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Atomic versus Ionized States in Many-Particle Systems and the Spectra of Reduced Density Matrices: A Model Study

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We study the spectrum of appropriate reduced density matrices for a model consisting of one quantum particle ("electron") in a classical fluid (of "protons") at thermal equilibrium. The quantum and classical particles interact by a short-range, attractive potential such that the quantum particle can form "atomic" bound states with a single classical particle. We consider two models for the classical component: an ideal gas and the "cell model of a fluid." We find that when the system is at low density the spectrum of the "electron–proton" pair density matrix has, in addition to a continuous part, a discrete part that is associated with "atomic" bound states. In the high-density limit the discrete eigenvalues disappear in the case of the cell model, indicating the existence of pressure ionization or a Mott effect according to a general criterion for characterizing bound and ionized electron–proton pairs in a plasma proposed recently by M. Girardeau. For the ideal gas model, on the other hand, eigenvalues remain even at high density.

KEY WORDS: Bound and ionized states; Mott effect; pressure ionization; reduced density matrix; discrete and continuous spectra; functional integrals; Birman–Schwinger principle.

1. INTRODUCTION

It is generally agreed that an appropriate fundamental description of bulk macroscopic matter in equilibrium is via the Gibbs density matrix $\rho \sim \exp(-\beta H)$, with H the Coulomb Hamiltonian of nuclei and electrons

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(we are excluding here domains of densities, temperatures, and sizes where nuclear, relativistic, and gravitational effects are important). In most situations this description is replaced by a much simpler one using an effective Hamiltonian $H_{\rm eff}$ where many of the degrees of freedom have been frozen out. For example, to obtain the properties of helium or nitrogen at moderate temperatures and pressures it certainly suffices, for all practical purposes, to consider the atoms or molecules as the basic units with an effective two- or three-body interaction between them. Similarly, for the analysis of sodium at 10^3 K we would use an atomic Hamiltonian at low densities and a "plasma Hamiltonian" corresponding to Na^+ ions and electrons (with no neutral atoms) at high densities where the system forms a liquid metal. For intermediate densities the effective description would involve the "degree of ionization" of the system.

While it is often clear intuitively how to go about finding an approximate $H_{\rm eff}$, there are important situations where this is not so. In fact, it is not even clear, in a general system, what one means by degree of ionization. An important theoretical and practical problem is therefore to find methods for obtaining the effective description from the basic Hamiltonian in a clear and systematic way. This has been achieved so far only for special limits of zero pressure and zero temperature,[2-4] where the approximate formula for the degree of ionization at low pressures given by the Saha formalism[1] has been given a rigorous foundation. The result (established modulo some reasonable assumptions) in the simplest case of the electron–proton system is as follows: if one fixes the chemical potential $\mu = \frac{1}{2}(\mu_e + \mu_p)$ below the ground-state energy of a hydrogen atom $E_{\rm at}$, then in the limit $\beta \to \infty$ the system consists of free electrons and protons (see also ref. 5 for a related result). On the other hand, when the chemical potential is fixed slightly above $E_{\rm at}$, the system will consist of independent hydrogen atoms when $\beta \to \infty$. One can obtain "ionization equilibrium phases" which consist of mixtures of free electrons, protons, and hydrogen atoms by letting the chemical potential (versus temperature) tend to $E_{\rm at}$ as $\beta \to \infty$. The degree of ionization then varies smoothly with the slope of the chemical potential at $E_{\rm at}$, and coincides with the usual Saha formula.[4] The techniques of refs. 2 and 3 generalize this picture to arbitrary mixtures of electrons and nuclei and also include molecules.

In the above limits both the particle density and the temperature go to zero. One therefore has to go beyond this formalism to gain an understanding of the degree of ionization in systems with finite density. This is necessary to describe the transition, continuous or abrupt, such as must occur in the sodium system mentioned earlier at pressures intermediate between the neutral gas and liquid metal regime. This "pressure-induced ionization" occurs when the density increases and the Debye radius of the plasma becomes of the order of the Bohr radius. In such a situation the electronic levels of the ions and atoms merge in the continuum and the chemical species become unstable (Mott effect).[6] This affects the equation of state, the transport properties, and the spectral lines of the system. These changes may be gradual or there may be a plasma ionization phase transition with the coexistence of two phases with different densities and degrees of ionization.[7]

A fundamental conceptual difficulty in dealing with these problems is the lack of an *a priori* distinction between "free or ionized" and "bound or atomic" states in the many-body quantum formalism. It would be extremely useful for a quantitative theory of pressure ionization to be able to characterize the degree of ionization, at least in a partial way, in terms of equilibrium quantities.

Recently Girardeau[8] made an interesting proposal for identifying "ionized" and "atomic" states in terms of the eigenvalues and eigenfunctions of an appropriate reduced equilibrium density matrix of the system. This scheme, which is related to Yang's description of bound pairs in superconductivity, considers the pair reduced density matrix $\rho_2(\mathbf{x}, \mathbf{X} \mid \mathbf{y}, \mathbf{Y})$, where $\mathbf{x}, \mathbf{y}$ and $\mathbf{X}, \mathbf{Y}$ denote the electron and proton coordinates, respectively. One can express it as a function of the relative $\mathbf{x}_{\mathrm{rel}} = \mathbf{x} - \mathbf{X}$, $\mathbf{y}_{\mathrm{rel}} = \mathbf{y} - \mathbf{Y}$ and center-of-mass coordinates $\mathbf{r} = (m\mathbf{x} + M\mathbf{X})/(m + M)$, $\mathbf{s} = (m\mathbf{y} + M\mathbf{Y})/(m + M)$, where m is the electron mass and M is the proton mass. In the thermodynamic limit the resulting function will, for translation-invariant phases, depend on $\mathbf{x}_{\mathrm{rel}}$, $\mathbf{y}_{\mathrm{rel}}$, and $\mathbf{r} - \mathbf{s}$. We set $\rho_2(\mathbf{x}, \mathbf{X} \mid \mathbf{y}, \mathbf{Y}) = \bar{\rho}_2(\mathbf{x}_{\mathrm{rel}}, \mathbf{y}_{\mathrm{rel}}, \mathbf{r} - \mathbf{s})$ and define, for a given wave number $\mathbf{q}$,

$$\rho_{\mathbf{q}}(\mathbf{x}_{\mathrm{rel}}, \mathbf{y}_{\mathrm{rel}}) = \int d\mathbf{r}\, e^{i\mathbf{q}\cdot\mathbf{r}} \bar{\rho}_2(\mathbf{x}_{\mathrm{rel}}, \mathbf{y}_{\mathrm{rel}}, \mathbf{r}) \tag{1.1}$$

This object is like a one-particle reduced density matrix describing the relative degree of freedom of an electron–proton pair with wavenumber $\mathbf{q}$ for its center of mass. For a given $\mathbf{q}$ one considers the spectrum of this density matrix. Girardeau's proposal is to associate the discrete part with "bound states" and the continuum with "ionized states." In particular, the discrete eigenvalues $\lambda_\nu(\mathbf{q})$ are interpreted as occupation numbers of electron "bound states" and their sum is assumed equal to the number of bound electrons. Ionization is then associated with the decrease of this number caused in part by the disappearance of eigenvalues $\lambda_\nu(\mathbf{q})$ which merge into the continuous part of the spectrum, as the density of the system increases. This definition is in agreement with the results of ref. 9 in the limits considered there.

In order to see whether Girardeau's ideas are valid in other cases, we study in this paper the spectral properties of such pair density matrices for very simplified models. In particular, we consider the ratio $m/M \to 0$. In this limit we have $\mathbf{r} \sim \mathbf{X}$, $\mathbf{s} \sim \mathbf{Y}$ and the center of mass becomes a classical variable, whereas the relative degree of freedom remains quantum mechanical. Consequently, the center-of-mass momentum will, in this limit, be distributed according to a Maxwellian and

$$\rho_{\mathbf{q}}(\mathbf{x}_{\text{rel}}, \mathbf{y}_{\text{rel}}) \sim e^{-\beta[\hbar^2 |\mathbf{q}|^2/2(M+m)]} \bar{\rho}_2(\mathbf{x}_{\text{rel}}, \mathbf{y}_{\text{rel}}, \mathbf{0}) \tag{1.2}$$

Our problem is thus reduced to the study of the spectrum of the integral operator with kernel $\bar{\rho}_2(\mathbf{x}_{\text{rel}}, \mathbf{y}_{\text{rel}}, \mathbf{0}) = \rho_2(\mathbf{x}, \mathbf{r} \mid \mathbf{y}, \mathbf{r})$.

Our models consist of one quantum particle (the q-particle or "electron") in thermal equilibrium with a system of classical particles (the c-particles or "protons"). We assume that there is an attractive short-range force between the q-particles and the c-particles so that an isolated pair can bind to form "atomic states." While the presence of only one q-particle is not realistic, it greatly simplifies the analysis and we are able to investigate low-density as well as high-density regimes of the classical fluid. In fact one can formally obtain our models by starting from a more realistic situation with a finite density of q-particles and c-particles and letting the density of the q-particles tend to zero. The reduced density matrices of our models then correspond to the first-order term of an expansion with respect to the q-particle density.

When the density of the c-particles is also small we expect that

$$\rho_2(\mathbf{x}, \mathbf{r} \mid \mathbf{y}, \mathbf{r}) \sim (\mathbf{x} \mid \exp(-\beta H[\mathbf{r}]) \mid \mathbf{y}) \tag{1.3}$$

where $H[\mathbf{r}] = H_0 + V$ is the Hamiltonian of the q-particle in the potential V of a single c-particle at position $\mathbf{r}$. In this limit the spectrum will consist of a continuous part plus some eigenvalues closely related to the exponentials of the bound-state energies of an isolated atom. The same behavior is expected at high temperature. This argument is not sensitive to the particular model of the classical fluid and indeed the results will be similar for the two models that will be considered. At high c-particle density, however, (1.3) does not hold and the situation can be very different. Let us write the pair density matrix as

$$\rho_2(\mathbf{x}, \mathbf{r} \mid \mathbf{y}, \mathbf{r}) = \rho\rho_1(\mathbf{x}, \mathbf{y}) + \rho\left[\frac{\rho_2(\mathbf{x}, \mathbf{r} \mid \mathbf{y}, \mathbf{r})}{\rho} - \rho_1(\mathbf{x}, \mathbf{y})\right] \tag{1.4}$$

where ρ is the density of the classical fluid. In (1.4), $\rho_1(\mathbf{x}, \mathbf{y})$ is the reduced density matrix of the q-particle. For $\mathbf{x} = \mathbf{y}$, $\rho_1(\mathbf{x}, \mathbf{x})$ is the probability density to find a q-particle at $\mathbf{x}$, while $\rho_2(\mathbf{x}, \mathbf{r} \mid \mathbf{x}, \mathbf{r})/\rho$ is the conditional probability density to find the q-particle at $\mathbf{x}$ when one c-particle is fixed at position $\mathbf{r}$. Thus, for $\mathbf{x}=\mathbf{y}$ the term in the bracket can be interpreted as the excess electron density at $\mathbf{x}$ when a c-particle is fixed at $\mathbf{r}$.

In view of (1.4) we will consider the perturbation problem for the pair of operators $(\rho\rho_1, \rho_2)$ defined, respectively, by the kernels $\rho\rho_1(\mathbf{x}, \mathbf{y})$ and $\rho_2(\mathbf{x}, \mathbf{r} \mid \mathbf{y}, \mathbf{r})$, $\mathbf{r}$ fixed, in close analogy with the usual Schrödinger problem for a pair of Hamiltonians (H_0, H_0+V).

