\mathrm{sol}} \rangle / L = R \exp(-E_{\mathrm{sol}}) \sim R\varepsilon^{2/\beta} \tag{141}$$

goes to zero with $\varepsilon \to 0$, if the factor R keeps a finite value in this limit. This situation would be ideal to employ the 'independent soliton approximation' (see AES). To

calculate R one is, however, also dependent on gaussian approximations of the functional integrals. Accepting even these approximations the evaluation of R and b_q still becomes very involved. But the main steps correspond to those in the 1DCG case and are described by AES (Appendix C). Only the results are therefore given here.

The factor R takes a finite value, indeed. However, this result is valid only for large z. The correlation function (133) is made up of two terms, $b_q = b_q^0 + b_q^{\mathrm{sol}}$, corresponding to small deviations from $\phi(r,\tau)=0$ and from solitons, respectively. The leading (gaussian) contribution to b_q^0 agrees with the HA result (61), and the first anharmonic correction to $b_{q=0}^0$ is zero. Most probably *all* anharmonic terms of $b_{q=0}^0$ vanish as in the 1DCG case (AES). Then deviations from the HA result can only arise from the soliton term b_q^{sol}. For the latter the single soliton (and antisoliton) contribution is sufficient due to (141). The leading term of this contribution turns out to be $-8\beta^{-1}w(q)R\exp(-E_{\mathrm{sol}})$ and vanishes with $\varepsilon\to 0$ (to describe the LG, note that the limit $\varepsilon\to 0$ has to be performed at finite wavevector q). Thus, independent of the temperature, at sufficient large density the LG is in the metallic state.

Acknowledgments

I am grateful to H-U Everts for his patience in numerous stimulating discussions, and W Apel, Ph Choquard, H Kunz and K D Schotte for their interest in the course of this work.

Appendix

Here various sums are evaluated containing the objects τ_k and γ_k. These are defined in the main text as functions of ζ by the equations (51) and (52). Note that for $\zeta = z$ and $\zeta = zE$ the special cases τ_{0k}, γ_{0k} and t_k, Γ_k, respectively, are obtained (cf §§ 4.1 and 6). All the following formulae apply to these special cases as well. Multiplying (51) with $\gamma_r^2/(\tau_r^2 - s^2)$ and summing over r gives

$$\sum_r \gamma_r^2/(\tau_r^2 - s^2) = \varepsilon/4\beta\zeta. \tag{A1}$$

Then, multiplying (A1) with $\lambda^{2s}/(s^2+p^2)$, where p is arbitrarily real, summing over s, using (5) and exploiting again (51), one obtains the key relation

$$\sum_r \gamma_r^2(\tau_r^2 + p^2) = \tfrac{1}{2}\varepsilon w(\varepsilon p)/(1 + 2\beta\zeta w(\varepsilon p)). \tag{A2}$$

The limits $p\to\infty$ and $p\to 0$ in (A2) imply

$$\sum_r \gamma_r^2 = 1/\varepsilon \tag{A3}$$

and

$$\sum_r \gamma_r^2/\tau_r^2 = (\varepsilon/4\beta\zeta)(1 + \varepsilon/4\beta\zeta I)^{-1}, \tag{A4}$$

respectively. Integrating (A2) over p gives

$$\sum_r \gamma_r^2/\tau_r = (1/\pi)\int_0^\infty \mathrm{d}q\, w(q)/(1 + 2\beta\zeta w(q)), \tag{A5}$$

which remains a finite expression, if $w(q) \to w_0(q)$ as $\varepsilon \to 0$ (see (6) and (7)). Differentiating (51) with respect to ζ and using (52), one obtains

$$\partial_\zeta \tau_r = 2\beta\gamma_r^2/\varepsilon\tau_r. \tag{A6}$$

Combining (A6) and (A5), integrating over ζ and noting that $\tau_r(0) = r$, one has

$$\sum_r (\tau_r - r) = (1/\varepsilon\pi) \int_0^\infty \mathrm{d}q \, \ln[1 + 2\beta\zeta w(q)] \tag{A7}$$

i.e. equation (56) in the main text. To evaluate the sum ℓ, (85), note that

$$\sum_r \gamma_r^2/\tau_r^3 = (2/\pi) \int_0^\infty \mathrm{d}p \, p^{-2} \Big(\sum_r \gamma_r^2/\tau_r^2 - \sum_r \gamma_r^2/(\tau_r^2 + p^2) \Big)$$

and use (A4) and (A2) to obtain

$$\ell = 4\pi\zeta(1 + \varepsilon/4\beta\zeta I)^2 \int_0^\infty \mathrm{d}q \, q^{-2}[(1 + 2\beta\zeta w(q))^{-1} - (1 + 2\beta\zeta w(0))^{-1}]. \tag{A8}$$

