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The Two-Dimensional One-Component Plasma in a Doubly Periodic Background: Exact Results

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We revisit the equilibrium classical statistical mechanics of the two-dimensional one-component plasma, for the special value $\Gamma = 2$ of the coupling constant. Using a new method, we find that the model is solvable (the n-body densities can be explicitly computed) for a larger class of inhomogeneous backgrounds. In particular, we can deal with a doubly periodic background; this is a classical model for a crystal made of fixed ions and mobile electrons. At $\Gamma = 2$, this system is conducting: the correlations have a fast decay, and the Stillinger–Lovett screening sum rule is obeyed.

KEY WORDS: One-component inhomogeneous plasma; doubly periodic background; conducting phase.

1. INTRODUCTION

In statistical mechanics, it is obviously of interest to have exactly solvable models for Coulomb systems (plasmas, electrolytes, metals, etc.). The simplest model of a Coulomb system is the one-component plasma (jellium): identical charged particles move in a rigid charged background, which ensures overall neutrality. In two dimensions, the Coulomb potential between two particles of charge e at a distance r from one another is $-e^2 \ln(r/L)$, where L is an arbitrary length scale, and the dimensionless coupling constant is $\Gamma = \beta e^2$, where β is the inverse temperature; for the special value $\Gamma = 2$, it has been previously found that the equilibrium

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classical statistical mechanics of the two-dimensional one-component plasma can be worked out exactly for several kinds of background charge distributions: one is able to obtain the n-particle densities. Besides the simplest case of a uniform background,[1,2] essentially one could deal with a background charge density depending on one space coordinate[3]; this covers a variety of charged interfaces (electrical double layers) of interest to electrochemists.

This previous work left unsolved the important case of a doubly periodic background. In the present paper, we solve this case, using a more general new method; a preliminary account has been given elsewhere by two of us.[4] Thus, we have an explicit solution for a model which can be understood as made of mobile (classical) "electrons" interacting between themselves and with a lattice of extended fixed "ions"; this one-component plasma in a periodic background can also be regarded as a two-component plasma in which the particles of one species have been fixed on a lattice. Like the symmetric two-component plasma, the present model is expected to undergo a Kosterlitz–Thouless phase transition between a low-temperature dielectric phase and a high-temperature conducting phase, and this transition is actually seen in computer simulations.[5,6] Here, we show that, in our system, criteria that characterize a conductor are satisfied: the correlations have a fast decay at large separations, and the Stillinger–Lovett sum rule[7] is obeyed. According to these criteria, at $\Gamma=2$, the system is in its conducting phase

The paper is organized as follows. In Section 2, the general method is reviewed. In Section 3, it is shown that this method provides a simpler approach to the known case where the background density is inhomogeneous in one direction only. The doubly periodic background is discussed in Section 4: we compute the n-particle densities and discuss sum rules.

2. METHOD

2.1. n-Particle Densities

We start with N particles of charge $-e$ in some background. The position of the ith particle is $\mathbf{r}_i=(x_i, y_i)$; we also use the complex number $z_i=x_i+iy_i$. The Hamiltonian is

$$H=e^2\sum_{i=1}^{N} V(\mathbf{r}_i)-e^2\sum_{1\leqslant i<j\leqslant N}\ln(|z_i-z_j|/L) \tag{2.1}$$

where e^2V is the background–particle interaction, and therefore, for an inverse temperature β such that $\Gamma = \beta e^2 = 2$, the Boltzmann factor is

$$\exp(-\beta H) = C\,|\det\{\exp[-V(\mathbf{r}_i)]\,z_i^{j-1}\}_{i,j=1,\dots,N}|^2 \tag{2.2}$$

where C is a constant.

In the simple case of a background potential of circular symmetry, $V(\mathbf{r}) = V(r)$, the functions $\exp[-V(\mathbf{r})]\,z^{j-1}$ are mutually orthogonal, and (2.2) has the same form as some squared wave function of a system of independent fermions; the determinant in (2.2) is just a Slater determinant, and to compute the n-body densities is a standard problem. All the previously solved cases could be obtained by starting with a circular geometry and taking a suitable limit.

In the present paper, we want to consider more general forms of the background potential, and the functions $\exp[-V(\mathbf{r})]\,z^{j-1}$ are not necessarily mutually orthogonal. However, we can choose an orthogonal basis $\Psi_j(\mathbf{r})$ for the space of these functions, and rewrite (2.2) as

$$\exp(-\beta H) = C\,|\det\{\Psi_j(\mathbf{r}_i)\}_{i,j=1,\dots,N}|^2 \tag{2.3}$$

since the new determinant is proportional to the former one. It is then easy to show that the n-particle truncated densities can be expressed in terms of the projector

$$\langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle = \sum_j \frac{\Psi_j(\mathbf{r}_1)\,\Psi_j^*(\mathbf{r}_2)}{\int d\mathbf{r}\,|\Psi_j(\mathbf{r})|^2} \tag{2.4}$$

as

$$\begin{aligned}
\rho(\mathbf{r}) &= \langle \mathbf{r} | P | \mathbf{r} \rangle \\
\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) &= -|\langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle|^2 \\
\rho^{(n)}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n) &= (-)^{n+1} \sum_{(i_1 i_2 \cdots i_n)} \langle \mathbf{r}_{i_1} | P | \mathbf{r}_{i_2} \rangle \cdots \langle \mathbf{r}_{i_n} | P | \mathbf{r}_{i_1} \rangle
\end{aligned} \tag{2.5}$$

where the summation runs over all cycles $(i_1 i_2 \cdots i_n)$ built with $\{1, 2, \dots, n\}$. In the thermodynamic limit, the functions $\exp[-V(\mathbf{r})]\,z^{j-1}$ span the subspace of Hilbert space defined by the entire functions of $z = x + iy$ times $\exp[-V(\mathbf{r})]$, and P becomes the projector on that subspace (of course, this is an intrinsic definition of P, independent of the choice of the orthogonal basis Ψ_j). Thus, the problem of obtaining the n-particle densities is reduced to computing the projector P.

In the simplest case of a uniform background density ρ_0, the background potential $V(\mathbf{r})$ can be chosen as $\frac{1}{2}\pi\rho_0 r^2$ (plus some irrelevant constant), $\Psi_j = \exp(-V) z^{j-1}$, and

$$\begin{aligned} \langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle &= \rho_0 \exp[-\tfrac{1}{2}\pi\rho_0(|z_1|^2 + |z_2|^2 - 2z_1 z_2^*)] \\ \rho(\mathbf{r}) &= \rho_0 \\ \rho_T^{(2)}(\mathbf{r}_1, \mathbf{r}_2) &= -\rho_0^2 \exp(-\pi\rho_0 |\mathbf{r}_1 - \mathbf{r}_2|^2) \end{aligned} \tag{2.6}$$

In the general case, the background density $\rho_B(\mathbf{r})$ can be considered as being the sum of a uniform contribution ρ_0 plus a nonuniform modulation $\tilde{\rho}(\mathbf{r})$. Correspondingly, the background potential $V(\mathbf{r})$ can be chosen of the form $V_0(\mathbf{r}) + \phi(\mathbf{r})$, where $V_0(\mathbf{r}) = \frac{1}{2}\pi\rho_0 r^2$ and $\Delta\phi(\mathbf{r}) = 2\pi\tilde{\rho}(\mathbf{r})$. As a first step toward the computation of the projector P on the space of the functions $\exp[-\phi(\mathbf{r}) - V_0(\mathbf{r})] z^j$, $j \in \mathbb{N}$, it will turn out to be convenient to replace the z^j by another basis for the entire functions

$$\varphi_k(z) = \exp\{-\tfrac{1}{2}\pi\rho_0[z - (k/\pi\rho_0)]^2\}, \qquad k \in \mathbb{R}$$

The φ_k are indeed such a basis, since

$$z^n = \pi^{-1/2} 2^{-n} \int_{-\infty}^{\infty} dt\, H_n(t) \exp[-(z-t)^2] \tag{2.7}$$

where the $H_n(t)$ are Hermite polynomials, and (2.7) becomes a superposition of φ_k functions through a rescaling of z and t. The basis $\exp[-V_0(r)]\, z^j$ is then replaced by

$$\begin{aligned} \exp[-V_0(r)]\, \varphi_k(z) &= \exp(-i\pi\rho_0 xy) \exp(-k^2/4\pi\rho_0) \\ &\quad \times \exp\{-\pi\rho_0[x - (k/2\pi\rho_0)]^2 + iky\} \end{aligned} \tag{2.8}$$

Actually, since (2.8) will be used for defining the projector P and thereafter computing the densities (2.5), we can omit in (2.8) the normalization factor $\exp(-k^2/4\pi\rho_0)$ (this leaves the projector unchanged) and the phase factor $\exp(-i\pi\rho_0 xy)$ (this leaves the densities unchanged because of their cyclic structure).