In a homogeneous system, we will have $\rho_1(\mathbf{x}, \mathbf{y})=\rho_1(\mathbf{x}-\mathbf{y}, \mathbf{0})$, so ρ_1 acts as a convolution operator, or equivalently, as the multiplication in Fourier space by the Fourier transform $\tilde{\rho}_1(\mathbf{k})$ of $\rho_1(\mathbf{x}, \mathbf{0})$. Therefore ρ_1 will have an absolutely continuous spectrum, whose spectral density is the kinetic energy distribution of the q-particle in the fluid. In fact, in a very dilute gas, or when the interaction is very small, $\tilde{\rho}_1(\mathbf{k})$ is close to the Maxwellian $(2\pi\beta\hbar^2/m)^{-3/2}\exp(-\beta(\hbar^2\mathbf{k}^2/2m))$. Thus, ρ_1 plays the role of the kinetic term, as does H_0 in the Schrödinger problem. The second term in (1.4) is the kernel of the truncated reduced density matrix $\rho_T \equiv \rho_2 - \rho\rho_1$. We observe that it vanishes if there is no interaction between the q-particle and the c-particles, and should tend to zero rapidly as $|\mathbf{x}-\mathbf{r}| \to \infty$ and $|\mathbf{y}-\mathbf{r}| \to \infty$, when the interaction is sufficiently short-ranged (clustering property). So ρ_T plays the role of a localized perturbation of ρ_1, as does the potential in the Schrödinger equation. It turns out in the models under consideration that ρ_T is a trace class operator (that is actually a stronger property than integrable clustering). Then by the basic theorems on perturbations by trace class operators, ρ_2 and $\rho\rho_1$ have the same absolutely continuous spectrum, so the knowledge of this part of the spectrum of ρ_2 is reduced to that of ρ_1.

The question is now to determine under what conditions the perturbation ρ_T creates eigenvalues in ρ_2. This will in general depend on the structure of the classical fluid.

We will consider two models for the system of c-particles: an ideal gas and a "cell model of a fluid."[10] In the cell model one basically divides space into a lattice of cells and allows each cell to be occupied by at most one c-particle with some probability distribution. This mimics a short-range repulsion between the particles and the variance of the number of particles in a given region tends to zero as the density increases. This is in contrast to the situation for the ideal gas, where this variance is proportional to the density and the particle configurations are Poissonian, which corresponds on a microscopic scale to large variations in the potential seen by the electron. For this reason, the q-particle excess density takes appreciable values, and clusters of c-particles may always bind with the q-particle; hence discrete eigenvalues of ρ_2 should persist at high density in the ideal gas model. In the cell model, the particle configurations become uniform at high density, and the q-particle will therefore see an essentially constant potential. Hence the excess particle density is small as ρ becomes large and only weakly perturbs ρ_1 in (1.4), leading to a disappearance of the eigenvalues of ρ_2 at high density. We note that the lattice model of the classical fluid where c-particles are forced to sit at fixed lattice sites is in many ways similar to the cell model and we expect it to have similar behavior. Its lack of translational invariance (which cannot be overcome by a simple averaging) makes it, however, more difficult to analyze rigorously. We comment on the lattice model at various points throughout the paper.

The main purpose of this paper is to establish the above-mentioned properties of the two models. The mathematical methods are the same as those used in the Schrödinger theory (perturbation of eigenvalues, equivalence of spectra, bounds on the number of eigenvalues), but we have in addition to control the spectral properties in terms of the thermodynamic parameters ρ and β. It is worth noting that our results are for three-dimensional space. The situation may be different in lower dimensions.

The disappearance of eigenvalues in the cell model can be viewed as an elementary prototype of a Mott transition in a partially ionized gas. Usually, a Mott transition is observed when some approximate two-body effective Hamiltonian $H_{\text{eff}}(\rho, \beta)$ loses its bound states as ρ varies.[6] Here, since ρ_2 is positive, an effective two-body Hamiltonian could be defined by $\rho_2 = \rho \exp[-\beta H_{\text{eff}}(\rho, \beta)]$: the spectrum of ρ_2 is simply the exponential of that of $H_{\text{eff}}(\rho, \beta)$. In this paper we do not attempt an approximate derivation of $H_{\text{eff}}(\rho, \beta)$, but rather study the spectral properties of ρ_2 without further approximation.

We note that the qualitative discussion presented here in the framework of simple models seems to be of general nature. The basic scheme (1.4) for the study of ρ_2 as a perturbation of ρ_1 should also work in a fully quantum mechanical many-body system. Clearly, the spectral properties of ρ_2 are intimately linked to the nature of the particle fluctuations: a Mott or a plasma ionization phase transition should correspond to a drastic reduction of these fluctuations in the system.

We are of course aware that this approach to the problem of bound states in a dense system is not the only one (see the discussion of this point in ref. 11). In particular, the definition of an effective Hamiltonian from purely static quantities such as the reduced density matrices may not be adapted to the study of line broadening or transport properties. It has, however, the virtue of leading to a well-posed spectral problem which can be treated by the mathematical tools developed in connection with the theory of Schrödinger operators.

We finally observe that for the specific models treated in this paper we are concerned with the spectral properties of an annealed problem: the q-particle is in thermal equilibrium with the c-particle. These spectral properties bear no evident relationship with those of the corresponding quenched problem, where one studies the spectral properties of the Hamiltonian of the q-particle for frozen configurations of c-particles. For instance, in one dimension, it is known that the spectrum is discrete for almost all configurations of c-particles,[12] whereas ρ_1 will still have a continuous spectrum. Also, the eigenfunctions belonging to the possible eigenvalues of ρ_2 have no obvious link to the localized states of random Schrödinger operators (here an attractive potential is needed while localization can occur independently of the sign of the potential). Clearly a better understanding of the connections between these two types of spectral problem would be of interest.

In Section 2, we first formulate the two models and then state the main results of the paper. The general spectral properties of ρ_1 and ρ_2 are established in Section 3. Section 4 is devoted to the low-density and high-temperature regimes, while the high-density limit is studied in Section 5. The appendices contain more technical material.

2. DESCRIPTION OF MODELS AND STATEMENT OF RESULTS

Given a configuration $\mathbf{r}_1 \cdots \mathbf{r}_n$ in $\mathbf{R}^3$ of classical particles, the Hamiltonian of the quantum particle is

$$H[\mathbf{r}_1 \cdots \mathbf{r}_n] = -\frac{1}{2} \Delta_{\mathbf{x}} + \sum_{i=1}^{n} V(\mathbf{x} - \mathbf{r}_i) \tag{2.1}$$

where $\Delta_{\mathbf{x}}$ is the Laplacian (we set $\hbar = m = 1$) and the potential $V(\mathbf{x})$ satisfies $V(\mathbf{x}) = V(-\mathbf{x})$, $V(\mathbf{x}) \leqslant 0$, and is six times continuously differentiable with

$$|\partial^k_{m_1 \cdots m_k} V(\mathbf{x})| \leqslant \frac{M}{(1 + |\mathbf{x}|^2)^{\eta/2}}, \qquad k = 0, 1, ..., 6 \tag{2.2}$$

and $\eta \geqslant 6$. It follows from (2.2) that the one-particle Hamiltonian $H[\mathbf{r}]$ has at most a finite number of bound states, $\phi_0, \phi_1, ..., \phi_g$, with energies $E_0 \leqslant E_1 \leqslant \cdots E_g \leqslant 0$.[16] We assume that this set is not empty.

For a bounded region $\Lambda \subset \mathbf{R}^3$, the reduced density matrix of the quantum particle is defined by the kernel

$$\rho_{1,\Lambda}(\mathbf{x}, \mathbf{y}) = \frac{1}{\Xi_\Lambda} \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_\Lambda d\mathbf{r}_1 \cdots \int_\Lambda d\mathbf{r}_n \, G_n(\mathbf{r}_1 \cdots \mathbf{r}_n) \, e^{-\beta H_\Lambda[\mathbf{r}_1 \cdots \mathbf{r}_n]}(\mathbf{x}, \mathbf{y}) \tag{2.3}$$

where $G_n(\mathbf{r}_1 \cdots \mathbf{r}_n)$ describes the probability density of classical particles in

Λ in the absence of the quantum particle and $H_\Lambda[\mathbf{r}_1 \cdots \mathbf{r}_n]$ denotes the Hamiltonian (2.1) with Dirichlet boundary conditions on $\partial\Lambda$. In (2.3), Ξ_Λ is the partition function obtained by taking the trace of the numerator. When one classical particle is fixed at position $\mathbf{r}$, the reduced density matrix of the pair of particles is

$$\rho_{2,\Lambda}(\mathbf{x}, \mathbf{y} \mid \mathbf{r}) = \frac{z}{\Xi_\Lambda} \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_\Lambda d\mathbf{r}_1 \cdots \int_\Lambda d\mathbf{r}_n \, G_{n+1}(\mathbf{r}, \mathbf{r}_1 \cdots \mathbf{r}_n) \times e^{-\beta H_\Lambda[\mathbf{r}, \mathbf{r}_1 \cdots \mathbf{r}_n]}(\mathbf{x}, \mathbf{y}) \tag{2.4}$$

In the simplest case where the classical fluid is just an ideal gas the function $G_n(\mathbf{r}_1 \cdots \mathbf{r}_n)$ is identically equal to one.

In the case of the cell model G_n is constructed as follows. We consider the lattice $\mathbf{L} = \{\mathbf{j}a \mid \mathbf{j} \in \mathbf{Z}^3,\ a > 0\}$ and call Δ the unit cell, centered at the origin, of volume $|\Delta| = a^3$. The characteristic function of Δ is χ_Δ. To a configuration $\mathbf{r}_1 \cdots \mathbf{r}_n$ of n classical particles we associate the weight function

$$G_n(\mathbf{r}_1 \cdots \mathbf{r}_n) = \frac{1}{|\Delta|} \int_\Delta d\tau \sum_{\mathbf{j}_1 \neq \mathbf{j}_2 \cdots \neq \mathbf{j}_n} \prod_{i=1}^{n} \frac{1}{|\Delta|} \chi_\Delta(\mathbf{r}_i - \mathbf{j}_i a - \tau) \tag{2.5}$$

This weight function selects, for each τ, configurations of n particles with at most one particle in a cell $\Delta + \mathbf{j}a + \tau$. Thus this function mimics a short-range repulsion between the particles. The extra integral over the translations $\tau \in \Delta$ of the lattice $\mathbf{L}$ will restore the translation invariance in the thermodynamic limit. As a consequence of the uniform distribution in every cell $G_n(\mathbf{r}_1, \ldots, \mathbf{r}_n) = G_1(\mathbf{r}_1)\, G_{n-1}(\mathbf{r}_2, \ldots, \mathbf{r}_n)$ for $|\mathbf{r}_1 - \mathbf{r}_i| > 2a$, $i = 2, \ldots, n$ and the cell model classical fluid has strong cluster properties at all densities.

If we replace $(1/|\Delta|)\, \chi_\Delta$ by the Dirac measure and remove the τ integral in (2.5), we obtain a usual lattice model for the classical system. However, the full translation invariance (in $\mathbf{R}^3$) turns out to be helpful for our purposes and in this respect the cell model is simpler than the lattice model.

