Properties of an Exact Crystalline Many-Body Ground State

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A new quantum many-body Hamiltonian is introduced, for which the exact ground state is a Jastrow-type product. This Hamiltonian is interpreted as a one-component $|x|$-potential Coulomb system in free boundary conditions, and by explicit calculation it is shown that the ground state is crystalline. The general n-body density matrix is calculated, and is related to the n-body density matrix calculated in periodic boundary conditions.

1. INTRODUCTION

1.1. Objective of the Paper

The Wigner transition refers to the freezing of the quantum mechanical one-component plasma (positive ions immersed in an inert neutralizing background). In two and three dimensions ($-\log r$ and $1/r$ potential, respectively), at large values of the dimensionless coupling characterizing the ratio of the potential to the kinetic energy, the ions become localized around the classical equilibrium points which form the Wigner lattice.[1] However, in one dimension ($|x|$ potential) the ground state is always crystalline.[2]

Although there is no phase transition in the one-dimensional system, it does have the noteworthy feature of allowing an exact evaluation of the ground-state wave function when an additional certain short-range pair potential is imposed and the particles are spinless fermions.[3] Our objective

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in this paper is to explore further this exact crystalline state by providing the analogous exact solution for the system in free boundary conditions (the calculation of ref. 3 was done in periodic boundary conditions), and relating the density matrices in each case.

Regarding this latter point, from the work of Choquard and Kunz[4, 5] on the classical one-dimensional one-component plasma we know that the distribution functions for a crystalline state in free (f) and periodic (p) boundary conditions are related by averaging the former over a period of oscillation (a say). Thus,

$$\rho_n^{(p)}(x_1,...,x_n) = \frac{1}{a} \int_0^a d\xi \, \rho_n^{(f)}(x_1 + \xi,..., x_n + \xi) \tag{1.1}$$

For the quantum system, we will show that (1.1) remains valid, being a special case of an analogous relationship between the density matrices of each system,

$$\rho_n^{(p)}(x_1,..., x_n \,|\, x_1',..., x_n')$$
$$= \frac{1}{a} \int_0^a d\xi \, \rho_n^{(f)}(x_1 + \xi,..., x_n + \xi \,|\, x_1' + \xi,..., x_n' + \xi) \tag{1.2}$$

1.2. Further Implications

We will evaluate the general n-body density matrix for the state

$$\psi_0(x_1,..., x_N) = \frac{1}{C_N} \exp\left(-\frac{a}{2} \sum_{j=1}^N x_j^2 \right) \prod_{1 \le j < k \le N} \sinh[\alpha(x_k - x_j)] \tag{1.3}$$

It is interesting to note that there are other physical problems in which the probability density function (1.3) occurs and for which the calculation of the density matrix (in the special case of it being a distribution function) is relevant.

With $a = 1/Dt$ and $\alpha = d/Dt$ we have previously observed[6] that (1.3) satisfies the n-dimensional heat equation

$$\sum_{j=1}^N \frac{\partial^2}{\partial x_j^2} \psi_0 = \frac{2}{D} \frac{\partial}{\partial t} \psi_0 \tag{1.4}$$

subject to the initial condition

$$\psi_0(x_1,..., x_N) \sim \prod_{j=1}^N \delta(x_j - d(j - [(N+1)/2])) \qquad \text{as} \quad t \to 0 \tag{1.5}$$

and boundary condition

$$\psi_0 = 0 \qquad \text{whenever} \quad x_j = x_{j'} \quad (j \neq j') \qquad (1.6)$$

It thus follows that ψ_0 is the probability density function for the event that N random walkers, initially equally spaced (spacing d) symmetrically about the origin, will arrive at the points $x_1,..., x_N$ without their paths crossing [this interpretation of (1.3) was first given in ref. 7]. With this interpretation, the n-particle distribution function for the state ψ_0 is proportional to the conditional probability that n of the N random walkers will arrive at the points $x_1,..., x_n$ in time t, given that after time $2t$ each walker has returned to its initial position.