Therefore, an alternative definition of P is to take it as the projector on the space of the functions

$$\psi_k(\mathbf{r}) = \exp[-\phi(\mathbf{r})] \exp\left[-\pi\rho_0\left(x - \frac{k}{2\pi\rho_0}\right)^2 + iky\right] \tag{2.9}$$

For the potentials $\phi(\mathbf{r})$ that will be considered here, strictly speaking the functions (2.9) do not belong to Hilbert space, because $|\exp(iky)|$ does not decrease at infinity. However, these functions do form a basis in the sense of distributions, just like the plane waves in quantum mechanics.

2.2. Arbitrariness in the Choice of $V(\mathbf{r})$

Let us remark that the background potential $V(\mathbf{r})$ is not uniquely determined by the background density $\rho_B(\mathbf{r})$. In the thermodynamic limit, $V(\mathbf{r})$ keeps a memory of the boundary conditions even after these boundaries have receded to infinity. The n-particle densities, however, should depend only on $\rho_B(\mathbf{r})$ for a system with screening properties that prevent the bulk from being affected by infinitely remote charged boundaries. It is satisfactory to check explicitly this independence upon the choice of $V(\mathbf{r})$, to which it should be always possible to add an arbitrary harmonic function. Actually, since the confinement of the particles must be preserved, the total background potential must increase fast enough at infinity, and we shall only consider the addition to $V(\mathbf{r})$ of a harmonic function of the form

$$f(\mathbf{r}) = a_2(x^2 - y^2) + b_2 xy + a_1 x + b_1 y + c$$

with coefficients a_2 and b_2 of sufficiently small absolute value; furthermore, the term $b_2 xy$ can be removed by a rotation of the axes. The potential $f(\mathbf{r})$ can be interpreted as determined by suitable external electrodes.

It is then easy to see that $\varphi_k(z)$ can be chosen again of the form $\exp\{-\alpha[z-(2\alpha)^{-1}(k+\gamma+i\delta)]^2\}$, where α, γ, δ are real constants, and by a suitable choice of these constants, $f(\mathbf{r})$ can be cancelled, except for irrelevant normalization and phase factors. Therefore, the projector P can be left unchanged.

Incidentally, the basis (2.9) can be directly obtained by choosing the potential contribution from the uniform background as $V_0 = \pi\rho_0 x^2$ and taking $\exp(kz)$ as the basis for the entire functions. Such a V_0 will be obtained if we reach the infinite-system limit starting from a strip geometry rather than from a circular one.

2.3. Magnetic Analogy

The arbitrariness in the choice of our background potential $V(\mathbf{r})$ has a quantum mechanical analog: a gauge transformation in a magnetic problem. Let us consider a particle of mass m and charge q moving in the xy plane and subjected to a uniform magnetic field $\mathbf{B}$ parallel to the z axis.[8] The ground state is infinitely degenerate. In the gauge where the vector potential is $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}$, a basis for the ground-state wave functions is $\exp[-(qB/4)r^2]\, z^j$, $j \in \mathbb{N}$; in the gauge where the vector potential is $\mathbf{A} = \mathbf{j}Bx$ ($\mathbf{j}$ is the unit vector along the y axis), a basis for the ground-state wave functions is $\exp\{-\frac{1}{2}qB[x-(k/qB)]^2 + iky\}$, $k \in \mathbb{R}$. Obviously, our change from the basis $\exp[-\frac{1}{2}\pi\rho_0 r^2]\, z^j$ to the basis $\exp\{-\pi\rho_0[x-$

$(k/2\pi\rho_0)]^2 + iky\}$ is exactly of the same form. If a Slater determinant is built with the ground-state wave functions, the corresponding n-body densities must be gauge-independent, just as our n-body densities are independent of our choice of basis.

3. BACKGROUND INHOMOGENEOUS IN ONE DIRECTION

We now revisit the case of a background density depending on one coordinate only[3]: $\rho_B(x)$. The potential ϕ can be chosen as $\phi(x)$, and we have at hand the orthogonal basis: (2.9) is orthogonal because of the plane-wave factor $\exp(iky)$. Adapting (2.4) to the case of a continuous index k, we find

$$\langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle = \exp[-\phi(x_1) - \phi(x_2)] \int_{-\infty}^{\infty} \frac{dk}{2\pi}$$

$$\times \frac{\exp[ik(y_1 - y_2)] \exp\{-\pi\rho_0[(x_1 - k/2\pi\rho_0)^2 + (x_2 - k/2\pi\rho_0)^2]\}}{\int_{-\infty}^{\infty} dx \exp[-2\phi(x) - 2\pi\rho_0(x - k/2\pi\rho_0)^2]} \quad (3.1)$$

Using (3.1) in (2.5), we retrieve at once the results of Ref. 3.

Some special care must be exercised for dealing with the case where the particles are confined to the half-space $x > 0$ by an impenetrable wall at $x = 0$. Then, in (3.1), the range of x must be restricted to $x > 0$, and the range of k must be restricted to $k > 0$. This is shown as follows. Since we have already taken the limit of an infinite system, we shall start[3] with a system in which an impenetrable barrier occupying the region $-l < x < 0$ separates the plasma into two regions $x < -l$ and $x > 0$. The impenetrable wall system will be obtained by taking the limit $l \to \infty$ in such a way that the remote regions $x > 0$ and $x < -l$ no longer see each other. The values $k < 0$ are suppressed in (3.1) because the norm in the denominator has a contribution from the remote region $x < -l$, which becomes infinite for $k < 0$ in the limit $l \to \infty$; on the contrary, this contribution vanishes for $k > 0$ in the limit $l \to \infty$. The independence of the regions $x > 0$ and $x < -l$ is achieved by requiring that each of them should be globally neutral, which will be the case if the background potential is symmetrical with respect to the barrier: $V(x) = \pi\rho_0 x^2 + \phi(x)$ for $x > 0$, $V(x) = +\infty$ for $-l < x < 0$, $V(x) = V(-x - l)$ for $x < -l$. Then, remembering that $\phi(x)$ is defined in *every* region as $V(x) - \pi\rho_0 x^2$, and changing $-x - l$ into x, we can rearrange the denominator of (3.1) as

$$f(k) = \exp(-2kl) \int_0^{\infty} dx \exp\left[-2\phi(x) - 2\pi\rho_0 \left(x + \frac{k}{2\pi\rho_0}\right)^2\right]$$

$$+ \int_0^{\infty} dx \exp\left[-2\phi(x) - 2\pi\rho_0 \left(x - \frac{k}{2\pi\rho_0}\right)^2\right] \quad (3.2)$$

In the limit $l \to \infty$, the first term of $f(k)$ (which is the contribution from the region $x < -l$) diverges if $k < 0$, and vanishes if $k > 0$. As a consequence, (3.1) becomes ($x_1, x_2 > 0$)

$$\langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle = \exp[-\phi(x_1) - \phi(x_2)] \int_0^\infty \frac{dk}{2\pi} \times \frac{\exp[ik(y_1 - y_2)] \exp\{-\pi\rho_0[(x_1 - k/2\pi\rho_0)^2 + (x_2 - k/2\pi\rho_0)^2]\}}{\int_0^\infty dx \exp[-2\phi(x) - 2\pi\rho_0(x - k/2\pi\rho_0)^2]} \tag{3.3}$$

(3.3) is in agreement with the results[9] about a hard wall carrying a surface charge density $e\sigma$, in which case $\phi(x) = 2\pi\sigma x$, $x > 0$; $\phi(x) = 0$, $x < 0$.