It is possible to show that $|\Lambda|\, \rho_{1,\Lambda}(\mathbf{x}, \mathbf{y})$ and $|\Lambda|\, \rho_{2,\Lambda}(\mathbf{x}, \mathbf{y} \mid \mathbf{r})$ have well-defined thermodynamic limits for all the models.[3] To compute them, we use a functional integral representation of the kernels,[13]

$$\exp(-\beta H_\Lambda[\mathbf{r}_1 \cdots \mathbf{r}_n])(\mathbf{x}, \mathbf{y}) = \frac{\exp[-(\mathbf{x}-\mathbf{y})^2/2\beta]}{(2\pi\beta)^{3/2}} \int \mathbf{D}\alpha\, \chi_\Lambda(\alpha_{\mathbf{xy}}) \times \prod_{i=1}^{n} \exp\left[-\beta \int_0^1 ds\, V(\alpha_{\mathbf{xy}}(s) - \mathbf{r}_i)\right] \tag{2.6}$$

[3] We introduce a volume factor $|\Lambda|$ to take into account that the density of the single quantum particle is $|\Lambda|^{-1}$.

where

$$\alpha_{\mathbf{xy}}(s) = \mathbf{x} + s(\mathbf{y} - \mathbf{x}) + \sqrt{\beta}\,\alpha(s)$$

and α is the Gaussian Brownian bridge process $\alpha(s) = (\alpha_1(s), \alpha_2(s), \alpha_3(s))$, $0 \leqslant s \leqslant 1$, $\alpha_j(0) = \alpha_j(1) = 0$, with zero mean and covariance $s(1-t)\,\delta_{ij}$ $(i, j = 1, 2, 3)$ for $s \leqslant t$. $\chi_\Lambda(\alpha_{\mathbf{xy}})$ represents the characteristic function of the paths $\alpha_{\mathbf{xy}}(s)$ that stay in Λ for all s, $0 \leqslant s \leqslant 1$. To obtain the thermodynamic limit of $\rho_{1,\Lambda}$ and $\rho_{2,\Lambda}$ it is convenient to divide the numerator and the denominator of (2.3) and (2.4) by the partition function of the classical system without the quantum particle. We give the explicit formulas only for the cell model and indicate the necessary modifications for the ideal gas and lattice models. We get for the cell model

$$\begin{aligned}\rho_1(\mathbf{x}, \mathbf{y}) &\equiv \lim_{\Lambda} |\Lambda|\, \rho_{1,\Lambda}(\mathbf{x}, \mathbf{y}) \\ &= \frac{1}{N(\rho, \beta)} \frac{\exp[-(\mathbf{x}-\mathbf{y})^2/2\beta]}{(2\pi\beta)^{3/2}} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \\ &\quad \times \int_\Delta \mathbf{d}\tau \exp\left[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha)\right] \end{aligned} \tag{2.7}$$

$$\begin{aligned}\rho_2(\mathbf{x}, \mathbf{y} \mid \mathbf{0}) &\equiv \lim_{\Lambda} |\Lambda|\, \rho_{2,\Lambda}(\mathbf{x}, \mathbf{y} \mid \mathbf{0}) \\ &= \frac{\rho}{N(\rho, \beta)} \frac{\exp[-(\mathbf{x}-\mathbf{y})^2/2\beta]}{(2\pi\beta)^{3/2}} \\ &\quad \times \int \mathbf{D}\alpha \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau \exp\left[\sum_{\mathbf{j} \neq \mathbf{0}} C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha)\right] \\ &\quad \times \exp\left[-\beta \int_0^1 ds\, V(\alpha_{\mathbf{xy}}(s))\right] \end{aligned} \tag{2.8}$$

where

$$\begin{aligned} N(\rho, \beta) &= (2\pi\beta)^{-3/2} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau \\ &\quad \times \exp\left[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{x}, \alpha)\right] \end{aligned} \tag{2.9}$$

$$\begin{aligned} C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha) &= \ln\Bigg(1 + \rho \int_\Delta \mathbf{dr} \\ &\quad \times \left\{\exp\left[-\beta \int_0^1 ds\, V(\alpha_{\mathbf{xy}}(s) - \mathbf{r} - \mathbf{j}a - \tau)\right] - 1\right\}\Bigg) \end{aligned} \tag{2.10}$$

and the parameter

$$\rho = \frac{z}{1+z} \frac{1}{|\Delta|}$$

is the density of the classical fluid, $z/(1+z)$ being the mean occupation number of one cell. In Appendix A we derive the formulas (2.7)–(2.10) and check that the reduced density matrices are translation invariant, i.e., $\rho_1(\mathbf{x}+\mathbf{x}_0, \mathbf{y}+\mathbf{x}_0) = \rho_1(\mathbf{x}, \mathbf{y})$ and $\rho_2(\mathbf{x}+\mathbf{x}_0, \mathbf{y}+\mathbf{x}_0 \,|\, \mathbf{0}) = \rho_2(\mathbf{x}, \mathbf{y} \,|\, -\mathbf{x}_0)$. This implies in particular that the integral operators with kernels $\rho_2(\mathbf{x}, \mathbf{y} \,|\, \mathbf{r})$ are, for different values of $\mathbf{r}$, unitarily equivalent. Since we will be concerned with the spectral properties, it is sufficient to study $\rho_2(\mathbf{x}, \mathbf{y} \,|\, \mathbf{0})$, as defined by (2.8).

From (2.7) and (2.8) we can form the truncated reduced density matrix

$$\begin{aligned} \rho_T(\mathbf{x}, \mathbf{y}) &= \rho_2(\mathbf{x}, \mathbf{y} \,|\, \mathbf{0}) - \rho\rho_1(\mathbf{x}, \mathbf{y}) \\ &= \frac{\rho}{N(\rho, \beta)} \frac{\exp[-(\mathbf{x}-\mathbf{y})^2/2\beta]}{(2\pi\beta)^{3/2}} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \\ &\quad \times \int_\Delta \mathbf{d}\tau \exp\left[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha)\right] \\ &\quad \times \left[\frac{\exp[-\beta \int_0^1 ds\, V(\alpha_{\mathbf{xy}}(s))]}{1 + \rho \int_\Delta \mathbf{dr}\, \{\exp[-\beta \int_0^1 ds\, V(\alpha_{\mathbf{xy}}(s) - \mathbf{r} - \mathbf{j}a - \tau)] - 1\}} - 1\right] \end{aligned} \tag{2.11}$$

which is also translation invariant.

Other Models. In the case of the ideal gas model the formulas for the reduced density matrices are the same as (2.7)–(2.8) with $\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha)$ replaced by the functional $\rho F(\mathbf{y}-\mathbf{x}, \alpha)$, where

$$F(\mathbf{x}, \alpha) = \int \mathbf{dr} \left\{\exp\left[-\beta \int_0^1 ds\, V(s\mathbf{x} + \sqrt{\beta}\, \alpha(s) - \mathbf{r})\right] - 1\right\} \tag{2.12}$$

For this model the density matrices are again translation invariant and $\rho = z$. In the corresponding reduced density matrix, the large bracket in (2.11) has to be replaced by

$$\left\{\exp\left[-\beta \int_0^1 ds\, V(\alpha_{\mathbf{xy}}(s))\right] - 1\right\} \tag{2.13}$$

To obtain the analogous formulas for the lattice model we just have to replace $(1/|\Delta|)\,\chi_\Delta$ by the Dirac measure. Then we get (2.7) and (2.8) with $C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha)$ replaced by

$$G_{\mathbf{j}}(\mathbf{x}, \mathbf{y}, \alpha) = \ln\left(1 + \frac{z}{1+z}\left\{\exp\left[-\beta\int_0^1 ds\; V(\alpha_{\mathbf{xy}}(s) - \mathbf{j}a)\right] - 1\right\}\right) \tag{2.14}$$

Here the parameter $z/(1+z)$ represents the occupation probability of a lattice site and the density matrices have the periodicity of the lattice.

Following the ideas presented in the Introduction, we have studied the spectrum of the pair reduced density matrix in the cases of the ideal gas and cell models. For the lattice model the lack of full translation invariance makes this study more difficult and we only present some comments at the end of this section. Averaging the position of the lattice over a unit cell makes the one-particle density matrix translation invariant but destroys the cluster property of the pair correlations.

The integral operator with kernel $\rho_2(\mathbf{x}, \mathbf{y}\,|\,\mathbf{0})$ will be denoted by ρ_2. It can be considered as an integral bounded self-adjoint operator from $L^2(\mathbf{R}^3)$ to $L^2(\mathbf{R}^3)$ (see the beginning of Section 3). Our main results on the spectra of ρ_2 for the ideal gas and cell models in three dimensions are summarized below.

I. *General Properties.* For any ρ, β the spectrum of ρ_2 has an absolutely continuous part spanning the interval $[0, \Sigma]$, with $\Sigma = \rho \int \mathbf{dx}\, \rho_1(\mathbf{x}, \mathbf{0})$. If the spectrum is not empty outside this interval, then it consists of a finite number of isolated eigenvalues all greater than Σ.

II. *Low-Density and High-Temperature Limits.* For a given β there exist densities ρ small enough (depending on β) such that the discrete part of the spectrum is not empty and there exist eigenvalues λ_ν that are related to the single-atom energy levels E_ν by

$$\lim_{\rho\to 0} \frac{\lambda_\nu}{\Sigma} = e^{-\beta E_\nu} \tag{2.15}$$

The edge Σ of the continuous spectrum is asymptotic to $\rho(2\pi\beta)^{3/2}$ for $\rho \to 0$.

There exist a $\bar{\rho}$, independent of β, such that for $\rho < \bar{\rho}$ and β small enough the discrete part of the spectrum is not empty. All eigenvalues are asymptotic to Σ as $\beta \to 0$, i.e., they merge in the continuous spectrum. The edge of the continuous spectrum is asymptotic to $\rho(2\pi\beta)^{3/2}$ for $\beta \to 0$. Moreover, in the case of the ideal gas model we have $\bar{\rho} = \infty$ and

$$\frac{(\phi_\nu, \rho_2 \phi_\nu)}{\Sigma} = e^{-\beta E_\nu(1 + o(1))} \tag{2.16}$$

III. *High-Density Limit.* In the ideal gas model, for fixed β and for ρ large enough the discrete part of the spectrum is not empty. Remarkably enough, this remains true for an arbitrarily weak attractive potential, i.e., even when the one-particle Hamiltonian $H[\mathbf{r}]$ has no bound states. Moreover, in this limit $\Sigma = O(\rho^{1/4})$.

In the case of the cell model for fixed β, $|\Delta|$ fixed small enough, and z large enough (depending on β and $|\Delta|$), the discrete part of the spectrum is empty. Moreover, in this limit $\Sigma = O(\rho^{3/4})$.

The results I–II will be shown rigorously. The derivation of III is not entirely rigorous insofar as it involves the formal computation of some functional integrals by the Laplace method. According to the above results, it is likely that in the ideal gas model the discrete part of the spectrum of ρ_2 is always nonempty. At low density or high temperature ρ_2 has some eigenvalues that are related to the energy levels of the isolated atom. However, we cannot exclude the existence of other eigenvalues regardless of density (and temperature). As already noted in the Introduction, we believe the existence of eigenvalues at high density for the ideal gas model to be a consequence of large density fluctuations (the variance of the particle number, in any region, divided by the region's volume being equal to ρ). Consequently, the quantum particle may form bound states with clusters of classical particles that happen to be near the same point, thus forming a trap for the quantum particle. This also explains why there exists eigenvalues even when the potential is so weak that the one-particle Hamiltonian $H[\mathbf{r}]$ does not have bound states. In a situation where the density of classical particles is uniform with little fluctuations we expect that the quantum particle cannot bind and the spectrum of the pair reduced density matrix will be entirely continuous. This is precisely the case for a classical fluid modeled by the cell model as we increase the density.