This integral diverges for $\varepsilon \to 0$ (see (6)). Since

$$w(q) = 2I/\varepsilon - 2I_0 q^2/\varepsilon^3 + \mathrm{O}(q^4/\varepsilon^5) \tag{A9}$$

there are only finite contributions to (A8) from $0 < q < \varepsilon$. Therefore, the leading term of ℓ towards $\varepsilon \to 0$ arises from $\varepsilon < q \ll 1$, where $w(q) \sim \pi/q$. Thus, (A8) leads to $\ell \sim (2/\beta) \int_\varepsilon^1 \mathrm{d}q \, q^{-1}$, i.e. to equation (86) in the main text. Among the overlap integrals (§ 4.3) and the soliton energy (§ 6) there is yet another quantity, which is determined by the sum ℓ, namely the half width of the (metallic) wavefunction ψ_0 in the easy direction. Consider ψ_0 in GA, (62), turn to the variables v_k by (101), $\boldsymbol{x}\boldsymbol{B}\boldsymbol{x} = \boldsymbol{v}\bar{\boldsymbol{B}}\boldsymbol{v}$, and evaluate $\bar{B}_{11}$. The result is

$$\bar{B}_{11} = \ell/2\pi^2 I \tag{A10}$$

and shows that on the metal side for $\varepsilon \to 0$ the wavefunction ψ_0 becomes infinitely sharply peaked.

Part of the above analysis can be extended even to negative values of the parameter ζ. Comparing equation (104), which determines the numbers c_r, with (51) implies

$$c_r = \tau_r(\zeta = -\varepsilon/4\beta I). \tag{A11}$$

However, note that the first solution of (104) is $c_1 = 0$, i.e. $\tau_1(\zeta)$ ceases to be real just at $\zeta = -\varepsilon/4\beta I$. Nevertheless (105) may be compared with (52) to obtain $d_r^2 = \gamma_r^2/I$. Also, (A3) may be used to derive

$$\sum_r{}' \, d_r^2 = 1/\varepsilon I - I/I_0. \tag{A12}$$

Moreover, from (A2) and (A12) the sum

$$\sum_r{}' \, c_r^2 d_r^2/(c_r^2 + p^2) = 1/\varepsilon I - \varepsilon p^2 w(\varepsilon p)[2I(1 - \varepsilon w(\varepsilon p)/2I)]^{-1} \tag{A13}$$

is obtained, which is needed to evaluate the function α, (120). Using (A13) this function becomes

$$\alpha = (1 - \varepsilon w(q)/2I)/\beta q w(q). \tag{A14}$$

It is also possible, of course, to derive (A12) and (A13) from (104) and (105) without reference to negative ζ-values.

Note added in proof. S A Bulgadaev kindly informed me of his general gas model (1979 *Phys. Lett.* B**87** 47–9, 1979 *JETP Lett.* **30** 426–9) of which the LG is a special case. In a recent preprint (submitted to *Phys. Lett.* A) Bulgadaev arrives at results which differ from mine. The reason for this discrepancy is not yet understood.

References

Anderson P W and Yuval G 1969 *Phys. Rev. Lett.* **23** 89–92
Apel W, Everts H U and Schulz H 1979 *Z. Phys.* B **34** 183–95
Baxter R J 1964 *Phys. Fluids* **7** 38–43
—— 1965 *Phys. Fluids* **8** 687–92
Behncke J and Schotte K D 1979 *Phys. Rev.* A **19** 834–45
Choquard Ph 1975 *Helv. Phys. Acta* **48** 585–98
Edwards S F and Lenard A 1962 *J. Math. Phys.* **3** 778–92
Everts H U and Koch W 1977 *Z. Phys.* B **28** 117–27
Gupta N and Sutherland B 1976 *Phys. Rev.* A **14** 1790–801
Hauge E H and Hemmer P C 1971 *Phys. Norvegica* **5** 209–17
Horovitz B, Krumhansl J A and Domany E 1977 *Phys. Rev. Lett.* **38** 778–81
Koch W 1980 *Z. Phys.* B **40** 249–56
Kogut J B 1979 *Rev. Mod. Phys.* **51** 659–713
Kosterlitz J M 1974 *J. Phys. C: Solid State Phys.* **7** 1046–60
Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181–203
Kunz H 1974 *Ann. Phys.* **85** 303–35
Lenard A 1961 *J. Math. Phys.* **2** 682–93
Luther A 1976 *Phys. Rev.* B **14** 2153–9
Minnhagen P, Rosengren A and Grinstein G 1978 *Phys. Rev.* B **18** 1356–70
Ohta T and Kawasaki K 1978 *Progr. Theor. Phys.* **60** 365–79
Saito Y and Müller-Krumbhaar H 1981 *Phys. Rev.* B **23** 308–15
Schotte K D 1970 *Z. Phys.* **230** 99–107
Schotte K D and Truong T T 1980 *Z. Phys.* B **37** 193–202
Schulz H 1977 *Z. Phys.* B **26** 377–88
Solyom J 1979 *Adv. Phys.* **28** 201–303
Zittartz J 1976 *Z. Phys.* B **23** 55–62