4. DOUBLY PERIODIC BACKGROUND

In this section, which is the core of the present paper, we study the case where the background density is doubly periodic. Thus, we consider a doubly periodic background potential modulation $\phi(\mathbf{r})$:

$$\phi(\mathbf{r} + n\mathbf{a} + m\mathbf{b}) = \phi(\mathbf{r}), \qquad n, m \in \mathbb{Z} \tag{4.1}$$

The unit cell is a parallelogram built with the vectors $\mathbf{a}$ and $\mathbf{b}$, of area $ab \sin \varphi$, where φ is the angle between $\mathbf{a}$ and $\mathbf{b}$. The system is neutral, with a particle density ρ_0 equal to the average of the total background density $\rho_0 + (2\pi)^{-1} \Delta\phi(\mathbf{r})$. In order to mimic a simple crystal of extended fixed ions and mobile electrons of opposite charges, we take $\rho_0 = (ab \sin \varphi)^{-1}$, which means there is one particle per unit cell.

4.1. *n*-Particles Densities

Although the functions (2.9) now are not orthogonal, they are a good starting point for computing the projector P. Choosing the y axis along the period vector $\mathbf{b}$, and defining $\zeta \in [0, 1]$ and n integer by $k = 2\pi(\zeta + n)/b$, we can rewrite Ψ_k as

$$\Psi_{\zeta,n}(\mathbf{r}) = \exp[-\phi(\mathbf{r})] \exp\left[-\pi\rho_0\left(x - \frac{\zeta + n}{\rho_0 b}\right)^2 + 2\pi i(\zeta + n)\frac{y}{b}\right] \tag{4.2}$$

As a consequence of the periodicity of ϕ along the y axis,

$$\int_{-\infty}^{\infty} dy\, \Psi^*_{\zeta',n'}(\mathbf{r})\, \Psi_{\zeta,n}(\mathbf{r}) \propto \delta(\zeta - \zeta') \tag{4.3}$$

Furthermore, if the unit cell is a rectangle ($\varphi = \pi/2$), $(\rho_0 b)^{-1} = a$ and the periodicity of ϕ along the x axis ensures that $\Psi_{\zeta,n}$ depends on x only through $x-na$; this suggests introducing the Bloch functions

$$\tilde{\Psi}_{\zeta,\eta}(\mathbf{r})=\sum_n \exp(-2\pi i\eta n)\,\Psi_{\zeta,n}(\mathbf{r}),\qquad \zeta,\eta\in[0,1] \tag{4.4}$$

which do have the desired orthogonality property

$$\int_{-\infty}^{\infty} dx\,\tilde{\Psi}^*_{\zeta,\eta'}(\mathbf{r})\,\tilde{\Psi}_{\zeta,\eta}(\mathbf{r})\propto\delta(\eta-\eta') \tag{4.5}$$

The argument can be easily extended to the more general case where the unit cell is a parallelogram, by introducing (dimensionless) oblique coordinates (X, Y) defined by $\mathbf{r}=X\mathbf{a}+Y\mathbf{b}$. Multiplying $\Psi_{\zeta,n}$ by an irrelevant phase factor $\exp\{-i\pi(a/b)\cos\varphi[X^2+(\zeta+n)^2]\}$, we obtain

$$\Psi_{\zeta,n}(\mathbf{r})=\exp[-\phi(\mathbf{r})]\exp[-(\pi/\tau)(X-\zeta-n)^2+2\pi i(\zeta+n)Y] \tag{4.6}$$

where $\tau=(b/a)\exp[i(\varphi-\frac{1}{2}\pi)]$; with these $\Psi_{\zeta,n}$ functions, which have the same form as (4.2), we can proceed as above, in oblique coordinates in the general case.

Thus, the $\tilde{\Psi}_{\zeta,\eta}$ are orthogonal:

$$\int d\mathbf{r}\,\tilde{\Psi}^*_{\zeta',\eta'}(\mathbf{r})\,\tilde{\Psi}_{\zeta,\eta}(\mathbf{r})=\delta(\zeta-\zeta')\,\delta(\eta-\eta')\,f(\zeta,\eta) \tag{4.7}$$

where

$$\begin{aligned} f(\zeta,\eta)=\frac{1}{\rho_0}\sum_N \exp(2\pi i\eta N)\int_{-\infty}^{\infty} dX\exp\left[-\frac{\pi}{\tau}(X-\zeta)^2-\frac{\pi}{\tau^*}(X-\zeta-N)^2\right]\\ \times\int_0^1 dY\exp[-2\phi(X,Y)]\exp(-2\pi iNY) \end{aligned} \tag{4.8}$$

These orthogonal $\tilde{\Psi}_{\zeta,\eta}$ can be used for building the projector (2.4), with the result

$$\begin{aligned} \langle\mathbf{r}_1|P|\mathbf{r}_2\rangle=\exp[-\phi(\mathbf{r}_1)-\phi(\mathbf{r}_2)]\int_0^1 d\zeta\int_0^1 d\eta\,\frac{1}{f(\zeta,\eta)}\sum_{nm}\exp[2\pi i\eta(m-n)]\\ \times\exp\left\{-\frac{\pi}{\tau}(X_1-\zeta-n)^2-\frac{\pi}{\tau^*}(X_2-\zeta-m)^2\right.\\ \left.+2\pi i[(\zeta+n)Y_1-(\zeta+m)Y_2]\right\} \end{aligned} \tag{4.9}$$

A more compact form can be obtained by using the Poisson identity

$$\sum_N \exp\left(-\frac{\pi}{\tau^*}N^2+2\pi izN\right)=\sqrt{\tau^*}\sum_N \exp[-\pi\tau^*(z-N)^2] \tag{4.10}$$

in (4.8), and also in (4.9), where we set $m=n+N$. The result is

$$\begin{aligned} f(\zeta,\eta)=&\frac{1}{\rho_0}\sqrt{\tau^*}\int_{-\infty}^{\infty}dX\int_{-\infty}^{\infty}dY\exp[-2\phi(X,Y)]\\ &\times\exp\left[-\frac{\pi}{\tau}(X-\zeta)^2-\pi\tau^*(Y-\eta)^2-2\pi i(X-\zeta)(Y-\eta)\right] \end{aligned} \tag{4.11}$$

and

$$\begin{aligned} \langle\mathbf{r}_1|P|\mathbf{r}_2\rangle=&\exp[-\phi(\mathbf{r}_1)-\phi(\mathbf{r}_2)]\sqrt{\tau^*}\int_{-\infty}^{\infty}d\zeta\int_{-\infty}^{\infty}d\eta\frac{1}{f(\zeta,\eta)}\\ &\times\exp\left[-\frac{\pi}{\tau}(X_1-\zeta)^2-\pi\tau^*(Y_2-\eta)^2-2\pi i(X_2-\zeta)(Y_2-\eta)\right.\\ &\left.+2\pi i\zeta(Y_1-Y_2)\right] \end{aligned} \tag{4.12}$$

Thus, we have obtained an integral representation of the projector P; when used in (2.5) it gives the n-body densities. Some symmetries of (4.12) are hidden; for instance, $\langle\mathbf{r}_1|P|\mathbf{r}_2\rangle=\langle\mathbf{r}_2|P|\mathbf{r}_1\rangle^*$. Others are apparent; for instance, the function $f(\zeta,\eta)$ is doubly periodic with period 1, and this ensures that the densities have the same periodicity properties as the background.