Ionization Equilibrium Limit. Another limit of interest is the "ionization equilibrium limit."[4,9] This case is obtained by setting the chemical potential $\mu(\beta) = E_0 + \sigma\beta^{-1} + o(\beta^{-1})$, $\sigma \in \mathbf{R}$, $z(2\pi\beta)^{3/2} = \exp(\beta\mu)$. Then it is possible to show in the case of the cell model that if $|\Delta|$ (the size of the cells) is large enough,

$$\lim_{\beta \to \infty} \rho_2(\mathbf{x}, \mathbf{y} \,|\, \mathbf{0}) = (1 - \alpha)\, \phi_0(\mathbf{x})\, \phi_0(\mathbf{y}) \tag{2.17}$$

with

$$\alpha = \lim_{\beta \to \infty} [1 + z(2\pi\beta)^{3/2}\, e^{-\beta E_0}]^{-1} = (1 + e^{\sigma})^{-1} \tag{2.18}$$

If we fix $\mu < E_0$, then (2.17) holds with $\alpha = 1$, which corresponds to

$\sigma = -\infty$. On the other hand, one can show that if μ is fixed slightly above E_0, then (2.17) holds with $\alpha = 0$. Formula (2.18) corresponds to the Saha formula for the degree of ionization (see ref. 9 for a discussion of this point). We note that Girardeau's definition for the fraction of bound particles[8] is consistent with (2.17). To obtain (2.17), it is crucial that the following operator inequality holds:

$$H[\mathbf{r}_1,..., \mathbf{r}_n] \geqslant -Kn, \qquad K < |E_0|, \qquad n \geqslant 2 \tag{2.19}$$

For the cell model, (2.19) is valid as long as $|\Delta|$ is large enough, but it is not for the ideal gas model. Equations (2.17)–(2.19) and their proofs are similar to those of the model considered in ref. 9 and we will not discuss them in what follows.

Outline of the Proofs. As described in the Introduction, our analysis is based on treating the integral operator ρ_1 with kernel $\rho_1(\mathbf{x}, \mathbf{y})$ [see (2.7)] as our unperturbed "reference system" and ρ_T as a "perturbation." The operator ρ_1 is bounded and self-adjoint from $L^2(\mathbf{R}^3)$ to $L^2(\mathbf{R}^3)$ (see beginning of Section 3). We also consider the Fourier transform

$$\tilde{\rho}_1(\mathbf{k}) = \int d\mathbf{x}\, e^{-i\mathbf{k}\cdot\mathbf{x}} \rho_1(\mathbf{x}, \mathbf{0}) \tag{2.20}$$

The following propositions, which we prove in Section 3, will play an important role.

Proposition 1. For any ρ and β, ρ_1 has an absolutely continuous spectrum given by $[0, \tilde{\rho}_1(0)]$.

Proposition 2. For any ρ and β, the truncated reduced density matrix $\rho_T = \rho_2 - \rho\rho_1$ is a trace class operator.

It follows from standard theorems on the stability of absolutely continuous spectra[14] that

$$\rho_2 = \rho\rho_1 + \rho_T \tag{2.21}$$

has an absolutely continuous part in its spectrum, covering the interval $[0, \rho\tilde{\rho}_1(0)]$. Moreover, by the Weyl–von Neumann theorem[14] this interval coincides with the essential spectrum. Thus, outside this interval the spectrum can consist only of isolated eigenvalues with finite multiplicities.[4] Moreover, these eigenvalues are all greater than $\Sigma = \rho\tilde{\rho}_1(0)$, since ρ_2 is a

[4] It cannot be excluded on general grounds that ρ_2 has also a singular continuous part in $[0, \rho\tilde{\rho}_1(0)]$. We will assume throughout the paper that this does not occur.

positive operator (the thermodynamic limit of positive operators). Thus, what remains to be proven for result I is that the number of eigenvalues is finite. This will be achieved by the Birman–Schwinger technique in Section 3. Let us remark at this point that since ρ_2 is a bounded operator, it could have an infinity of eigenvalues only if Σ is an accumulation point of the discrete spectrum.

The low-density limit is the easiest part and is treated in Section 4. In this case the properties of the discrete spectrum can easily be derived by perturbation theory around $\rho = 0$.

We can construct a variational principle which will be useful in some cases to prove the existence of eigenvalues. In view of the properties of the spectrum that we outlined before we know that the discrete part is not empty if we can find a function $\phi \in L^2(\mathbf{R}^3)$ such that $\|\phi\|_2 = 1$ and

$$\frac{(\phi, \rho_2 \phi)}{\Sigma} > 1 \tag{2.22}$$

This will be used for the investigation of the high-temperature limit in Section 4.

The high-density limit is the subject of Section 5. For the case of the ideal gas we use again the variational principle (2.22). The absence of a discrete spectrum for the cell model is proven with the aid of a Birman–Schwinger technique.

Lattice Model. Before closing this section, we comment on the lattice model defined by (2.14). For all $z > 0$, ρ_1 is only invariant under the discrete lattice translations, so it can have an absolutely continuous band spectrum with a number of gaps. It can be checked that ρ_T satisfies Proposition 2, hence ρ_2 will have the same band spectrum as $\rho\rho_1$.

As far as the existence of eigenvalues is concerned, we observe that there is a limiting situation, i.e., the full occupancy of the lattice $z/(1+z) = 1$, where ρ_2 has certainly no eigenvalues. Indeed, in the limit of full occupancy when $z/(1+z) = 1$, ρ_2 reduces to $\rho\rho_1 \sim \exp(-\beta H_{\text{per}})$, where $H_{\text{per}} = -\frac{1}{2}\Delta_{\mathbf{x}} + \sum_{\mathbf{j}} V(\mathbf{x} - \mathbf{j}a)$ is the Hamiltonian of an electron in a perfectly periodic crystal. Thus ρ_2 has a continuous band spectrum and no discrete part. On the other hand, for a sufficiently small occupation number $z/(1+z)$ of the lattice, one can reproduce the analysis of Section 4 to show that there exist at least eigenvalues $\lambda_\nu \sim \exp(-\beta E_\nu)$ above the supremum Σ of the band spectrum.

Therefore as the occupancy number increases to 1 it will reach a value where all eigenvalues above Σ disappear [certainly at $z/(1+z) = 1$, but presumably in some range of values close to 1].

The main difference with the cell model is that this will occur irrespective of the lattice spacing a, which we can choose as large as we wish. The disappearance of the discrete spectrum in the lattice model is thus a result of quantum mechanical coherence due to the strict periodicity of the lattice. This coherence due to the absence of fluctuations remains even when we send all the classical particles far apart by letting $a \to \infty$. So the cell model and the lattice model share the common feature that the disappearance of eigenvalues is caused by a reduction of the particle fluctuations.

3. GENERAL PROPERTIES OF THE REDUCED DENSITY MATRICES

It follows from the definitions (2.3) and (2.4) that the finite-volume kernels $\rho_{1,\Lambda}$ and $\rho_{2,\Lambda}$ are symmetric and positive definite. These properties are preserved in the thermodynamic limit.

We now derive some useful pointwise estimates on the infinite volume kernels (2.7), (2.8), and (2.11) for the cell model.

Using $\ln(1+x) \leqslant x$ for $x \geqslant 0$ in (2.10), we have

$$C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha) \leqslant \rho \int_{\Lambda} d\mathbf{r} \left\{ \exp\left[-\beta \int_0^1 ds\, V(\alpha_{\mathbf{xy}}(s) - \mathbf{r} - \mathbf{j}a - \tau) \right] - 1 \right\} \tag{3.1}$$

Applying the Jensen inequality to the integral over s in the right-hand side of (3.1) then gives

$$\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha) \leqslant \rho \int d\mathbf{r}\, (e^{-\beta V(\mathbf{r})} - 1) = \rho v(\beta) \tag{3.2}$$

Thus from (2.7)

$$\rho_1(\mathbf{x}, \mathbf{y}) \leqslant \frac{e^{\rho v(\beta)}}{N(\rho, \beta)} \frac{e^{-(\mathbf{x}-\mathbf{y})^2/2\beta}}{(2\pi\beta)^{3/2}} \tag{3.3}$$

Since the potential V is assumed to be bounded, we obtain from (2.8) a similar bound for $\rho_2(\mathbf{x}, \mathbf{y} \mid \mathbf{0})$

$$\rho_2(\mathbf{x}, \mathbf{y} \mid \mathbf{0}) \leqslant \frac{e^{\rho v(\beta)} e^{\beta \sup |V|}}{N(\rho, \beta)} \frac{e^{-(\mathbf{x}-\mathbf{y})^2/2\beta}}{(2\pi\beta)^{3/2}} \tag{3.4}$$

The inequality (3.4) implies that

$$\tilde{M} \equiv \max\left[\sup_{\mathbf{x}} \int d\mathbf{y}\, |\rho(\mathbf{x}, \mathbf{y})|, \sup_{\mathbf{y}} \int d\mathbf{x}\, |\rho(\mathbf{x}, \mathbf{y})| \right] < \infty \tag{3.5}$$

where $\rho(\mathbf{x}, \mathbf{y})$ stands for $\rho_1(\mathbf{x}, \mathbf{y})$ or $\rho_2(\mathbf{x}, \mathbf{y} \mid \mathbf{0})$. We conclude[14] that the two symmetric kernels (2.7) and (2.8) represent bounded self-adjoint operators on $L^2(\mathbf{R}^3)$.

Since V is negative, the denominator in the bracket in (2.11) is larger than one. Using $e^x - 1 \leqslant xe^x$, $x \geqslant 0$, and (2.2), we find that this bracket is less than

$$\beta e^{\beta \sup |V|} \int_0^1 ds \, |V(\alpha_{\mathbf{xy}}(s))| \leqslant \beta e^{\beta \sup |V|} M \int_0^1 ds \, [1 + |\alpha_{\mathbf{xy}}(s)|^2]^{-\eta/2} \tag{3.6}$$

and then, from (3.2), we have for the kernel of the truncated density matrix

$$|\rho_T(\mathbf{x}, \mathbf{y})| \leqslant C(\rho, \beta) \frac{e^{-(\mathbf{x}-\mathbf{y})^2/2\beta}}{(2\pi\beta)^{3/2}} \int \mathbf{D}\alpha \int_0^1 ds \, [1 + |\alpha_{\mathbf{xy}}(s)|^2]^{-\eta/2} \tag{3.7}$$

where $C(\rho, \beta)$ depends only on density and temperature. The estimates (3.3), (3.4), and (3.7) are also true for the ideal gas model.

For the cell model, we can obtain a better estimate on $\rho_T(\mathbf{x}, \mathbf{y})$ for small a if we use the condition (2.2) on the derivative of the potential. By the truncated Taylor expansion, this condition implies that for $\mathbf{r}$, $\tau \in \Lambda$

$$\int_0^1 ds \, [V(\alpha_{\mathbf{xy}}(s) - \mathbf{r} - \tau) - V(\alpha_{\mathbf{xy}}(s))] \leqslant aC \int_0^1 ds \, [1 + |\alpha_{\mathbf{xy}}(s)|^2]^{-\eta/2} \tag{3.8}$$

with C independent of a for a small. Using again that V is negative, (3.6), and (3.8), we obtain that the bracket in (2.11) is majorized by

$$\begin{aligned} &\frac{1}{1+z} \left\{ \exp\left[-\beta \int_0^1 ds \, V(\alpha_{\mathbf{xy}}(s)) \right] - 1 \right\} \\ &\quad + \frac{z}{1+z} \frac{1}{|\Lambda|} \int_\Lambda \mathbf{dr} \\ &\quad \times \left| \exp\left[-\beta \int_0^1 ds \, V(\alpha_{\mathbf{xy}}(s) - \mathbf{r} - \tau) \right] - \exp\left[-\beta \int_0^1 ds \, V(\alpha_{\mathbf{xy}}(s)) \right] \right| \\ &\leqslant A\beta [\exp(\beta \sup |V|)](z^{-1} + a) \int_0^1 ds \, [1 + |\alpha_{\mathbf{xy}}(s)|^2]^{-\eta/2} \end{aligned} \tag{3.9}$$

with A constant.

Thus, contrary to the ideal gas model [see (2.13)], the bracket in (2.11) is vanishingly small at high density (i.e., z large and a small enough).