We have also noted[6] that $|\psi_0|^2$ is proportional to the Boltzmann factor of a classical log-potential Coulomb gas system, consisting of one species of mobile charge on a line with periodic boundary conditions, period π/α, perpendicular to the line. This follows since

$$\phi(x) = -\log |\sinh \alpha x| \qquad (1.7)$$

is the pair potential between mobile particles in such a system, while the potential energy of the particle–background interaction, for a suitable value of α, gives the Gaussian in (1.3).

A further interpretation of (1.3) follows from the form given in (3.4) below:

$$\psi_0 = \frac{1}{\hat{C}_n} \prod_{k=1}^{N} e^{-\mu^2 \log^2 \lambda_k} \prod_{1 \leqslant j < k \leqslant N} (\lambda_k - \lambda_j), \qquad \lambda_j \geqslant 0 \qquad (1.8)$$

which results from a change of variables in (1.3). We see that $|\psi_0|^2$ can be interpreted as the eigenvalue density function of a generalized ensemble of Gaussian Hermitian matrices.[8]

2. THE HAMILTONIAN AND ITS EXACT WAVE FUNCTION

2.1. Solution of the Schrödinger Equation

We have the following result:

Theorem 1. Let

$$H = -\sum_{p=1}^{N} \frac{\partial^2}{\partial x_p^2} + a^2 \sum_{p=1}^{N} x_p^2 - 2\alpha ab \sum_{1 \leqslant j < k \leqslant N} (x_k - x_j) \coth \alpha(x_k - x_j)$$

$$+ 2\alpha^2 b(b-1) \sum_{1 \leqslant j < k \leqslant N} \frac{1}{\sinh^2 \alpha(x_k - x_j)} \qquad (2.1)$$

and

$$\psi_{0,b} = \frac{1}{C_{N,b}} \exp\left(-\frac{a}{2}\sum_{j=1}^{N} x_j^2\right)\left(\prod_{1 \le j < k \le N} \sinh[\alpha(x_k - x_j)]\right)^b \quad (2.2)$$

where the ordering $x_1 < x_2 < \cdots < x_N$ is assumed (for other orderings $\psi_{0,b}$ may change sign depending on the particle type, boson or fermion). Then $\psi_{0,b}$ satisfies the Schrödinger equation

$$H\psi_{0,b} = E_0\psi_{0,b} \quad (2.3)$$

with

$$E_0 = -\tfrac{1}{3}\alpha^2 b^2 N(N-1)(N-2) + aN - \alpha^2 b^2 N(N-1) \quad (2.4)$$

Remarks. (i) The same Hamiltonian in which the one-body harmonic well is replaced by a pairwise harmonic attraction between particles has been considered by Calegero.[9]

(ii) Reference 10 claims to provide an exhaustive list of Hamiltonians with one- and two-body potentials which have wave functions of the same structure as (2.2). However, (2.1) does not appear on the list.

Theorem 1 can be verified by a direct computation of the r.h.s. of (2.3). The apparent three-body terms which result reduce to a constant because of the identity

$$\coth a \coth b + \coth a \coth c + \coth b \coth c = -1 \quad (2.5a)$$

for

$$a + b + c = 0 \quad (2.5b)$$

2.2. Plasma Interpretation

In this subsection we will show that the long-range (lr) portion of the potential energy in (2.1) has a Coulombic origin. For this purpose we decompose the potential energy V as

$$V = V_{lr} + V_{sr} \quad (2.6a)$$

where

$$V_{lr} = a^2 \sum_{p=1}^{N} x_p^2 - 2\alpha ab \sum_{1 \le j < k \le N} |x_k - x_j| \quad (2.6b)$$

and

$$V_{sr} = -4\alpha ab \sum_{1 \leqslant j < k \leqslant N} \frac{|x_k - x_j|}{e^{2\alpha |x_k - x_j|} - 1}$$

$$+ 2\alpha^2 b(b-1) \sum_{1 \leqslant j < k \leqslant N} \frac{1}{\sinh^2 \alpha(x_k - x_j)} \qquad (2.6c)$$