As an illustration, we consider the case of a square unit cell ($a=b$, $\varphi=\pi/2$, $\tau=1$) with the simplest choice

$$\exp[-2\phi(\mathbf{r})]=1+\lambda(\cos 2\pi X+\cos 2\pi Y),\qquad |\lambda|\leqslant 1/2 \tag{4.13}$$

The total background density is

$$\rho_B(r)=\rho_0+(2\pi)^{-1}\Delta\phi \tag{4.14}$$

and from (4.11) and (4.12), we find for the particle density

$$\begin{aligned} \rho(\mathbf{r})=&\langle\mathbf{r}|P|\mathbf{r}\rangle\\ =&\rho_0\sqrt{2}\exp[-2\phi(\mathbf{r})]\int_{-\infty}^{\infty}d\zeta\int_{-\infty}^{\infty}d\eta\\ &\times\frac{\exp[-\pi(X-\zeta)^2-\pi(Y-\eta)^2]\cos[2\pi(X-\zeta)(Y-\eta)]}{1+\lambda[\exp(-\pi/2)](\cos 2\pi\zeta+\cos 2\pi\eta)} \end{aligned} \tag{4.15}$$

The potential modulation $\phi(X, Y)$, the background density $\rho_B(X, Y)$, and the particle density $\rho(X, Y)$ are displayed in Fig. 1 for $\lambda = 0.49$. With this choice of a large amplitude λ, the background density is a rather tormented landscape; the particle density tries to follow, but it does not quite succeed and it exhibits much smoother oscillations.

Another representation of $\rho(\mathbf{r})$ might be of interest. The normalization factor (4.8) can be written as

$$f(\zeta, \eta) = \frac{1}{\rho_0} \int_0^1 dX \int_0^1 dY \, |\tilde{\Psi}_{\zeta,\eta}(X, Y)|^2 \tag{4.16}$$

and therefore

$$\rho(X, Y) = \rho_0 \int_0^1 d\zeta \int_0^1 d\eta \, \frac{|\tilde{\Psi}_{\zeta,\eta}(X, Y)|^2}{\int_0^1 dX_1 \int_0^1 dY_1 \, |\tilde{\Psi}_{\zeta,\eta}(X_1, Y_1)|^2} \tag{4.17}$$

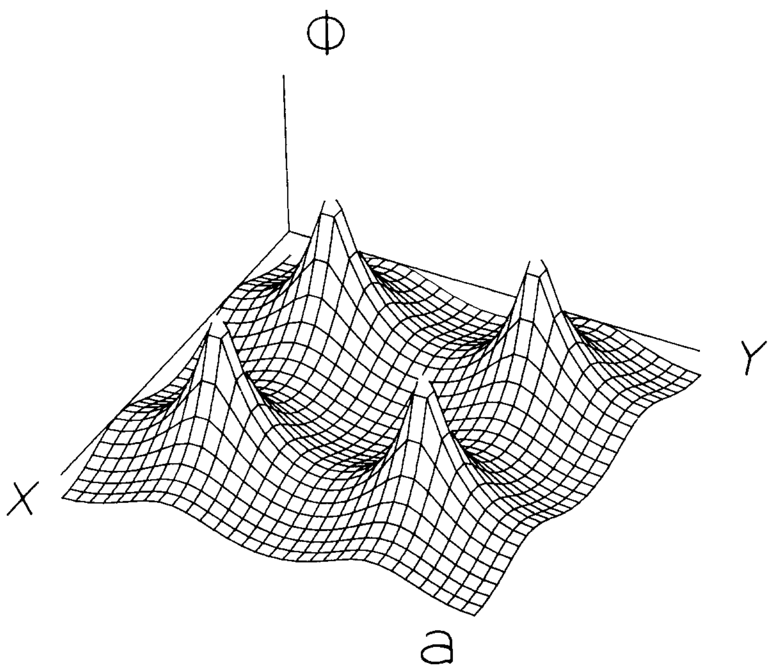
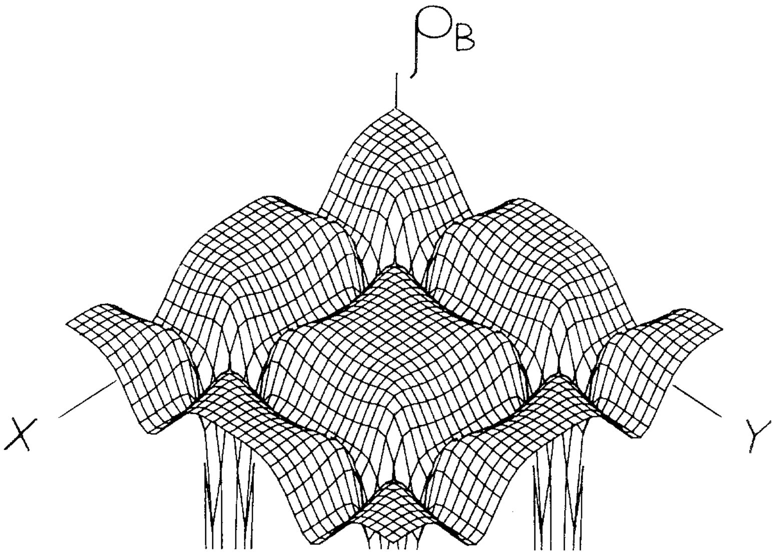


Fig. 1. A simple example. (a) The potential modulation $\phi(\mathbf{r})$. (b) The background density $\rho_B(\mathbf{r})$. (c) The particle density $\rho(\mathbf{r})$.



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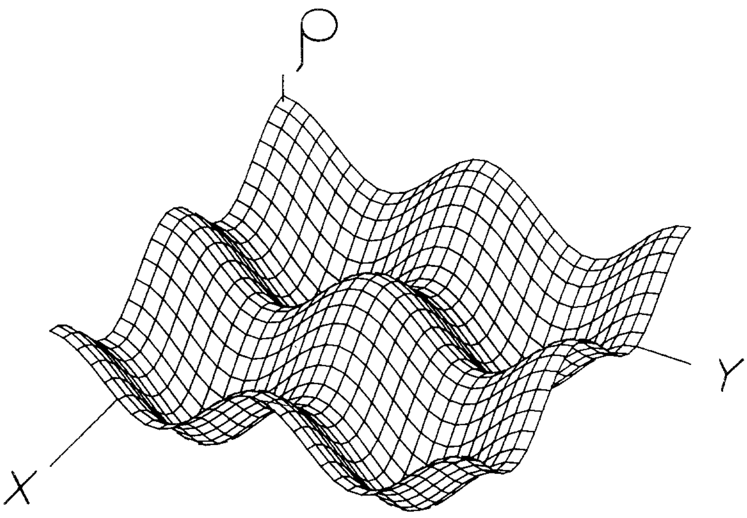

c

Fig. 1 (*continued*)

If we restrict ourselves to the case of a rectangular unit cell, τ is real, and

$$|\tilde{\Psi}_{\zeta,\eta}(X, Y)|^2 = \exp[-2\phi(X, Y)] \sum_{mn} \exp\left[-\frac{\pi}{\tau}(X-\zeta-n)^2 - \frac{\pi}{\tau}(X-\zeta-m)^2 + 2\pi i(n-m)(Y-\eta)\right] \tag{4.18}$$