Proof of Proposition 1. Because of translation invariance we have for any $\phi \in L^2(\mathbf{R}^3)$

$$(\rho_1 \phi)(\mathbf{x}) = \int \mathbf{dy}\, \rho_1(\mathbf{x}-\mathbf{y}, 0)\, \phi(\mathbf{y}) \tag{3.10}$$

Note that by (3.3), $\rho_1(\mathbf{x}, \mathbf{0})$ is in $L^2(\mathbf{R}^3) \cap L^1(\mathbf{R}^3)$, so ρ_1 acts as a multiplication operator in the Fourier representation

$$\widetilde{(\rho_1 \phi)}(\mathbf{k}) = \tilde{\rho}_1(\mathbf{k})\, \tilde{\phi}(\mathbf{k}) \tag{3.11}$$

Because of the bound (3.3), $\tilde{\rho}_1(\mathbf{k})$ is an entire function of the component of $\mathbf{k}$, so it cannot be constant on open sets of $\mathbf{R}^3$. Thus ρ_1 has an absolutely continuous spectrum given by the image of the function $\tilde{\rho}_1(\mathbf{k})$. Since $\tilde{\rho}_1(\mathbf{k}) \geqslant 0$ and $\lim_{|\mathbf{k}| \to \infty} \tilde{\rho}_1(\mathbf{k}) = 0$, the spectrum is $[0, \sup_{\mathbf{k}} \tilde{\rho}_1(\mathbf{k})]$. Finally, since $\rho_1(\mathbf{x}, \mathbf{0}) \geqslant 0$ we have

$$\tilde{\rho}_1(\mathbf{0}) \leqslant \sup_{\mathbf{k}} \tilde{\rho}_1(\mathbf{k}) \leqslant \int \mathbf{dx}\, |\rho_1(\mathbf{x}, \mathbf{0})| = \int \mathbf{dx}\, \rho_1(\mathbf{x}, \mathbf{0}) = \tilde{\rho}_1(\mathbf{0}) \tag{3.12}$$

This completes the proof of Proposition 1.

Remark. The function $\tilde{\rho}_1(\mathbf{k})$ attains its maximum only for $\mathbf{k} = \mathbf{0}$. Indeed, we see from (2.7) that $\rho_1(\mathbf{x}, \mathbf{0}) = \rho_1(-\mathbf{x}, \mathbf{0})$ and that $\rho_1(\mathbf{x}, \mathbf{0})$ is strictly positive for finite $\mathbf{x}$,

$$\rho_1(\mathbf{x}, \mathbf{0}) \geqslant \frac{1}{N(\rho, \beta)} \frac{e^{-(\mathbf{x})^2/2\beta}}{(2\pi\beta)^{3/2}}$$

since $V(\mathbf{x}) < 0$. Thus, for any $\mathbf{k} \neq \mathbf{0}$, the integrand of

$$\tilde{\rho}_1(\mathbf{k}) = \int \mathbf{dx}\, \cos(\mathbf{k} \cdot \mathbf{x})\, \rho_1(\mathbf{x}, \mathbf{0}) \tag{3.13}$$

is strictly less than $\rho_1(\mathbf{x}, \mathbf{0})$ on some open set not containing the points $\mathbf{k} \cdot \mathbf{x} \in 2\pi\mathbf{Z}$. Hence $\tilde{\rho}_1(\mathbf{k}) < \tilde{\rho}_1(\mathbf{0})$, $\mathbf{k} \neq \mathbf{0}$.

Proof of Proposition 2. To prove that ρ_T belongs to the trace class, it is sufficient to represent it as a product of two Hilbert–Schmidt operators.[14] Let $h(\mathbf{x}) = 1$ for $|\mathbf{x}| \leqslant 1$ and $h(\mathbf{x}) = |\mathbf{x}|^{-(3/2+\varepsilon)}$ for $|\mathbf{x}| \geqslant 1$, with $\varepsilon > 0$. We denote by h the multiplication operator by this function. One can easily check that the operator

$$K = (-\Delta + 1)^{-1}\, h \tag{3.14}$$

is Hilbert–Schmidt. Since $\rho_T = K(K^{-1}\rho_T)$, it is sufficient to prove that $(K^{-1}\rho_T)$ is Hilbert–Schmidt, i.e.,

$$\int \mathbf{dx} \int \mathbf{dy}\, |h(\mathbf{x})|^{-2}\, |(-\Delta_{\mathbf{x}} + 1)\, \rho_T(\mathbf{x}, \mathbf{y})|^2 < \infty \tag{3.15}$$

With the explicit formula (2.11) for $\rho_T(\mathbf{x}, \mathbf{y})$ we check in Appendix B that (3.15) holds.

For the proof of I we will need the following result.

Lemma 3.1. Let $|\rho_T| = [(\rho_T)^2]^{1/2}$. The kernel of this operator satisfies

$$J_1 \equiv \int \mathbf{dx} \int \mathbf{dy}\, |(|\rho_T|)(\mathbf{x}, \mathbf{y})| < \infty \tag{3.16}$$

$$J_2 \equiv \int \mathbf{dx} \int \mathbf{dy} \left[\int \mathbf{dz}\, |(|\rho_T|)(\mathbf{x}, \mathbf{z})|\; |(|\rho_T|)(\mathbf{z}, \mathbf{y})| \right] < \infty \tag{3.17}$$

Here the nontrivial point is that we have to deal with the kernel of $|\rho_T|$ instead of ρ_T.

Proof. From Schwartz's inequality

$$\begin{aligned} J_2 &\leqslant \int \mathbf{dx} \int \mathbf{dy} \left[\int \mathbf{dz}\, |(|\rho_T|)(\mathbf{x}, \mathbf{z})|^2 \right]^{1/2} \left[\int \mathbf{dz}\, |(|\rho_T|)(\mathbf{z}, \mathbf{y})|^2 \right]^{1/2} \\ &= \left\{ \int \mathbf{dx} \left[\int \mathbf{dz}\, |(|\rho_T|)(\mathbf{x}, \mathbf{z})|^2 \right]^{1/2} \right\}^2 \end{aligned} \tag{3.18}$$

We introduce again the same function $h(\mathbf{x})$ as in the proof of Proposition 2. By (3.18) and the Schwartz inequality

$$\begin{aligned} J_2 &\leqslant \left\{ \int \mathbf{dx}\, h(\mathbf{x})[h(\mathbf{x})]^{-1} \left[\int \mathbf{dz}\, |(|\rho_T|)(\mathbf{x}, \mathbf{z})|^2 \right]^{1/2} \right\}^2 \\ &\leqslant \left[\int \mathbf{dx}\, |h(\mathbf{x})|^2 \right] \left[\int \mathbf{dx}\, |h(\mathbf{x})|^{-2} \int \mathbf{dz}\, |(|\rho_T|)(\mathbf{x}, \mathbf{z})|^2 \right] \end{aligned} \tag{3.19}$$

We recall that the multiplication operator by the function $h(\mathbf{x})$ is denoted simply by h. The last bracket in (3.19) is the square of the Hilbert–Schmidt norm of $h^{-1}\, |\rho_T|$. Introducing the polar decomposition of the self-adjoint operator ρ_T (i.e., $|\rho_T| = \rho_T U$, U unitary) we notice $\|h^{-1}|\rho_T|\|_2 = \|h^{-1}\rho_T\|_2$, and therefore

$$J_2 \leqslant \left[\int \mathbf{dx}\, |h(\mathbf{x})|^2\right]\left[\int \mathbf{dx} \int \mathbf{dy}\, |h(\mathbf{x})|^{-2}\, |\rho_T(\mathbf{x}, \mathbf{y})|^2\right] \tag{3.20}$$

Now with the help of the estimate (3.7) it is possible to check that $J_2 < \infty$ [for ε small enough in the function $h(\mathbf{x})$].

For J_1 we write

$$\begin{aligned} J_1 &= \int \mathbf{dx} \int \mathbf{dy}\, h(\mathbf{x})\, h(\mathbf{y})[h(\mathbf{x})\, h(\mathbf{y})]^{-1}\, |(|\rho_T|)(\mathbf{x}, \mathbf{y})| \\ &\leqslant \left[\int \mathbf{dx}\, |h(\mathbf{x})|^2\right]\left\{\int \mathbf{dx} \int \mathbf{dy}\, [h(\mathbf{x})\, h(\mathbf{y})]^{-2}\, |(|\rho_T|)(\mathbf{x}, \mathbf{y})|^2\right\}^{1/2} \\ &\leqslant \left[\int \mathbf{dx}\, |h(\mathbf{x})|^2\right]\left\{\int \mathbf{dx} \int \mathbf{dy}\, [h(\mathbf{x})]^{-4}\, |(|\rho_T|)(\mathbf{x}, \mathbf{y})|^2\right\}^{1/2} \end{aligned} \tag{3.21}$$

The first inequality is Schwartz and for the second we use $g(1/2) \leqslant \frac{1}{2}[g(0) + g(1)]$ for the convex function of t,

$$g(t) \equiv \left\{\int \mathbf{dx} \int \mathbf{dy}\, [h(\mathbf{x})]^{-4t}\, [h(\mathbf{y})]^{-4(1-t)}\, |(|\rho_T|)(\mathbf{x}, \mathbf{y})|^2\right\} \tag{3.22}$$

The bound (3.21) involves the Hilbert–Schmidt norm of $h^{-2}|\rho_T|$, which is equal to that of $h^{-2}\rho_T$. Thus, in the last line of (3.21) we can replace $|\rho_T|$ by ρ_T and explicitly show that the bound is finite as for (3.20) (for ε small enough). Let us just remark that this time the fourth power of $h(\mathbf{x})$ [instead of the square in (3.20)] appears, so we really need that the potential V is $O(|\mathbf{x}|^{-\eta})$, $\eta \geqslant 6$, at infinity. This completes the proof of Lemma 3.1.

Let N be the number of eigenvalues of ρ_2 that are greater than Σ. According to the discussion after Propositions 1 and 2, the proof of I will be complete if we show $N < \infty$. For this we introduce N', the number of eigenvalues of $\rho\rho_1 + |\rho_T|$. The following inequality holds:

$$N \leqslant N' \tag{3.23}$$

This is a special case of the following result.

Lemma 3.2. Let A, B be self-adjoint operators such that $A \leqslant B$. Let σ be the supremum of the essential spectrum of B. Let $N(A, \sigma)$ and $N(B, \sigma)$

be the number of bound states of A and B above σ. Then $N(A, \sigma) \leqslant N(B, \sigma)$.

This Lemma is stated in ref. 15, p. 54, and can easily be proven by the minmax principle.

If we set $A = \rho_2$, $B = \rho\rho_1 + |\rho_T|$, we have $A \leqslant B$ and $\sigma = \Sigma$ as a consequence of Propositions 1 and 2. Thus we can apply Lemma 3.2 to our choice of A and B to obtain (3.23).