To relate V_{lr} to the potential energy of a Coulomb system, recall that the one-dimensional Coulomb potential between a charge of strength Q at x and a charge of strength Q' at x' is

$$\phi(|x - x'|) = -QQ' |x - x'| \qquad (2.7)$$

One-component Coulomb systems require a neutralizing background for thermodynamic stability. Thus suppose that in the interval $[-L/2, L/2]$ there is a background of charge density $-QN/L := -Q\eta$. A short calculation gives that the electrostatic energy of the particle–particle, particle–background, and background–background interactions is

$$V_{lr} = -Q^2 \sum_{1 \leqslant j < k \leqslant N} |x_k - x_j| + Q^2\eta \sum_{j=1}^{N} x_j^2 + \tfrac{1}{12}Q^2 N^2 L \qquad (2.8)$$

The derivation of (2.8) assumes that $x_j \in [-L/2, L/2]$. When the particles lie outside this interval the one-body potential is linear rather than quadratic in x_j. However, we must retain the quadratic potential for all $x_j \in \mathbb{R}$ in the quantum Hamiltonian. This approximation should not affect the value of bulk quantities in the thermodynamic limit.

By comparing (2.6b) and (2.8) we see that if

$$2\alpha ab = Q^2 \qquad \text{and} \qquad a^2 = \eta Q^2 \qquad (2.9)$$

then

$$V_{lr} = V_e - \tfrac{1}{12}Q^2 N^2 L \qquad (2.10)$$

Hence from (2.6a) and (2.4) the ground-state energy E_0' of the Hamiltonian with potential energy

$$V_e + V_{sr} \qquad (2.11)$$

is given by

$$E_0' = N\left(\frac{Q^2}{12\eta} + Q\sqrt{\eta}\right) \qquad (2.12)$$

Note that this is extensive. It agrees with the analogous result for the system in periodic boundary conditions [ref. 3, Eq. (21) with the identifications $\gamma = 4\pi^2/Q^2$ and $d = \eta$].

3. THE EXACT n-BODY DENSITY MATRIX

3.1. Wave Function in Terms of Stieltjes–Wigert Polynomials

For the remainder of the paper we will consider the case $b = 1$, when $\psi_{0,b}$ reduces to ψ_0 as given by (1.3). From (2.9) and (2.6b) we see that this does not affect the generality of the Coulomb portion of the Hamiltonian (2.1). The only effect is on the short-range part (2.6c)—the $1/\sinh^2 \alpha r$ pair potential is not present in this case.

The significance of the choice $b = 1$ is that the corresponding wave function (1.3) can be expressed as a Slater determinant of orthogonal functions, which allows an explicit calculation of the n-body density matrix. The orthogonal functions are formed by the product of the log-normal distribution and the Stieltjes–Wigert polynomials.

The Stieltjes–Wigert polynomials, to be denoted $S_l(y; q)$, are polynomials of order l in a variable y, say, and also depend on a parameter q. Explicitly[11]

$$S_l(y; q) = \frac{(-1)^l q^{l/2 + 1/4}}{\{(1-q)(1-q^2) \cdots (1-q^l)\}^{1/2}} \sum_{v=0}^{l} \begin{bmatrix} l \\ v \end{bmatrix}_q q^{v^2}(-q^{1/2}y)^v \quad (3.1)$$

where

$$\begin{bmatrix} l \\ v \end{bmatrix}_q$$

denotes the Gaussian polynomial (see, e.g., ref. 12). The Stieltjes–Wigert polynomials have the orthonormality property

$$\int_0^\infty w(y; q)\, s_m(y; q)\, s_n(y; q)\, dy = \delta_{m,n} \quad (3.2a)$$

where

$$w(y; q) = \pi^{-1/2} k e^{-k^2 \log^2 y} \qquad \text{and} \qquad q = e^{-1/(2k^2)} \quad (3.2b)$$

To rewrite the wave function (1.3) we make the change of variables

$$y_j = e^{2\alpha(x_j + \alpha N/a)} \quad (3.3)$$

After adjusting the normalization C_N this gives

$$\psi_0 = \frac{1}{C_N} \prod_{k=1}^{N} [2\alpha y_k w(y_k; e^{-2\alpha^2/a})]^{1/2} \prod_{1 \leqslant j < k \leqslant N} (y_k - y_j) \qquad (3.4)$$

Now, from the van der Monde determinant expansion,

$$\prod_{1 \leqslant j < k \leqslant N} (y_k - y_j) = \det[y_j^{k-1}]_{j,k=1,\dots,N} \qquad (3.5)$$