The sum on n and m can be replaced by a sum on $\mu = m - n$ and $\nu = m + n$, with μ and ν of the same parity. The contributions from (μ, ν) even and (μ, ν) odd, respectively, can be expressed in terms of Jacobi theta functions. The result is

$$\tilde{\Psi}_{\zeta,\eta}(X, Y)|^2 = \exp[-2\phi(X, Y)] \left(\frac{\tau}{2}\right)^{1/2} \left[\theta_3\left(2\eta - 2Y, \frac{2}{\tau}\right)\theta_3\left(X-\zeta, \frac{\tau}{2}\right) + \theta_2\left(2\eta - 2Y, \frac{2}{\tau}\right)\theta_4\left(X-\zeta, \frac{\tau}{2}\right)\right] \tag{4.19}$$

where the θ functions are defined by

$$\begin{aligned} \theta_3(x, t) &= \sum_n \exp(-\pi t n^2 + 2\pi i n x) \\ &= t^{-1/2} \sum_n \exp[-(\pi/t)(x-n)^2] \\ \theta_2(x, t) &= \sum_n \exp[-\pi t(n+\tfrac{1}{2})^2 + 2\pi i(n+\tfrac{1}{2})x] \\ &= t^{-1/2} \sum_n (-1)^n \exp[-(\pi/t)(x-n)^2] \\ \theta_4(x, t) &= \sum_n \exp[-\pi t n^2 + 2\pi i n(x+\tfrac{1}{2})] \\ &= t^{-1/2} \sum_n \exp[-(\pi/t)(x-n-\tfrac{1}{2})^2] \end{aligned} \tag{4.20}$$

The particle density is obtained by substituting (4.19) into (4.17).

4.2. Decay of the Correlations

The decay of the truncated densities (2.5) at large separations is faster than any inverse power law. This can be seen as follows. The decay of the densities is governed by the decay of P: we can study this behavior from (4.12) written in the form

$$\langle \mathbf{r}_1|P|\mathbf{r}_2\rangle = \exp[-\phi(\mathbf{r}_1)-\phi(\mathbf{r}_2)]\exp[2\pi i X_1(Y_1-Y_2)]$$
$$\times\sqrt{\tau^*}\int_{-\infty}^{\infty}d\zeta\int_{-\infty}^{\infty}d\eta\,\frac{1}{f(\zeta+X_1,\eta+Y_2)}$$
$$\times\exp\left[-\frac{\pi}{\tau}\zeta^2-\pi\tau^*\eta^2-2\pi i\zeta\eta+2\pi i\zeta(Y_1-Y_2)-2\pi i\eta(X_1-X_2)\right] \tag{4.21}$$

Let us study the behavior of (4.21), for a fixed value of $\mathbf{r}_1$, as $\mathbf{r}_2$ recedes to infinity. Since f is periodic in $\eta+Y_2$, we can define $\bar{Y}_2$ by $Y_2=\bar{Y}_2+n$, $\bar{Y}_2\in[0,1]$, n integer, and replace Y_2 by $\bar{Y}_2$ in f. If we restrict ourselves to a fixed value for $\bar{Y}_2$, i.e., if $\mathbf{r}_2$ recedes to infinity by integral steps in Y_2, the integral in (4.21) is the Fourier transform of a well-behaved function of ζ and η, and it decays faster than any inverse power law.

The resulting fast decay of the correlations is one of the criteria that is believed to characterize a conducting phase.

4.3. Sum Rules

The one- and two-particle densities can be shown to obey several sum rules, which characterize a conductor.

Neutrality. The averages, on a unit cell, of the particle density and of the background density are equal:

$$\int_0^1 dX\int_0^1 dY\,\rho(X,Y)=\rho_0 \tag{4.22}$$

This sum rule is satisfied by (4.17).

Screening of a Particle of the System. This screening rule means that a particle of the system induces a polarization cloud of exactly opposite charge:

$$\int d\mathbf{r}_2\,\rho_T^{(2)}(\mathbf{r}_1,\mathbf{r}_2)=-\rho(\mathbf{r}_1) \tag{4.23}$$

The structure of (2.5) ensures that this rule is obeyed, because of the closure property

$$\int d\mathbf{r}_2\,\langle\mathbf{r}_1|P|\mathbf{r}_2\rangle\langle\mathbf{r}_2|P|\mathbf{r}_1\rangle=\langle\mathbf{r}_1|P|\mathbf{r}_1\rangle \tag{4.24}$$

The rule can also be checked explicitly on the representation (4.9), after some algebra.

Screening of an Infinitesimal Test Charge (Stillinger–Lovett Rule). This screening rule means that an external infinitesimal test charge induces in the system a polarization cloud of exactly opposite charge. Through linear response theory, this statement becomes a sum rule for the truncated two-body density, the Carnie and Chan generalization[10] of the Stillinger–Lovett rule[7] to an inhomogeneous system, written here for two dimensions:

$$-\beta \int d\mathbf{r}_1 \int d\mathbf{r}_2 \ln r_2 S(\mathbf{r}_1, \mathbf{r}_2) = 1 \tag{4.25}$$

where S is the total charge structure factor

$$S(\mathbf{r}_1, \mathbf{r}_2) = e^2[\rho_T^{(2)}(\mathbf{r}_1, \mathbf{r}_2) + \rho(\mathbf{r}_1)\,\delta(\mathbf{r}_2 - \mathbf{r}_1)] \tag{4.26}$$

In the present case of a periodic system, (4.25) can be written in other forms. Because of its periodicity properties, $S(\mathbf{r}_1, \mathbf{r}_2)$ is completely described by its double Fourier transform

$$\tilde{S}_{\mathbf{G}}(\mathbf{k}) = \frac{1}{A}\int_U d\mathbf{r}_1 \int d\mathbf{r}_2 \exp[i\mathbf{G}\cdot\mathbf{r}_1 + i\mathbf{k}\cdot(\mathbf{r}_2 - \mathbf{r}_1)]\, S(\mathbf{r}_1, \mathbf{r}_2) \tag{4.27}$$

where U means that the integration domain of $\mathbf{r}_1$ is the unit cell, of area $A = ab \sin\varphi$; $\mathbf{G}$ is a vector of the reciprocal lattice. From (4.23), one finds $\tilde{S}_{\mathbf{G}}(\mathbf{G}) = 0$. Then, (4.25) can be reexpressed in terms of $\tilde{S}_{\mathbf{G}}(\mathbf{k})$ and of the Fourier transform $2\pi/k^2$ of $-\ln r$ as

$$2\pi\beta \lim_{k\to 0} \frac{\tilde{S}_{\mathbf{0}}(\mathbf{k})}{k^2} = 1 \tag{4.28}$$

In other words

$$\frac{1}{A}\int_U d\mathbf{r}_1 \int d\mathbf{r}_2 \exp[i\mathbf{k}\cdot(\mathbf{r}_2 - \mathbf{r}_1)]\, S(\mathbf{r}_1, \mathbf{r}_2) \underset{k\to 0}{\sim} \frac{k^2}{2\pi\beta} \tag{4.29}$$

Expanding the exponential in (4.29), we find the generalization to a periodic system of the Stillinger–Lovett second moment rule

$$\frac{1}{A}\int_U d\mathbf{r}_1 \int d\mathbf{r}_2\, (\mathbf{r}_2 - \mathbf{r}_1)_\alpha (\mathbf{r}_2 - \mathbf{r}_1)_\gamma\, \rho_T^{(2)}(\mathbf{r}_2 - \mathbf{r}_1) = -\frac{\delta_{\alpha\gamma}}{\pi\beta e^2} \tag{4.30}$$

where α, $\gamma = 1, 2$ are the Cartesian components of $\mathbf{r}$. Equations (4.29) and (4.30) are of the same form as in a homogeneous system, except for the average on $\mathbf{r}_1$, which is taken over the unit cell.