Proof of I Completed. For $\lambda > \Sigma$ we define

$$K(\lambda) = |\rho_T|^{1/2} (\lambda - \rho\rho_1)^{-1} |\rho_T|^{1/2} \tag{3.24}$$

From Proposition 2 we know that $|\rho_T|^{1/2}$ is Hilbert–Schmidt. For a given $\lambda > \Sigma$, $(\lambda - \rho\rho_1)^{-1}$ is bounded, so $K(\lambda)$ is also Hilbert–Schmidt (even trace class). Consequently we can apply the Birman–Schwinger principle in the form[16] (see also ref. 17)

$$N' \leqslant \lim_{\lambda \to \Sigma} \operatorname{Tr} K(\lambda)\, K(\lambda)^+ \tag{3.25}$$

In (3.25) the limit may be finite or infinite. We will show that it is in fact finite and therefore, using (3.23), $N < \infty$. We make the following decomposition:

$$\operatorname{Tr} K(\lambda)\, K(\lambda)^+ = \operatorname{Tr} |\rho_T|\, S(\lambda)\, |\rho_T|\, S(\lambda) + \frac{2}{\lambda} \operatorname{Tr} |\rho_T|\, S(\lambda)\, |\rho_T| - \frac{1}{\lambda^2} \operatorname{Tr} |\rho_T|^2 \tag{3.26}$$

where

$$S(\lambda) = (\lambda - \rho\rho_1)^{-1} - \lambda^{-1} = \rho\rho_1 (\lambda - \rho\rho_1)^{-1} \tag{3.27}$$

Obviously the last term on the right-hand side of (3.26) has a finite limit when λ tends to Σ. Let us first control the limit of the second term. Since $|\rho_T|$ and $S(\lambda)\, |\rho_T|$ are Hilbert–Schmidt, the trace can be represented as follows:

$$\operatorname{Tr} |\rho_T|\, S(\lambda)\, |\rho_T| = \int \mathbf{dx} \int \mathbf{dy}\, (|\rho_T|)(\mathbf{x}, \mathbf{y})(S(\lambda)\, |\rho_T|)(\mathbf{y}, \mathbf{x}) \tag{3.28}$$

From the proof of Proposition 1 we see that

$$(S(\lambda))(\mathbf{x}, \mathbf{y}) = \int \mathbf{dk}\, e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})} \frac{\rho\tilde{\rho}_1(\mathbf{k})}{\lambda - \rho\tilde{\rho}_1(\mathbf{k})} \tag{3.29}$$

The integral (3.29) is absolutely convergent for $\lambda > \Sigma = \rho\tilde{\rho}(\mathbf{0})$, since (i) $\tilde{\rho}_1(\mathbf{k}) \leqslant \tilde{\rho}(\mathbf{0})$, and (ii) $\tilde{\rho}_1(\mathbf{k})$ has an integrable decay because $\rho_1(\mathbf{x}, \mathbf{0})$ has integrable derivatives as a consequence of the smoothness of the potential (2.2). From (3.28) and (3.29)

$$
\begin{aligned}
&|\mathrm{Tr}\, |\rho_T|\, S(\lambda)\, |\rho_T|\, | \\
&\quad = \left| \int \mathbf{dx} \int \mathbf{dy} \int \mathbf{dz} \int \mathbf{dk}\, (|\rho_T|)(\mathbf{x}, \mathbf{y})\, e^{i\mathbf{k}\cdot(\mathbf{y}-\mathbf{z})} \frac{\rho\tilde{\rho}_1(\mathbf{k})}{\lambda - \rho\tilde{\rho}_1(\mathbf{k})} (|\rho_T|)(\mathbf{z}, \mathbf{x}) \right| \\
&\quad \leqslant \left\{ \int \mathbf{dz} \int \mathbf{dy} \left[\int \mathbf{dx}\, |(|\rho_T|)(\mathbf{z}, \mathbf{x})(|\rho_T|)(\mathbf{x}, \mathbf{y})| \right] \right\} \\
&\qquad \times \left[\int \mathbf{dk} \frac{\rho\tilde{\rho}_1(\mathbf{k})}{\lambda - \rho\tilde{\rho}_1(\mathbf{k})} \right]
\end{aligned}
\tag{3.30}
$$

We know from Lemma 3.1 that the integrals in the large braces of the right-hand side of (3.30) are finite. This also justifies the interchange of integrals. Let us check that

$$
\lim_{\lambda \to \Sigma} \int \mathbf{dk} \frac{\rho\tilde{\rho}_1(\mathbf{k})}{\lambda - \rho\tilde{\rho}_1(\mathbf{k})} = \int \mathbf{dk} \frac{\tilde{\rho}_1(\mathbf{k})}{\tilde{\rho}(\mathbf{0}) - \tilde{\rho}_1(\mathbf{k})} < \infty \tag{3.31}
$$

We know that the integrand on the right-hand side of (3.27) has a unique singularity at $\mathbf{k} = 0$ (by the remark after the proof of Proposition 1). For the two models $\rho_1(\mathbf{x}, \mathbf{0}) = \rho_1(-\mathbf{x}, \mathbf{0})$ and $\rho_1(\mathbf{x}, \mathbf{0}) \geqslant 0$, so

$$
\int \mathbf{dx}\, \mathbf{x}\rho_1(\mathbf{x}, \mathbf{0}) = 0, \qquad 0 \leqslant \int \mathbf{dx}\, |\mathbf{x}|^2\, \rho_1(\mathbf{x}, \mathbf{0}) \leqslant \infty \tag{3.32}
$$

Thus the singularity at $\mathbf{k} = 0$ is $O(|\mathbf{k}|^{-2})$, an integrable one in three dimensions. Since $\tilde{\rho}_1(\mathbf{k})$ has an integrable decay at infinity, (3.31) follows by monotone convergence.

It remains to control the limit of the first term on the right-hand side of (3.26). We have again a product of Hilbert–Schmidt operators, so we can represent the trace as

$$
\mathrm{Tr}\, |\rho_T|\, S(\lambda)\, |\rho_T|\, S(\lambda) = \int \mathbf{dx} \int \mathbf{dy}\, (|\rho_T|\, S(\lambda))(\mathbf{x}, \mathbf{y})(|\rho_T|\, S(\lambda))(\mathbf{y}, \mathbf{x}) \tag{3.33}
$$

With (3.29) we get

$$|\mathrm{Tr}\,|\rho_T|\,S(\lambda)\,|\rho_T|\,S(\lambda)|$$

$$=\left|\int \mathbf{dx}\int \mathbf{dy}\int \mathbf{dz}\int \mathbf{dk}\int \mathbf{dz'}\int \mathbf{dk'}\,(|\rho_T|)(\mathbf{x},\mathbf{z})\right.$$

$$\left.\times e^{i\mathbf{k}\cdot(\mathbf{z}-\mathbf{y})}\frac{\rho\tilde{\rho}_1(\mathbf{k})}{\lambda-\rho\tilde{\rho}_1(\mathbf{k})}(|\rho_T|)(\mathbf{y},\mathbf{z'})\,e^{i\mathbf{k'}\cdot(\mathbf{z'}-\mathbf{x})}\frac{\rho\tilde{\rho}_1(\mathbf{k'})}{\lambda-\rho\tilde{\rho}(\mathbf{k'})}\right|$$

$$\leqslant\left[\int \mathbf{dx}\int \mathbf{dz}\,|(|\rho_T|)(\mathbf{x},\mathbf{z})|\right]^2\left[\int \mathbf{dk}\,\frac{\rho\tilde{\rho}_1(\mathbf{k})}{\lambda-\rho\tilde{\rho}_1(\mathbf{k})}\right]^2 \tag{3.34}$$

The first bracket in the last line of (3.34) is finite because of Lemma 3.1. The limit of the second as $\lambda\to\Sigma$ is the same as (3.31). This completes the proof of I.

4. THE LOW-DENSITY AND HIGH-TEMPERATURE LIMITS

In this section we will prove the results in II for the cell model. The arguments for the ideal gas model are similar. Let us begin with the low-density limit. From I we know that the edge of the continuous spectrum is

$$\Sigma=\rho\int \mathbf{dx}\,\rho_1(\mathbf{x},\mathbf{0})$$

$$=\frac{\rho}{N(\rho,\beta)}\int \mathbf{dx}\,\frac{\exp[-(\mathbf{x})^2/2\beta]}{(2\pi\beta)^{3/2}}$$

$$\times\int \mathbf{D}\alpha\,\frac{1}{|\Delta|}\int_\Delta d\tau\,\exp\left[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x},\mathbf{0},\alpha)\right] \tag{4.1}$$

Using the estimate (3.2), it is easy to deduce that $\lim_{\rho\to 0}N(\rho,\beta)=(2\pi\beta)^{-3/2}$ and $\lim_{\rho\to 0}[\Sigma/\rho(2\pi\beta)^{3/2}]=1$ by dominated convergence. To prove that the discrete part of the spectrum is not empty, we make the following decomposition:

$$\rho_2=\frac{\rho}{N(\rho,\beta)}\,[e^{-\beta H[\mathbf{0}]}+R] \tag{4.2}$$

where R is an operator with kernel

$$R(\mathbf{x}, \mathbf{y}) = \frac{\exp[-(\mathbf{x}-\mathbf{y})^2/2\beta]}{(2\pi\beta)^{3/2}} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau$$

$$\times \exp\left[-\beta \int_0^1 ds\, V(\alpha_{\mathbf{xy}}(s))\right]$$

$$\times \left\{\exp\left[\sum_{\mathbf{j}\neq \mathbf{0}} C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha)\right] - 1\right\} \tag{4.3}$$

We estimate the operator norm of R by[14]

$$\|R\| \leqslant \operatorname{Max}\left[\sup_x \int \mathbf{dy}\, |R(\mathbf{x}, \mathbf{y})|, \sup_y \int \mathbf{dx}\, |R(\mathbf{x}, \mathbf{y})|\right]$$

$$\leqslant e^{\beta \sup V}(e^{\rho v(\beta)} - 1) \tag{4.4}$$

where we have used (3.2). Thus $\|R\| = O(\rho)$. So by the regular perturbation theory, for β fixed and ρ small enough, ρ_2 has isolated eigenvalues λ_ν satisfying (2.15).

For the high-temperature limit we cannot use the same method because [as can be seen from (4.4) and $v(\beta) = O(\beta)$] the perturbation term in (4.2) is $O(\beta)$, whereas the spacing between the eigenvalues of $\exp(\beta H[\mathbf{0}])$ is also $O(\beta)$.

We first look at the edge of the continuous spectrum as $\beta \to 0$ and prove that all possible eigenvalues must merge in the continuous spectrum in this limit. For this to be true it is sufficient to have

$$\lim_{\beta \to 0} \frac{\|\rho_2\|}{\Sigma} = 1 \tag{4.5}$$

We have

$$\Sigma \leqslant \|\rho_2\| \leqslant \operatorname{Max}\left[\sup_x \int \mathbf{dy}\, |\rho_2(\mathbf{x}, \mathbf{y})|, \sup_y \int \mathbf{dx}\, |\rho_2(\mathbf{x}, \mathbf{y})|\right] \tag{4.6}$$

The operator ρ_2 is self-adjoint, so $|(\rho_2)(\mathbf{x}, \mathbf{y})|$ is symmetric; thus,

$$1 \leqslant \frac{\|\rho_2\|}{\Sigma} \leqslant \frac{\sup_x \int \mathbf{dy}\, |\rho_2(\mathbf{x}, \mathbf{y})|}{\Sigma} \tag{4.7}$$

We have from (2.8), after the change of variables $\mathbf{y} \to \sqrt{\beta}\,\mathbf{y} + \mathbf{x}$,

$$\frac{\int \mathbf{dy}\, |\rho_2(\mathbf{x}, \mathbf{y})|}{\Sigma}$$

$$= \left\{ \int \mathbf{dy} \exp\left(-\frac{\mathbf{y}^2}{2}\right) \int \mathbf{D}\alpha \int_\Delta \mathbf{d}\tau \exp\left[\sum_{\mathbf{j} \neq \mathbf{0}} C_{\mathbf{j},\tau}(\mathbf{x}, \sqrt{\beta}\,\mathbf{y} + \mathbf{x}, \alpha)\right] \right.$$

$$\left. \times \exp\left[-\beta \int_0^1 ds\, V(\mathbf{x} + \sqrt{\beta}\,\mathbf{y} + \sqrt{\beta}\,\alpha(s))\right] \right\}$$

$$\times \left\{ \int \mathbf{dy} \exp\left(-\frac{\mathbf{y}^2}{2}\right) \int \mathbf{D}\alpha \int \mathbf{d}\tau \right.$$

$$\left. \times \exp\left[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x}, \sqrt{\beta}\,\mathbf{y} + \mathbf{x}, \alpha)\right] \right\}^{-1} \tag{4.8}$$

From (3.2) it follows that

$$\sum_{\mathbf{j}} |C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha)| \leqslant \beta e^{\beta \sup |V|} \int \mathbf{dr}\, |V(\mathbf{r})| \tag{4.9}$$

showing that the integrands in the numerator and the denominator of (4.8) are bounded by and tend to $e^{-\mathbf{y}^2/2}$ uniformly with respect to all the arguments as $\beta \to 0$. Hence the ratio (4.8) tends to 1 uniformly with respect to $\mathbf{x}$ by dominated convergence. Thus we have (4.5). One can also prove, using (4.1) and (4.9), that $\lim_{\beta \to 0}[\Sigma/\rho(2\pi\beta)^{3/2}] = 1$ by dominated convergence.