By adding an appropriate multiple of column $1, 2,\dots, k-1$ to column k for each column $N, N-1,\dots, 1$ successively, we see that up to a multiplicative constant this can be rewritten as

$$\det[S_{k-1}(y_j; e^{-2\alpha^2/a})]_{j,k=1,\dots,N} \qquad (3.6)$$

The normalized wave function, in terms of the variable (3.3), therefore has the Slater determinant form

$$\psi_0 = \left(\frac{1}{N!}\right)^{1/2} \prod_{k=1}^{N} [2\alpha y_k w(y_k; e^{-2\alpha^2/a})]^{1/2}$$

$$\times \det[S_{k-1}(y_j; e^{-2\alpha^2/a})]_{j,k=1,\dots,N} \qquad (3.7)$$

3.2. A Determinant Formula for the Density Matrix

The n-body density matrix is defined as

$$\rho(x_1,\dots, x_n \,|\, x_1',\dots, x_n')$$

$$= \frac{N!}{(N-n)!} \left(\prod_{l=n+1}^{N} \int_{-\infty}^{\infty} dx_l\, \delta_{x_l,x_l'} \right) \psi_0(x_1,\dots, x_N)\, \psi_0(x_1',\dots, x_N') \qquad (3.8)$$

Making the change of variables (3.3) gives

$$\rho(y_1,\dots, y_n \,|\, y_1',\dots, y_n')$$

$$= (2\alpha)^n \frac{1}{(N-n)!} \prod_{j=1}^{n} [y_j y_j' w(y_j; e^{-2\alpha^2/a})\, w(y_j'; e^{-2\alpha^2/a})]^{1/2}$$

$$\times \left(\prod_{l=n+1}^{N} \int_{0}^{\infty} dy_l\, w(y_l)\, \delta_{y_l, y_l'} \right) \det[S_{k-1}(y_j, e^{-2\alpha^2/a})]_{j,k=1,\dots,N}$$

$$\times \det[S_{k-1}(y_j', e^{-2\alpha^2/a})]_{j,k=1,\dots,N} \qquad (3.9)$$

Due to the orthonormality property (3.2a), the multiple integral in (3.9) can be evaluated to give

$$
\rho(y_1,\dots,y_n \,|\, y_1',\dots,y_n')
$$

$$
= (2\alpha)^n \prod_{j=1}^{n} [y_j\, y_j'\, w(y_j; e^{-2\alpha^2/a})\, w(y_j'; e^{-2\alpha^2/a})]^{1/2}
$$

$$
\times \det\left[\sum_{p=1}^{N} S_{p-1}(y_j; e^{-2\alpha^2/a})\, S_{p-1}(y_k'; e^{-2\alpha^2/a})\right]_{j,k=1,\dots,n}
\tag{3.10}
$$

Furthermore, the sum in (3.10) can be evaluated by using the Christoffel–Darboux formula (see, e.g., ref. 11):

$$
\sum_{p=1}^{N} S_{p-1}(y; q)\, S_{p-1}(y'; q)
$$

$$
= \frac{C_{N-1}}{C_N}\left(\frac{S_N(y; q)\, S_{N-1}(y'; q) - S_{N-1}(y; q)\, S_N(y'; q)}{y - y'}\right)
\tag{3.11a}
$$

where C_N is the coefficient of y^N in $S_N(y; q)$, which from (3.1) is given by

$$
C_N = \frac{q^{N^2 + N + 1/4}}{\{(1-q)\cdots(1-q^N)\}^{1/2}}
\tag{3.11b}
$$

3.3. The Thermodynamic Limit

With the notation

$$
q = e^{-2\alpha^2/a}, \qquad y = e^{2\alpha(x + \alpha N/a)}; \qquad y' = e^{2\alpha(x' + \alpha N/a)}
\tag{3.12}
$$

from (3.3), (3.10), and (3.11) we see that in the thermodynamic limit the density matrix is given by

$$
\rho(x_1,\dots,x_n \,|\, x_1',\dots,x_n') = \det[L(x_j, x_k')]_{j,k=1,\dots,n}
\tag{3.13a}
$$

where

$$
L(x, x') := (2\alpha)\lim_{N \to \infty}\left\{[yy'w(y; q)\, w(y'; q)]^{1/2}\right.
$$

$$
\left.\times \frac{C_{N-1}}{C_N}\left(\frac{S_N(y; q)\, S_{N-1}(y'; q) - S_{N-1}(y; q)\, S_N(y'; q)}{y - y'}\right)\right\}
\tag{3.13b}
$$