In terms of the dimensionless oblique coordinates X, Y, when $\beta e^2 = 2$, (4.30) becomes

$$I_X = \int_0^1 dX_1 \int_0^1 dY_1 \int_{-\infty}^{\infty} dX_2 \int_{-\infty}^{\infty} dY_2\, (X_2 - X_1)^2\, \rho_T^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$$
$$= -\frac{\rho_0^2 b}{2\pi a \sin\varphi} \tag{4.31a}$$

$$I_Y = \int_0^1 dX_1 \int_0^1 dY_1 \int_{-\infty}^{\infty} dX_2 \int_{-\infty}^{\infty} dY_2\, (Y_2 - Y_1)^2\, \rho_T^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$$
$$= -\frac{\rho_0^2 a}{2\pi b \sin\varphi} \tag{4.31b}$$

$$I_{XY} = \int_0^1 dX_1 \int_0^1 dY_1 \int_{-\infty}^{\infty} dX_2 \int_{-\infty}^{\infty} dY_2\, (X_2 - X_1)(Y_2 - Y_1)\, \rho_T^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$$
$$= \frac{\rho_0^2 \cos\varphi}{2\pi \sin\varphi} \tag{4.31c}$$

In Appendix A, we show that these sum rules (4.31) are indeed obeyed. For this purpose, it is convenient to express $\rho_T^{(2)}$ in terms of the projector P in its form (4.9), which explicitly exhibits the periodicity properties.

The above-mentioned proof applies to any periodic background, including the special case of a lattice of fixed charges of negligible size. For this limiting case, however, we can also give an alternative proof, which is described in Appendix B.

4.4. Irrational Values of the Number of Particles per Cell

Up to this point, we have assumed the value 1 for $\rho_0 A$, the average number of mobile particles per unit cell. If $\rho_0 A = p/q$ (p, q integers), choosing a unit cell q times larger reduces the problem to $\rho_0 A = p$, and it is easy to see that this case is solved by diagonalizing a $p \times p$ matrix.

What about irrational values of $\rho_0 A$? In terms of a model of a crystal, it would be a rather academic situation, since $-\rho_0 A$ is the ratio between the charge of an ion and the charge of an electron. Nevertheless, this is a mathematically interesting situation. Furthermore, our problem is closely related to a magnetic analog[11] of importance for the theory of the quantum Hall effect[12] and also to problems that arise in the theories of incommensurate structures.[13]

We have not been able to compute the densities for irrational values of $\rho_0 A$. We only want to point out that, in the simplest case, the problem reduces to studying the solutions of an almost-Mathieu equation.

We start again with the functions (4.2), for a square unit cell of side a, and a potential modulation of the form (4.13):

$$\Psi_{\zeta,n}(\mathbf{r}) = [1+\lambda(\cos 2\pi X + \cos 2\pi Y)]^{1/2} \times \exp\left[-\pi\mu\left(X - \frac{\zeta+n}{\mu}\right)^2 + 2\pi i(\zeta+n)Y\right] \tag{4.32}$$

where $\mu = \rho_0 A = \rho_0 a^2$. Computing the projector P on the space of these functions amounts to diagonalizing the matrix formed by the scalar products

$$\int d\mathbf{r}\ \Psi^*_{\zeta,n}(\mathbf{r})\ \Psi_{\zeta',m}(\mathbf{r}) = \delta(\zeta-\zeta')\ A_{nm} \tag{4.33}$$

A simple calculation gives

$$A_{nm} = (2\mu)^{-1/2}\left\{\left[1+\lambda e^{-\pi/2\mu}\cos\frac{2\pi(\zeta+n)}{\mu}\right]\delta_{mn} + \frac{1}{2}\lambda e^{-\pi/2\mu}(\delta_{n,m-1}+\delta_{n,m+1})\right\} \tag{4.34}$$

The problem of diagonalizing A_{nm} leads to

$$\frac{1}{2}(u_{n+1}+u_{n-1}) + \left[\cos\frac{2\pi(\zeta+n)}{\mu}\right]u_n = su_n \tag{4.35}$$

If $\mu=1$, the solution is $u_n = \exp(-2\pi i\eta n)$, and we retrieve (4.4). If μ is irrational, (4.35) is the almost-Mathieu equation in its full glory, and we leave the computation of the projector P as an open problem.

5. CONCLUSION

At $\Gamma=2$, we have obtained an exact solution for the equilibrium statistical mechanics of the model of fixed ions and mobile electrons introduced by Hansen *et al.*[5,6] We have shown that, at $\Gamma=2$, the model exhibits the features of a conducting phase: the correlations at large separations decay faster than any inverse power law, and the system has good screening properties (the Stillinger–Lovett rule is obeyed). Our results are also valid when the potential modulation ϕ is a nonelectrostatic periodic potential. Furthermore, ϕ may have arbitrarily large oscillations.

On the basis of computer simulation results, it has been claimed by Hansen and his collaborators that the conductor–dielectric phase transition occurs at a coupling Γ that is larger than 2 for finite-size ions and goes to 2 as the ion radius goes to zero. Our exact results at $\Gamma=2$ do not contradict this claim.

APPENDIX A. STILLINGER–LOVETT SUM RULE

We check the sum rules (4.31), where

$$\rho_T^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = -\langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle \langle \mathbf{r}_2 | P | \mathbf{r}_1 \rangle \tag{A.1}$$

using for $\langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle$ the representation (4.9).

We first consider

$$\begin{aligned} I_Y = &-\int_0^1 dX_1 \int_0^1 dY_1 \exp[-2\phi(\mathbf{r}_1)] \\ &\times \sum_{\substack{nm\\ n'm'}} \int_0^1 d\zeta \int_0^1 d\eta \int_0^1 d\zeta' \int_0^1 d\eta' \, [f(\zeta, \eta) f(\zeta', \eta')]^{-1} \\ &\times \exp\Big\{ -2\pi i [\eta(n-m) - \eta'(n'-m')] \\ &- \frac{\pi}{\tau} (X_1 - \zeta - n)^2 - \frac{\pi}{\tau^*} (X_1 - \zeta' - n')^2 + 2\pi i (n - n') Y_1 \Big\} \\ &\times \int_{-\infty}^{\infty} dX_2 \exp\left[-\frac{\pi}{\tau^*} (X_2 - \zeta - m)^2 - \frac{\pi}{\tau} (X_2 - \zeta' - m')^2 \right] \\ &\times \int_{-\infty}^{\infty} dY_2 \, (Y_2 - Y_1)^2 \exp[-2\phi(\mathbf{r}_2) - 2\pi i (\zeta - \zeta')(Y_2 - Y_1) \\ &- 2\pi i (m - m') Y_2] \end{aligned} \tag{A.2}$$

Using the periodicity of ϕ, we find for the integral over Y_2 in (A.2)

$$-\frac{1}{(2\pi)^2} \frac{\partial^2}{\partial \zeta^2} \delta(\zeta - \zeta') \sum_M \delta_{m', m+M} \int_0^1 dY_2 \exp[-2\phi(\mathbf{r}_2) + 2\pi i M Y_2]$$

In (A.2), we can replace m' by $m+M$ and n' by $n+N$. Using the periodicity of ϕ, we can replace $X_2 - m$ by X_2 and perform the sum over m, which gives a $\delta(\eta - \eta')$; we can also replace $X_1 - n$ by X_1 and $\sum_n \int_0^1 dX_1 \ldots$ by $\int_{-\infty}^{\infty} dX_1 \ldots$. We obtain

$$
\begin{aligned}
I_Y = {} & \frac{\rho_0^2}{(2\pi)^2} \int_0^1 d\zeta \int_0^1 d\eta \, \frac{1}{f(\zeta, \eta)} \\
& \times \frac{1}{\rho_0} \sum_N \exp(2\pi i \eta N) \int_{-\infty}^{\infty} dX_1 \exp\left[-\frac{\pi}{\tau^*} (X_1 - \zeta - N)^2 \right] \\
& \times \int_0^1 dY_1 \exp[-2\phi(\mathbf{r}_1) - 2\pi i N Y_1] \\
& \times \frac{1}{\rho_0} \sum_M \exp(-2\pi i \eta M) \int_{-\infty}^{\infty} dX_2 \exp\left[-\frac{\pi}{\tau} (X_2 - \zeta - M)^2 \right] \\
& \times \int_0^1 dY_2 \exp[-2\phi(\mathbf{r}_2) + 2\pi i M Y_2] \\
& \times \frac{\partial^2}{\partial \zeta^2} \left\{ \frac{1}{f(\zeta, \eta)} \exp\left[-\frac{\pi}{\tau} (X_1 - \zeta)^2 - \frac{\pi}{\tau^*} (X_2 - \zeta)^2 \right] \right\}
\end{aligned} \tag{A.3}
$$