To prove the existence of eigenvalues in the high-temperature limit we use the variational principle (2.20). We choose an eigenfunction ϕ_ν corresponding to an eigenvalue E_ν of $H[\mathbf{0}]$. Then a computation presented in Appendix C gives for β small enough

$$\frac{(\phi_\nu, \rho_2 \phi_\nu)}{\Sigma} = 1 - \beta\left[\frac{1}{2\bar{m}(\beta)} \int \mathbf{dx}\, |\nabla\phi_\nu(\mathbf{x})|^2 \right.$$

$$\left. + \int \mathbf{dx}\, V^{\text{eff}}(\mathbf{x})\, |\phi_\nu(\mathbf{x})|^2 \right] + O(\beta^{3/2}) \tag{4.10}$$

where the effective potential $V^{\text{eff}}(\mathbf{x})$ is

$$V^{\text{eff}}(\mathbf{x}) = V(\mathbf{x}) - \frac{z}{1+z} \frac{1}{\Delta^2} \int_\Delta \mathbf{dr} \int_\Delta \mathbf{d}\tau\, V(\mathbf{x} - \mathbf{r} - \tau) \tag{4.11}$$

and the effective mass $\bar{m}(\beta)$ is given by the formula (C.8) in Appendix C. Since $\bar{m}(\beta) = 1 + o(1)$, for β small enough we have

$$\frac{(\phi_\nu, \rho_2 \phi_\nu)}{\Sigma} = 1 - \beta \left\{ E_\nu \,[1 + o(1)] + \frac{z}{1+z} \frac{1}{|\Delta|^2} \int_\Delta \mathbf{dr} \int_\Delta \mathbf{d}\tau \, |V(\mathbf{x} - \mathbf{r} - \tau)| \, |\phi_\nu(\mathbf{x})|^2 \right\} \tag{4.12}$$

There exists $\bar{z}(\Delta)$ small enough (independent of β) such that for $z < \bar{z}(\Delta)$ the brace is negative (since $E_\nu < 0$) and thus (4.12) is greater than one. This proves the existence of eigenvalues for $\rho \leqslant \bar{\rho}$ and β small enough; here

$$\bar{\rho} = \frac{\bar{z}(\Delta)}{1 + \bar{z}(\Delta)} \frac{1}{|\Delta|}$$

Let us also remark that if $|\Delta| \to \infty$, $V^{\text{eff}}(\mathbf{x}) \to V(\mathbf{x})$, so we have $\bar{z}(\Delta) \to \infty$. On the other hand, if $|\Delta| \to 0$, $V^{\text{eff}}(\mathbf{x}) \to [1/(1+z)]\, V(\mathbf{x})$, so that $\bar{z}(|\Delta| = 0) < z_c$ for some fixed number z_c.

In the case of the ideal gas model one proceeds in the same way. This leads to (4.10) with $V^{\text{eff}}(\mathbf{x}) = V(\mathbf{x})$. Thus, in the ideal gas, (4.12) becomes

$$\frac{(\phi_\nu, \rho_2 \phi_\nu)}{\Sigma} = 1 - \beta E_\nu [1 + o(1)] = e^{-\beta E_\nu (1 + o(1))} \tag{4.13}$$

showing that for small β there exist bound states for all values of the density.

5. HIGH-DENSITY LIMIT

Our analysis of the high-density limit involves the computation of functional integrals by the Laplace method. We begin with the ideal gas model.

Ideal Gas Model. To show that there remains an eigenvalue at high density, we will use again the variational principle (2.22). This leads to the computation of some functional integrals which we first explain. Let Ω be the space of $(\mathbf{x}, \alpha)$, $\mathbf{x} \in \mathbf{R}^3$, α a Brownian path such that $\alpha(0) = \alpha(1) = 0$ and $g(\mathbf{x}, \alpha)$ a functional from Ω to $\mathbf{R}$. The behavior of the integral $I(\rho)$

$$I(\rho) \equiv \int \mathbf{dx} \, \frac{\exp[-(\mathbf{x})^2/2\beta]}{(2\pi\beta)^{3/2}} \, \mathbf{D}\alpha \, g(\mathbf{x}, \alpha) \exp\left[\rho \int \mathbf{dr} \, F(\mathbf{x}, \alpha)\right] \tag{5.1}$$

is given for ρ sufficiently large by

$$I(\rho)=[1+o(1)]\, g(\mathbf{0},\mathbf{0})\, 2^{3/2}[\sqrt{\rho}\, K(\beta)]^{-1/2} \times \exp\left[-\frac{1}{2}\sqrt{\rho}\, K(\beta)\right] \exp\left(\rho \int d\mathbf{r}\, \{\exp[-\beta V(\mathbf{r})]-1\}\right) \tag{5.2}$$

where $K(\beta)$ is given by (5.8) and $F(\mathbf{x}, \alpha)$ is the positive functional (2.12). One can see that $(\mathbf{x}=\mathbf{0}, \alpha=\mathbf{0})$ is a stationary point of $F(\mathbf{x}, \alpha)$ in the space Ω. Indeed, the first derivatives are

$$\nabla_{\mathbf{x}} F(\mathbf{x}, \alpha)= -\int d\mathbf{r}\, \beta \int_0^1 ds\, s\, \nabla V(s\mathbf{x}+\sqrt{\beta}\, \alpha(s)-\mathbf{r}) \times \exp\left[-\beta \int_0^1 ds\, V(s\mathbf{x}+\sqrt{\beta}\, \alpha(s)-\mathbf{r})\right] \tag{5.3}$$

$$\frac{\delta}{\delta\alpha(t)} F(\mathbf{x}, \alpha)= -\int d\mathbf{r}\, \beta^{3/2}\, \nabla V(t\mathbf{x}+\sqrt{\beta}\, \alpha(t)-\mathbf{r}) \times \exp\left[-\beta \int_0^1 ds\, V(s\mathbf{x}+\sqrt{\beta}\, \alpha(s)-\mathbf{r})\right] \tag{5.4}$$

If we specialize (5.3), (5.4) to $(\mathbf{x}=\mathbf{0}, \alpha=\mathbf{0})$, we get

$$(\nabla_{\mathbf{x}} F)(\mathbf{0},\mathbf{0})= -\frac{\beta}{2}\int d\mathbf{r}\, \nabla V(\mathbf{r})\, e^{-\beta V(\mathbf{r})} = \frac{1}{2}\int d\mathbf{r}\, \nabla(e^{-\beta V(\mathbf{r})}-1)=0 \tag{5.5}$$

$$\left(\frac{\delta}{\delta\alpha(t)} F\right)(\mathbf{0},\mathbf{0})= -\beta^{3/2}\int d\mathbf{r}\, \nabla V(\mathbf{r})\, e^{-\beta V(\mathbf{r})} = \sqrt{\beta}\int d\mathbf{r}\, \nabla(e^{-\beta V(\mathbf{r})}-1)=0 \tag{5.6}$$

Moreover,

$$F(\mathbf{0},\mathbf{0})=\int d\mathbf{r}\, (e^{-\beta V(\mathbf{r})}-1)$$

so by applying Jensen's inequality to the s integral in (2.12) one readily concludes that this stationary point is also an absolute maximum for the functional. Expanding $F(\mathbf{x}, \alpha)$ around $(\mathbf{x}=\mathbf{0}, \alpha=\mathbf{0})$, we find up to second order

$$F(\mathbf{x}, \alpha) = F(\mathbf{0}, \mathbf{0}) - \frac{1}{2}[K(\beta)]^2 \int_0^1 du \int_0^1 dv \times [\delta(u-v)-1][\sqrt{\beta}\,\alpha(u)+u\mathbf{x}] \cdot [\sqrt{\beta}\,\alpha(v)+v\mathbf{x}] \quad (5.7)$$

with

$$[K(\beta)]^2 = \frac{\beta^2}{3}\int \mathbf{dr}\,|\nabla V(\mathbf{r})|^2 \exp[-\beta V(\mathbf{r})] \quad (5.8)$$

We now prove that the quadratic form in (5.7) is not degenerate and negative definite.

Lemma 5.1. For any $(\mathbf{x}, \alpha) \in \Omega$ not equal to $(\mathbf{x}=\mathbf{0}, \alpha=\mathbf{0})$ we have the strict inequality

$$\int_0^1 du \int_0^1 dv\,[\delta(u-v)-1][\sqrt{\beta}\,\alpha(u)+u\mathbf{x}] \cdot [\sqrt{\beta}\,\alpha(v)+v\mathbf{x}] > 0 \quad (5.9)$$

Proof. First we notice

$$\int_0^1 du \int_0^1 dv\,[\delta(u-v)-1][\sqrt{\beta}\,\alpha(u)+u\mathbf{x}] \cdot [\sqrt{\beta}\,\alpha(v)+v\mathbf{x}] = \int_0^1 du \left\{[\sqrt{\beta}\,\alpha(u)+u\mathbf{x}] - \int_0^1 ds\,[\sqrt{\beta}\,\alpha(s)+s\mathbf{x}]\right\}^2 \geqslant 0 \quad (5.10)$$

Since the Brownian paths are continuous, (5.10) implies that (5.9) can vanish if and only if we have

$$\sqrt{\beta}\,\alpha(u)+u\mathbf{x} = \int_0^1 ds\,[\sqrt{\beta}\,\alpha(s)+s\mathbf{x}] \quad (5.11)$$

for all $0 \leqslant u \leqslant 1$. Specifying (5.11) to $u=0$ and $u=1$, one sees that $\mathbf{x}=0=\int_0^1 ds\,[\sqrt{\beta}\,\alpha(s)+s\mathbf{x}]$. Thus, by (5.11), $\alpha(u)=0$ for all $0 \leqslant u \leqslant 1$.

Having established that $(\mathbf{x}=\mathbf{0}, \alpha=\mathbf{0})$ is an absolute maximum and a nondegenerate stationary point, it is legitimate to compute the asymptotic behavior of $I(\rho)$ in the Gaussian approximation,

$$I(\rho) = [1 + o(1)]\; g(\mathbf{0}, \mathbf{0}) \exp\left(\rho \int \mathbf{dr}\; \{\exp[-\beta V(\mathbf{r})] - 1\}\right)$$
$$\times \int \mathbf{dx}\, \frac{\exp[-(\mathbf{x})^2/2\beta]}{(2\pi\beta)^{3/2}}\, \mathbf{D}\alpha$$
$$\times \exp\left\{-\frac{\rho}{2}[K(\beta)]^2 \int_0^1 du \int_0^1 dv\right.$$
$$\left.\times [\delta(u-v) - 1][\sqrt{\beta}\,\alpha(u) + u\mathbf{x}] \cdot [\sqrt{\beta}\,\alpha(v) + v\mathbf{x}]\right\} \qquad (5.12)$$

The Gaussian integral in (5.12) can be exactly computed, and one obtains the result (5.2). The computation is carried out in Appendix D.