To evaluate the limit in (3.13b), we note from (3.11b) and the definition of the Gaussian polynomial that

$$\frac{C_{N-1}}{C_N} \sim q^{-2N} \quad \text{and} \quad \begin{bmatrix} N-1 \\ v \end{bmatrix}_q \sim (1-q^{N-v}) \begin{bmatrix} N \\ v \end{bmatrix}_q \qquad (3.14)$$

so from (3.1)

$$\frac{C_{N-1}}{C_N} S_N(y; q) S_{N-1}(y'; q)$$

$$\sim -\frac{q^{-N}}{(1-q) \cdots (1-q^N)} \left(\sum_{v=0}^{N} \begin{bmatrix} N \\ v \end{bmatrix}_q q^{v^2 + v/2}(-y)^v \right)$$

$$\times \left(\sum_{v=0}^{N} \begin{bmatrix} N \\ v \end{bmatrix}_q (1-q^{N-v}) q^{v^2 + v/2}(-y')^v \right) \qquad (3.15)$$

Completing the square in v gives exponents

$$(v - N/2 + 1/4 - ax/2\alpha)^2 \quad \text{and} \quad (v - N/2 - 1/4 - ax/2\alpha)^2 \quad (3.16)$$

for the two terms in (3.15). The next step is to change the summation variable

$$v - [N/2] \mapsto v \qquad (3.17)$$

where $[\cdot]$ denotes the integer part, and to note that

$$\begin{bmatrix} N \\ v + [N/2] \end{bmatrix}_q \sim \frac{1}{(q;q)_\infty} \qquad (3.18a)$$

where

$$(q; q)_\infty := \prod_{l=1}^{\infty} (1 - q^l) \qquad (3.18b)$$

The change of summation variable (3.17) implies a different limit depending on the parity of N (even or odd). This is a signature of a crystalline state [for N odd (even) $x = 0$ corresponds to a maximum (minimum) of the particle density] and is a feature of the exact solution of the classical one-dimensional one-component plasma in free boundary conditions.[5]

From the above working we find

$$L(x, x') = \left(\frac{a}{\pi} \right)^{1/2} \frac{q^{-1/8}}{(q;q)_\infty^3} \left(\frac{l(x; q) l(-x'; q) - l(x'; q) l(-x; q)}{\sinh \alpha(x - x')} \right) \qquad (3.19a)$$

where

$$l(x; q) := e^{\chi \alpha x/2} \sum_{v = -\infty}^{\infty} (-1)^v q^{(v + 1/4 - ax/2\alpha)^2} \tag{3.19b}$$

and

$$\chi := \begin{cases} 1 & N \text{ even} \\ -1 & N \text{ odd} \end{cases} \tag{3.19c}$$

This result can be transformed to involve the parameter

$$q' := e^{-\pi^2 a/2\alpha^2} \tag{3.20}$$

instead of q (the periodic boundary conditions results of ref. 3 involve q'). Using the theory of the Jacobian theta functions,[13] we obtain

$$L(x, x') = \frac{\alpha}{\pi} \frac{1}{\theta'_1(0; (q')^2)} \left(\frac{\hat{l}(x; q')(\hat{l}(-x'; q') - \hat{l}(x'; q') \hat{l}(-x; q'))}{\sinh \alpha(x - x')} \right) \tag{3.21a}$$

where

$$\hat{l}(x; q') := e^{-\chi \alpha x/2} \theta_1 \left(\pi \left(\frac{1}{4} + \frac{ax}{2\alpha} \right); q' \right) \tag{3.21b}$$

The above results relate to the bulk properties of the system. It is also possible to obtain explicit results for the density matrix in the edge region. The existence of an edge near $x = \pm N/2\eta = \pm N\alpha/a$ is predicted from the plasma interpretation of Section 2.2: the positively charged particles prefer the interval $[-N/2\eta, N/2\eta]$ due to the neutralizing background in this interval.