In (A.3), as a function of X_1 the derivative $(\partial^2/\partial\zeta^2)\cdots$ is a combination of terms of the form $\exp[-(\pi/\tau)(X_1 - \zeta)^2]$ or $(X_1 - \zeta)\exp[-(\pi/\tau)(X_1 - \zeta)^2]$ or $(X_1 - \zeta)^2 \exp[-(\pi/\tau)(X_1 - \zeta)^2]$. These terms enter the integral over X_1 and generate

$$
\begin{aligned}
& \frac{1}{\rho_0} \sum_N \exp(2\pi i \eta N) \int_{-\infty}^{\infty} dX_1 \exp\left[-\frac{\pi}{\tau} (X_1 - \zeta)^2 - \frac{\pi}{\tau^*} (X_1 - \zeta - N)^2 \right] \\
& \quad \times \int_0^1 dY_1 \exp[-2\phi(\mathbf{r}_1) - 2\pi i N Y_1]
\end{aligned}
$$

multiplied on the right by 1 or $X_1 - \zeta$ or $(X_1 - \zeta)^2$, i.e., either $f(\zeta, \eta)$ as given by (4.8), or combinations of $\partial f/\partial\zeta$, $\partial f/\partial\eta$, and $\partial^2 f/\partial\zeta\,\partial\eta$. The same identifications can be made with $\exp[-(\pi/\tau^*)(X_2 - \zeta)^2]$ and its derivatives. The result of these identifications is

$$
\begin{aligned}
I_Y = {} & -\frac{\rho_0^2}{(2\pi)^2} \int_0^1 d\zeta \int_0^1 d\eta \left\{ \frac{4\pi}{\tau + \tau^*} + \frac{\partial}{\partial \eta} \left[\frac{1}{(\tau + \tau^*)^2} \frac{1}{f} \frac{\partial f}{\partial \eta} \right.\right. \\
& \left.\left. + \frac{2i(\tau^* - \tau)}{(\tau + \tau^*)^2} \frac{1}{f} \frac{\partial f}{\partial \zeta} \right] \right\}
\end{aligned} \tag{A.4}
$$

Since f is periodic in ζ and η with periods 1, the contribution from the derivative $(\partial/\partial\eta)\cdots$ vanishes, and we obtain (4.31b).

The computation of I_{XY} follows the same lines. Instead of (A3), we obtain

$$I_{XY}=\frac{i\rho_0^2}{2\pi}\int_0^1 d\zeta\int_0^1 d\eta\,\frac{1}{f(\zeta,\eta)}$$
$$\times\frac{1}{\rho_0}\sum_N \exp(2\pi i\eta N)\int_{-\infty}^{\infty} dX_1\exp\left[-\frac{\pi}{\tau^*}(X_1-\zeta-N)^2\right]$$
$$\times\int_0^1 dY_1\exp[-2\phi(\mathbf{r}_1)-2\pi iNY_1]$$
$$\times\frac{1}{\rho_0}\sum_M \exp(-2\pi i\eta M)\int_{-\infty}^{\infty} dX_2\exp\left[-\frac{\pi}{\tau}(X_2-\zeta-M)^2\right]$$
$$\times\int_0^1 dY_2\exp[-2\phi(\mathbf{r}_2)+2\pi iMY_2]$$
$$\times\left(X_2-X_1-\frac{1}{2\pi i}\frac{\partial}{\partial\eta}\right)\frac{\partial}{\partial\zeta}\left\{\frac{1}{f(\zeta,\eta)}\exp\left[-\frac{\pi}{\tau}(X_1-\zeta)^2-\frac{\pi}{\tau^*}(X_2-\zeta)^2\right]\right\} \tag{A.5}$$

Again, we manage to recognize derivatives of $f(\zeta,\eta)$, with the result (4.31c).

Exchanging the X and Y axes in (4.31b) proves (4.31a).

APPENDIX B. LATTICE OF POINT PARTICLES

We take as the periodic background a lattice of fixed charged particles and consider the limiting case of point particles. We give a direct proof that the Stillinger–Lovett rule is obeyed.

Let $z_i=x_i+iy_i$ be the complex number that defines the position of the ith mobile particle; similarly, let Z_j define the position of the jth fixed particle. At $\Gamma=2$, the Boltzmann factor of a system of N mobile and N fixed point particles is

$$\exp(-\beta H)=L^{2N}\left|\frac{\prod_{i<k}(z_i-z_k)\prod_{j<l}(Z_j-Z_l)}{\prod_{i,j}(z_i-Z_j)}\right|^2$$
$$=L^{2N}\left|\det\left\{\frac{1}{z_i-Z_j}\right\}_{i,j=1,\ldots,N}\right|^2 \tag{B.1}$$

where the second form is obtained by using an algebraic identity of Cauchy. In order to avoid short-distance divergences, we introduce a cutoff at some small distance σ, and replace (B.1) by

$$\exp(-\beta H)=L^{2N}\left|\det\left\{\frac{1-\exp[-|z_i-Z_j|^2/2\sigma^2]}{z_i-Z_j}\right\}_{i,j=1,\ldots,N}\right|^2 \tag{B.2}$$

The limit $\sigma \to 0$ will be taken at the end of the calculation. Equation (B.2) is again a squared determinant, and therefore the n-body truncated densities are again of the form (2.5), where now P is the projector on the space spanned by the functions $(z-Z_j)^{-1}[1-\exp(-|z-Z_j|^2/2\sigma^2)]$. An orthogonal basis for this space is obtained by constructing Bloch functions. Assuming for simplicity that the fixed particles are on the square lattice $Z=m+in$, m, $n \in \mathbb{Z}$, we define the Bloch functions

$$\Psi_{\zeta,\eta}(x, y) = \sum_{mn} \exp[2\pi i(\zeta m + \eta n)] \frac{1-\exp\{-[(x-m)^2+(y-n)^2]/2\sigma^2\}}{x+iy-(m+in)} \tag{B.3}$$

Using the Fourier transform

$$\begin{aligned} g(\zeta, \eta) &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \exp[2\pi i(\zeta x + \eta y)] \frac{1-\exp[-(x^2+y^2)/2\sigma^2]}{x+iy} \\ &= i\frac{\exp[-2\pi^2\sigma^2(\zeta^2+\eta^2)]}{\zeta+i\eta} \end{aligned} \tag{B.4}$$

and the Poisson summation formula, we can rewrite Ψ as

$$\Psi_{\zeta,\eta}(x, y) = -\sum_{mn} \exp\{2\pi i[(\zeta+m)x+(\eta+n)y]\}\, g(\zeta+m, \eta+n) \tag{B.5}$$

and we find for the projector

$$\begin{aligned} \langle \mathbf{r}_1|P|\mathbf{r}_2\rangle &= \int_{-1/2}^{1/2} d\zeta \int_{-1/2}^{1/2} d\eta \frac{\Psi_{\zeta,\eta}(x_1, y_1)\, \Psi^*_{\zeta,\eta}(x_2, y_2)}{\int_{-1/2}^{1/2} dx \int_{-1/2}^{1/2} dy\, |\Psi_{\zeta,\eta}(x, y)|^2} \\ &= \int_{-1/2}^{1/2} d\zeta \int_{-1/2}^{1/2} d\eta \\ &\quad \times \Bigg(\sum_{m_1 n_1 m_2 n_2} \exp\{2\pi i[(\zeta+m_1)x_1+(\eta+n_1)y_1-(\zeta+m_2)x_2 \\ &\quad -(\eta+n_2)y_2]\}\, g(\zeta+m_1, \eta+n_1)\, g^*(\zeta+m_2, \eta+n_2)\Bigg) \\ &\quad \times \left[\sum_{mn} g(\zeta+m, \eta+n)\, g^*(\zeta+m, \eta+n)\right]^{-1} \end{aligned} \tag{B.6}$$