To study the system about one of these edges, say $x = -N\alpha/a$, we introduce the coordinates X, X':

$$X = x + \alpha N/a, \qquad X' = x' + \alpha N/a \tag{3.22}$$

In terms of X and X', for the limit in (3.14) we find

$$\begin{aligned} L(X, X') = \left(\frac{a}{\pi} \right)^{1/2} \frac{1}{(q; q)_\infty} \frac{e^{-a(X^2 + (X')^2)/2}}{\sinh \alpha(X - X')} \\ \times \{ F(-q^{1/2} e^{2\alpha X}; q) F(-q^{-1/2} e^{2\alpha X'}; q) \\ - F(-q^{1/2} e^{2\alpha X'}; q) F(-q^{-1/2} e^{2\alpha X}; q) \} \end{aligned} \tag{3.23a}$$

where

$$F(z; q) = \sum_{v=0}^{\infty} \frac{q^{v^2} z^v}{(1-q) \cdots (1-q^v)} \qquad (3.23b)$$

[The function $F(z; q)$ occurs in the theory of partitions.[12]] It is easy to check that (3.21) for N even (odd) is reclaimed by making the replacements $X \mapsto M + x$ $(M - 1/2 + x)$, $X' \mapsto M + x'$ $(M - 1/2 + x')$, $M \in \mathbb{Z}^+$, and taking the limit $M \to \infty$.

4. FEATURES OF THE CRYSTALLINE STATE

4.1. The Particle Density

The particle density $\rho(x)$ is the diagonal element of the one-body density matrix:

$$\rho(x) = \rho(x \,|\, x) \qquad (4.1)$$

Thus, from (3.13) and (3.21), in the bulk of the system we have

$$\rho(x) = \frac{1}{\pi \theta_1'(0; (q')^2)} \left(\frac{\partial}{\partial x} \hat{l}(x; q') \, \hat{l}(-x; q') - \hat{l}(x; q') \frac{\partial}{\partial x} \hat{l}(-x, q') \right) \qquad (4.2)$$

which is a periodic function of period $2\alpha/a$. Numerical plots show that for N odd (even) the density exhibits a maximum (minimum) at $x = 0$.

4.2. Relationship Between the State in Free and Periodic Boundary Conditions

In this subsection, we will verify the sum rule (1.2), which relates the n-particle density matrix obtained using free boundary conditions to the n-particle density matrix in periodic boundary conditions. The density matrix in free boundary conditions is given by (3.21) above, while in periodic boundary conditions, from the results of refs. 3 and 14 we have that

$$\rho(x_1, \ldots, x_n \,|\, x_1', \ldots, x_n')$$

$$= \int_0^1 d\xi \, \det[G(ax/2\alpha + \xi, \, ax'/2\alpha + \xi; \, e^{-\pi^2 a/2\alpha^2})] \qquad (4.3a)$$

where

$$G(X, X'; q) := \frac{a}{2\alpha} \int_0^1 dt \, \frac{\theta_3(\pi X + \pi i \tau t; q) \, \theta_3(\pi X' - \pi i \tau t; q)}{\theta_3(2i\tau t; q^2)} e^{2\pi i t(X - X')} \qquad (4.3b)$$

with

$$q = e^{\pi i \tau} \tag{4.3c}$$

This result applies independent of the limit having been taken with N even or odd.

To verify (1.2), we first note that the value of the right-hand side of (1.2) is independent of the values of χ, (3.19c). This follows from (3.21b) and the fact that

$$\int_0^1 d\xi \, \rho_n^{(f)}(x_1 + \xi, \ldots, x_n + \xi \, | \, x'_1 + \xi, \ldots, x'_n + \xi)$$

$$= \int_0^1 d\xi \, \rho_n^{(f)}(x_1 - \xi, \ldots, x_n - \xi \, | \, x'_1 - \xi, \ldots, x'_n - \xi) \tag{4.4}$$

Comparison of (3.13), (3.21), and (4.3) then shows that a sufficient condition for the validity of (1.2) is

$$G(ax/2\alpha, \, ax'/2\alpha; \, e^{-\pi^2 a/2\alpha^2}) = L(x, x') \tag{4.5}$$

where we can choose either $\chi = 1$ or $\chi = -1$ in (3.21b). Let us now verify this identity.

To do this, we consider the integrand of (4.3b) as the integrand of a contour integral about the closed contour $C_1 + C_2 + C_3 + C_4$, where each C_j $(j = 1, \ldots, 4)$ is a straight line segment in the complex plane. In an obvious notation, these segments are $[0, 1]$, $[1, 1 - 1/\tau]$, $[1 - 1/\tau, -1/\tau]$, and $[-1/\tau, 0]$, respectively. Let us denote the value of the integral along each of these contours by $I_1, \ldots, I_4$, respectively. Since the integrand is periodic of period 1, I_2 and I_4 cancel. Furthermore, since

$$\theta_3(z + \pi\tau; q) = q^{-1} e^{-2\pi i z} \theta_1(z; q) \tag{4.6}$$

it follows that

$$I_1 + I_3 = (1 - e^{-2\pi i (X - X')/\tau}) \, G(X, X'; q) \tag{4.7}$$

On the other hand, we can calculate the contour integral using the residue theorem. Inside the closed contour there are poles at

$$t = \frac{1}{2} - \frac{1}{4\tau} \quad \text{and} \quad t = \frac{1}{2} - \frac{3}{4\tau} \tag{4.8}$$

A straightforward calculation gives that the sum of the residues is

$$-\frac{1}{2\pi\tau}\frac{1}{\theta_1'(0;q^2)}\left(e^{-\pi i(X-X')/\tau}\theta_1\left(\pi X+\frac{\pi}{4};q\right)\theta_1\left(\pi X'-\frac{\pi}{4};q\right)\right.$$

$$\left.-e^{-3\pi i(X-X')/\tau}\theta_1\left(\pi X-\frac{\pi}{4};q\right)\theta_1\left(\pi X'+\frac{\pi}{4};q\right)\right) \tag{4.9}$$

The residue theorem then gives that the right-hand side of (4.7) is equal to $2\pi i$ times (4.9). This gives a formula for $G(X, X'; q)$ equivalent to (4.5) (with $\chi = -1$), as required.

4.3. Perfect Screening and Second Moment Sum Rules

The averaged truncated two-particle distribution function

$$\bar{\rho}^T(\alpha) := \eta \int_0^{1/\eta} \rho^T(s+x, s)\, ds \tag{4.10}$$

$[\eta := a/2\alpha$; recall (2.9)] satisfies a perfect screening and second moment sum rule [(4.18) and (4.19) below], which in turn imply a special small-k behavior of the structure factor

$$S(k) := 1 + \frac{1}{\eta}\int_{-\infty}^{\infty} e^{ikx}\bar{\rho}^T(x)\, dx \tag{4.11}$$

[(4.20) below].

To understand the physical origin of this latter result, we recall that for one-component plasma systems, quantum or classical, consisting of particles of charge Q and mass m at number density η, the collective excitations are plasma waves with angular frequency (see, e.g., ref. 15)

$$\omega = \left(\frac{c_d Q^2 \eta}{m}\right)^{1/2} \tag{4.12}$$

Here c_d is the dimensionality-dependent constant in Poisson's equation for the potential $\phi(x)$:

$$\nabla^2\phi(x) = -c_d\delta(x) \tag{4.13}$$

In particular, from (2.7), in one dimension

$$c_d = 2 \tag{4.14}$$

For the quantum mechanical one-component plasma, the energy Δ between

fundamental modes of the plasma waves, and in particular between the ground state and the lowest energy excitation, is therefore given by

$$\Delta = \hbar\omega \tag{4.15}$$

On the other hand, this energy gap is given in terms of the structure factor by the Bijl–Feynman formula (see, e.g., ref. 16):

$$\Delta(k) \sim \frac{(\hbar k)^2/2m}{S(k)} \qquad \text{as} \quad k \to 0 \tag{4.16}$$