The structure of (B.6) allows us at once to check the average density sum rule

$$\int_{-1/2}^{1/2} dx \int_{-1/2}^{1/2} dy\, \rho(\mathbf{r}) = \int_{-1/2}^{1/2} dx \int_{-1/2}^{1/2} dy\, \langle \mathbf{r}|P|\mathbf{r}\rangle = 1 \tag{B.7}$$

and the neutrality sum rule

$$\int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dy_2\, \rho_T^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$$
$$= -\int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dy_2\, \langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle \langle \mathbf{r}_2 | P | \mathbf{r}_1 \rangle$$
$$= -\langle \mathbf{r}_1 | P | \mathbf{r}_1 \rangle = -\rho(\mathbf{r}_1) \tag{B.8}$$

We turn to the Stillinger–Lovett second moment

$$I = 2\int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dy_2 \int_{-1/2}^{1/2} dx_1 \int_{-1/2}^{1/2} dy_1\, \rho_T^{(2)}(\mathbf{r}_1, \mathbf{r}_2)(x_1 - x_2)^2$$
$$= -2\int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dy_2 \int_{-1/2}^{1/2} dx_1 \int_{-1/2}^{1/2} dy_1\, \langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle \langle \mathbf{r}_2 | P | \mathbf{r}_1 \rangle (x_1 - x_2)^2 \tag{B.9}$$

Using the representation (B.6) of the projector, we perform the space integrals with variables $\mathbf{r}_1$ and $\mathbf{r}_2 - \mathbf{r}_1$; we find

$$I = \frac{1}{2\pi^2} \int_{-1/2}^{1/2} d\zeta \int_{-1/2}^{1/2} d\eta \int_{-1/2}^{1/2} d\zeta' \int_{-1/2}^{1/2} d\eta'$$
$$\times \delta''(\zeta - \zeta')\, \delta(\eta - \eta') \frac{f(\zeta, \eta; \zeta', \eta')\, f(\zeta', \eta'; \zeta, \eta)}{f(\zeta, \eta; \zeta, \eta)\, f(\zeta', \eta'; \zeta', \eta')} \tag{B.10}$$

where

$$f(\zeta, \eta; \zeta', \eta') = \sum_{mn} g(\zeta + m, \eta + n)\, g^*(\zeta' + m, \eta' + n) \tag{B.11}$$

Replacing $\delta''(\zeta - \zeta')$ by $\delta(\zeta - \zeta')(\partial^2/\partial\zeta'^2)$, we obtain

$$I = -\frac{1}{\pi^2} \int_{-1/2}^{1/2} d\zeta \int_{-1/2}^{1/2} d\eta \left[\frac{1}{f(\zeta, \eta; \zeta, \eta)} \frac{\partial^2 f(\zeta, \eta; \zeta', \eta)}{\partial\zeta\, \partial\zeta'} \right.$$
$$\left. - \frac{1}{f^2(\zeta, \eta; \zeta, \eta)} \frac{\partial f(\zeta, \eta; \zeta', \eta)}{\partial\zeta} \frac{\partial f(\zeta, \eta; \zeta', \eta)}{\partial\zeta'} \right]_{\zeta' = \zeta} \tag{B.12}$$

The function $f(\zeta, \eta; \zeta, \eta)$ defined by (B.4) and (B.11) is

$$f(\zeta, \eta; \zeta, \eta) = \sum_{mn} \frac{\exp\{-4\pi^2\sigma^2[(\zeta + m)^2 + (\eta + n)^2]\}}{(\zeta + m)^2 + (\eta + n)^2} \tag{B.13}$$

It is convenient to display the singularity at $\zeta = \eta = 0$, coming from the term $m = n = 0$, and to represent f, in the integration domain $|\zeta|$, $|\eta| < 1/2$, by its Laurent expansion

$$f(\zeta, \eta; \zeta, \eta) = \frac{1}{\zeta^2 + \eta^2} + A + \cdots \tag{B.14}$$

In the point-particle limit, $\sigma \to 0$, the sum in (B.13) diverges for large (m, n) and A becomes infinite; however, the terms of higher order in (ζ, η) represented by dots in (B.14) remain finite and can be neglected. If a similar analysis is performed for the derivatives of f appearing in (B.12), it is easily seen that only the term $m = n = 0$ plays a role as $\sigma \to 0$, because the sums on (m, n) that define these derivatives do *not* diverge for large (m, n); therefore

$$\left. \frac{\partial^2 f(\zeta, \eta; \zeta', \eta)}{\partial\zeta\, \partial\zeta'} \right|_{\zeta' = \zeta} \sim \left| \frac{\partial g(\zeta, \eta)}{\partial\zeta} \right|^2 \sim \frac{1}{(\zeta^2 + \eta^2)^2} \tag{B.15}$$

and

$$\left. \frac{\partial f(\zeta, \eta; \zeta', \eta)}{\partial\zeta} \frac{\partial f(\zeta, \eta; \zeta', \eta)}{\partial\zeta'} \right|_{\zeta' = \zeta} \sim \left| g(\zeta, \eta) \frac{\partial g(\zeta, \eta)}{\partial\zeta} \right|^2 \sim \frac{1}{(\zeta^2 + \eta^2)^3} \tag{B.16}$$

Using (B.14)–(B.16) in (B.12), we find

$$I \sim -\frac{1}{\pi^2} \int_{-1/2}^{-1/2} d\zeta \int_{-1/2}^{-1/2} d\eta \, \frac{A}{[1 + A(\zeta^2 + \eta^2)]^2} \tag{B.17}$$

As A goes to infinity, the integration domain in (B.17) can be extended to infinity and the integral evaluated in polar coordinates. Thus,

$$\lim_{\sigma \to 0} I = -1/\pi \tag{B.18}$$

This proves that the Stillinger–Lovett rules holds in the point-particle limit $\sigma \to 0$.

We have not been able to compute I for a finite value of σ. It should be remarked that the Boltzmann factor (B.2) corresponds, when σ is nonzero, to a complicated many-body interaction, which would become the Coulomb law only if all particles were far apart from one another. There is no obvious reason for believing that such a system obeys or does not obey the Stillinger–Lovett rule. This is in contrast with the case of a bona fide system with extended fixed particles, which does obey the rule, as shown in Appendix A.

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REFERENCES

1. B. Jancovici, *Phys. Rev. Lett.* **46**:386 (1981).
2. Ph. Choquard, P. J. Forrester, and E. R. Smith, *J. Stat. Phys.* **33**:13 (1983).
3. A. Alastuey and J. L. Lebowitz, *J. Phys. (Paris)* **45**:1859 (1984), and references quoted therein.
4. F. Cornu and B. Jancovici, *Europhys. Lett.* **5**:125 (1988).
5. J. Clérouin and J. P. Hansen, *Phys. Rev. Lett.* **54**:2277 (1985).
6. J. Clérouin, J. P. Hansen, and B. Piller, *Phys. Rev. A* **36**:2793 (1987).
7. F. H. Stillinger and R. Lovett, *J. Chem. Phys.* **49**:1991 (1968).
8. C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Mécanique Quantique* (Hermann, Paris, 1977).
9. B. Jancovici, *J. Stat. Phys.* **28**:43 (1982).
10. S. L. Carnie and D. Y. C. Chan, *Chem. Phys. Lett.* **77**:437 (1981).
11. D. R. Hofstadter, *Phys. Rev. B* **14**:2239 (1976).
12. D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. denNijs, *Phys. Rev. Lett.* **49**:405 (1982).
13. B. Souillard, *Phys. Rep.* **103**:41 (1984).