Below we use the exact result

$$\rho^T(x_1, x_2) = -|G(\eta x_1, \eta x_2; e^{-\pi a/2\alpha^2})|^2 \tag{4.17}$$

proved in the previous subsection to verify the perfect screening and second moment sum rules:

$$\int_{-\infty}^{\infty} \rho^T(x)\, dx = -\eta \tag{4.18}$$

and

$$\int_{-\infty}^{\infty} x^2 \rho^T(x)\, dx = -\frac{1}{2\alpha} \tag{4.19}$$

By expanding the complex exponential in (4.11) we see from (4.18) and (4.19) that

$$S(k) \sim -\frac{k^2}{4\eta\alpha} = -\frac{k^2}{(\eta Q^2)^{1/2}} \tag{4.20}$$

where to obtain the equality we have used (2.9) with $b = 1$. Since in the original Hamiltonian (2.1) the units are such that $\hbar^2/2m = 1$, we see from the Bijl–Feynman formula (4.16) that (4.20) is precisely the behavior required to reproduce (4.15) [ω in the latter formula is given by (4.12) with c_d given by (4.14)].

Let us now present the derivation of the sum rule (4.19). The derivation of (4.18) is less complicated and will not be given. In (4.17) G is given by (4.3b), which allows us to write

$$x^2 \rho^T(x+s, s) = \left(\frac{1}{2\pi}\right)^2 \left| \int_0^1 \left(\frac{\partial}{\partial t} e^{2\pi i \eta x}\right) \right.$$
$$\left. \times \frac{\theta_3(\pi\eta(x+s) + \pi i \tau t; q)\, \theta_3(\pi\eta s - \pi i \tau t; q)}{\theta_3(2\pi i \tau t; q^2)}\, dt \right|^2 \tag{4.21a}$$

where

$$q := e^{\pi i \tau} = e^{-\pi^2 a/2\alpha^2} \tag{4.21b}$$

An integration by parts in (4.21a) gives

$$x^2 \rho^T(x+s, s) = \left(\frac{1}{2\pi}\right)^2 \left| \int_0^1 e^{2\pi i \eta x} \frac{\partial}{\partial t} \right.$$

$$\left. \times \left(\frac{\theta_3(\pi\eta(x+s) + \pi i \tau t; q)\, \theta_3(\pi\eta s - \pi i \tau t; q)}{\theta_3(2\pi i \tau t; q^2)}\right) dt \right|^2 \tag{4.21c}$$

With (4.21c), we see from (4.10) and (4.17) that (4.19) consists of four integrations. We interchange the order of these integrations so that the integration over x is being performed first. Since

$$\int_{-\infty}^{\infty} e^{2\pi i \eta x(t - t')} \theta_3(\pi\eta(s+x) + \pi i \tau t; q)\, \theta_3(\pi\eta(s+x) - \pi i \tau t'; q)\, dx$$

$$= \frac{1}{\eta} \delta(t - t')\, \theta_3(\pi i \tau(t - t'); q^2) \tag{4.22}$$

we have

$$\int_{-\infty}^{\infty} x^2 \bar{\rho}^T(x)\, dx = \left(\frac{1}{2\pi}\right)^2 \int_0^{1/\eta} ds \int_0^1 dt \int_0^1 dt'\, \delta(t - t')$$

$$\times \left[\frac{\partial}{\partial t} \frac{\theta_3(\pi\eta s - \pi i \tau t; q)}{\theta_3(2\pi i \tau t; q^2)}\right.$$

$$\left. \times \left(\frac{\partial}{\partial t'} \frac{\theta_3(\pi\eta s + \pi i \tau t'; q)\, \theta_3(\pi i \tau(t + t'); q^2)}{\theta_3(2\pi i \tau t'; q^2)}\right)\right] \tag{4.23}$$

Integration over s and use of the Dirac delta function in (4.23) then gives, after some minor manipulation,

$$\int_{-\infty}^{\infty} x^2 \rho^T(x)\, dx = \left(\frac{1}{2\pi}\right)^2 \frac{1}{2\eta} \int_0^1 \frac{\partial^2}{\partial t^2} \log \theta_3(2\pi i \tau t; q^2)\, dt \tag{4.24}$$

The desired formula (4.19) now follows by evaluating (4.24) according to the fundamental theorem of calculus, and using the functional equation (4.6) to evaluate the resulting expression.

ACKNOWLEDGMENT

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