To compute the ratio (2.22), we choose a sufficiently regular function $\phi(\mathbf{x})$ such that $\|\phi\|_2 = 1$ and ϕ does not vanish on the support of $V(\mathbf{x})$. Then

$$(\phi, \rho_2 \phi) = \frac{\rho}{N(\rho, \beta)} \int \mathbf{dy}\; \phi(\mathbf{y}) \int \mathbf{dx}\, \frac{\exp[-(\mathbf{x})^2/2\beta]}{(2\pi\beta)^{3/2}}\, \mathbf{D}\alpha\; \phi(\mathbf{y} + \mathbf{x})$$
$$\times \exp\left[-\beta \int_0^1 ds\; V(\mathbf{y} + s\mathbf{x} + \sqrt{\beta}\,\alpha(s))\right] \exp[\rho F(\mathbf{x}, \alpha)] \qquad (5.13)$$

and

$$\Sigma = \frac{\rho}{N(\rho, \beta)} \int \mathbf{dx}\, \frac{\exp[-(\mathbf{x})^2/2\beta]}{(2\pi\beta)^{3/2}}\, \mathbf{D}\alpha \exp[\rho F(\mathbf{x}, \alpha)] \qquad (5.14)$$

Using (5.2) for $g(\mathbf{x}, \alpha)$ equal to

$$\phi(\mathbf{y} + \mathbf{x}) \exp\left[-\beta \int_0^1 ds\; V(\mathbf{y} + s\mathbf{x} + \sqrt{\beta}\,\alpha(s))\right]$$

and equal to 1, respectively, we obtain

$$\lim_{\rho \to \infty} \frac{(\phi, \rho_2 \phi)}{\Sigma} = \int \mathbf{dy}\; |\phi(\mathbf{y})|^2\, e^{-\beta V(\mathbf{y})} > 1 \qquad (5.15)$$

If we replace V by κV, where κ is a coupling constant, we note that (5.15) is still strictly greater than one for any value of the coupling constant. So even if κ is small enough so that $-\frac{1}{2}\Delta + \kappa V$ has no bound states, we will have discrete spectrum in ρ_2 at large enough densities. The significance of this point was discussed in Section 2.

We also remark that to derive (5.15) one does not need to compute the Gaussian integral in (5.12). However, this computation is useful for latter purposes.

To derive the asymptotic behavior of Σ, we still need to compute the asymptotic behavior of the normalization factor $N(\rho, \beta)$ as $\rho \to \infty$. For this quantity one gets a Gaussian integral similar to the one in (5.12). The calculations are sketched in Appendix D.

We now turn to the discussion of the cell model.

Cell Model. In this paragraph we want to show that the discrete spectrum of ρ_2 is empty at high density. We will use the Birman–Schwinger operator, as in Section 3, i.e.,

$$K(\lambda) = |\rho_T|^{1/2} (\lambda - \rho\rho_1)^{-1} |\rho_T|^{1/2} \tag{5.16}$$

We recall that the edge of the continuous spectrum of ρ_2 is $\Sigma = \rho\tilde{\rho}(0)$. The Birman–Schwinger operator has the following property: ρ_2 has no eigenvalues if and only if

$$\sup_{\lambda > \Sigma} \|K(\lambda)\| < 1 \tag{5.17}$$

where $\|\cdot\|$ denotes the operator norm.[17] To estimate the operator norm, one could try to use $\|K(\lambda)\| \leqslant \|K(\lambda)\|_2$, where $\|\cdot\|_2$ is the Hilbert–Schmidt norm, and then make estimates similar to those of Section 3. However, it turns out that this does not give sharp enough inequalities. Instead we will use the following two lemmas.

Lemma 5.2. Let $h(\mathbf{x})$ be the function defined in Section 3, i.e., $h(\mathbf{x}) = 1$ for $|\mathbf{x}| \leqslant 1$, $h(\mathbf{x}) = |\mathbf{x}|^{-(3/2+\varepsilon)}$ for $|\mathbf{x}| \geqslant 1$. Then the following quantities are finite:

$$m_0 \equiv \sup_{\mathbf{x}} \int \mathbf{dy}\, |\rho_T(\mathbf{x}, \mathbf{y})| = \sup_{\mathbf{y}} \int \mathbf{dx}\, |\rho_T(\mathbf{x}, \mathbf{y})| \tag{5.18}$$

$$m_1 \equiv \sup_{\mathbf{y}} \int \mathbf{dx}\, [h(\mathbf{x})]^{-2} |\rho_T(\mathbf{x}, \mathbf{y})| \tag{5.19}$$

$$m_2 \equiv \sup_{\mathbf{x}} \left\{ [h(\mathbf{x})]^{-2} \int \mathbf{dy}\, |\rho_T(\mathbf{x}, \mathbf{y})| \right\} \tag{5.20}$$

Lemma 5.3. One has the inequality

$$\sup_{\lambda > \Sigma} \|K(\lambda)\| \leqslant \frac{m_0}{\Sigma} + \|h\|_2^2 \frac{\max(m_1, m_2)}{\Sigma} \int \mathbf{dk}\, \frac{\rho\tilde{\rho}_1(\mathbf{k})}{\Sigma - \rho\tilde{\rho}_1(\mathbf{k})} \tag{5.21}$$

We do not give the details of the proof of Lemma 5.2, which is based on the bound (3.7) for $\rho_T(\mathbf{x}, \mathbf{y})$. Here we give the proof of Lemma 5.3.

Proof of Lemma 5.3. First we make the decomposition

$$K(\lambda) = \lambda^{-1} |\rho_T| + |\rho_T|^{1/2} S(\lambda) |\rho_T|^{1/2} \tag{5.22}$$

where $S(\lambda) = (\lambda - \rho\rho_1)^{-1} - \lambda^{-1}$, as in (3.27). Then

$$\|K(\lambda)\| \leqslant \lambda^{-1} \|\rho_T\| + \| |\rho_T|^{1/2} S(\lambda) |\rho_T|^{1/2}\| \tag{5.23}$$

and since $\|\rho_T\| \leqslant m_0$

$$\sup_{\lambda > \Sigma} \|K(\lambda)\| \leqslant \frac{m_0}{\Sigma} + \sup_{\lambda > \Sigma} \| |\rho_T|^{1/2} S(\lambda) |\rho_T|^{1/2}\| \tag{5.24}$$

Now it remains to estimate the second term on the right-hand side of (5.24). We remark that $S(\lambda)$ is a positive self-adjoint operator, so

$$\begin{aligned} \| |\rho_T|^{1/2} S(\lambda) |\rho_T|^{1/2}\| &= \|(|\rho_T|^{1/2} [S(\lambda)]^{1/2})([S(\lambda)]^{1/2} |\rho_T|^{1/2})\| \\ &\leqslant \|(|\rho_T|^{1/2} [S(\lambda)]^{1/2})(|\rho_T|^{1/2} [S(\lambda)]^{1/2})^+\|_2 \\ &= \|(|\rho_T|^{1/2} [S(\lambda)]^{1/2})^+ (|\rho_T|^{1/2} [S(\lambda)]^{1/2})\|_2 \\ &= \|[S(\lambda)]^{1/2} hh^{-1} |\rho_T| h^{-1}h[S(\lambda)]^{1/2}\|_2 \\ &\leqslant \|h^{-1} |\rho_T| h^{-1}\| \cdot \|[S(\lambda)]^{1/2} h\|_2^2 \end{aligned} \tag{5.25}$$

where h denotes the multiplication operator by the function $h(\mathbf{x})$. Since ρ_1 is the multiplication operator by $\tilde{\rho}_1(\mathbf{k})$ (see Section 3) we have

$$\|[S(\lambda)]^{1/2} h\|_2^2 = \int d\mathbf{k} \int d\mathbf{k}' \frac{\rho\tilde{\rho}_1(\mathbf{k})}{\lambda[\lambda - \rho\tilde{\rho}_1(\mathbf{k})]} |\tilde{h}(\mathbf{k} - \mathbf{k}')|^2 \tag{5.26}$$

where $\tilde{h}$ denotes the Fourier transform of the function $h(\mathbf{x})$. Evidently $\tilde{h}$ is square integrable. Thus, using (3.31), it is clear from (5.26) that

$$\sup_{\lambda > \Sigma} \|(S(\lambda))^{1/2} h\|_2^2 = \left[\int d\mathbf{k} \, |\tilde{h}(\mathbf{k})|^2\right] \int d\mathbf{k} \frac{\rho\tilde{\rho}_1(\mathbf{k})}{\Sigma[\Sigma - \rho\tilde{\rho}_1(\mathbf{k})]} \tag{5.27}$$

To obtain (5.21), it remains to prove

$$\|h^{-1} |\rho_T| h^{-1}\| \leqslant \max(m_1, m_2) \tag{5.28}$$

For given $\phi, \psi \in L^2(\mathbf{R}^3)$, $\|\phi\|_2 = \|\psi\|_2 = 1$, we define the function of the complex variable ζ,

$$F_{\phi,\psi}(\zeta) = \int \mathbf{dx} \int \mathbf{dy}\, \overline{\phi(\mathbf{x})}[h(\mathbf{x})]^{-2\zeta} (|\rho_T|)(\mathbf{x}, \mathbf{y})[h(\mathbf{y})]^{-2(1-\zeta)} \psi(\mathbf{y}) \tag{5.29}$$

We will show later that $F_{\phi,\psi}(\zeta)$ is analytic and bounded for ζ in the strip $\{\zeta \mid 0 < \operatorname{Re} \zeta < 1\}$. Thus, by the Hadamard three-line lemma[18]

$$|F_{\phi,\psi}(\zeta)| \leqslant |F_{\phi,\psi}(0)|^{\operatorname{Re}\zeta}\, |F_{\phi,\psi}(1)|^{1-\operatorname{Re}\zeta} \tag{5.30}$$

for ζ in the strip. Applying (5.30) to $\zeta = 1/2$ gives

$$\begin{aligned}(\phi, h^{-1} |\rho_T|\, h^{-1}\psi) &\leqslant |(\phi, |\rho_T|\, h^{-2}\psi)|^{1/2}\, |(\phi, h^{-2}\, |\rho_T|\, \psi)|^{1/2} \\ &\leqslant \|\phi\|_2\, \|\, |\rho_T|\, h^{-2}\psi\|_2^{1/2}\, \|h^{-2}\, |\rho_T|\, \psi\|_2^{1/2} \\ &\leqslant \|\, |\rho_T|\, h^{-2}\|^{1/2}\, \|h^{-2}\, |\rho_T|\, \|^{1/2} \\ &= \|\rho_T h^{-2}\|^{1/2}\, \|h^{-2}\rho_T\|^{1/2}\end{aligned} \tag{5.31}$$

For the second inequality in (5.31) we used the Schwartz inequality, for the third the fact that $\|\phi\|_2 = \|\psi\|_2 = 1$, and the last one follows from the polar decomposition of ρ_T. Since (5.31) is valid for any normalized ϕ, we choose $\phi = (h^{-1}\, |\rho_T|\, h^{-1}\psi)/\|h^{-1}\, |\rho_T|\, h^{-1}\psi\|$, which gives

$$\|h^{-1}\, |\rho_T|\, h^{-1}\psi\|_2 \leqslant \|\rho_T h^{-2}\|^{1/2}\, \|h^{-2}\rho_T\|^{1/2} \tag{5.32}$$

Finally, we deduce (5.28) thanks to the operator norm estimates

$$\|\rho_T h^{-2}\| \leqslant \operatorname{Max}(m_1, m_2), \qquad \|h^{-2}\rho_T\| \leqslant \operatorname{Max}(m_1, m_2) \tag{5.33}$$

We conclude the proof of this lemma by showing that $F_{\phi,\psi}(\zeta)$ is analytic and bounded in the strip $\{\zeta \mid 0 < \operatorname{Re}\zeta < 1\}$. Since $h(\mathbf{x})$ is strictly positive, the integrand of (5.29) is analytic in the strip for each fixed $\mathbf{x}$ and $\mathbf{y}$. Let $\operatorname{Re}\zeta = t$; then by the Schwartz inequality

$$|F_{\phi,\psi}(\zeta)| \leqslant \|\phi\|_2\, \|\psi\|_2 \left\{\int \mathbf{dx} \int \mathbf{dy}\, [h(\mathbf{x})]^{-4t}\, [|\rho_T|(\mathbf{x}, \mathbf{y})]^2\, [h(\mathbf{y})]^{-4(1-t)}\right\}^{1/2} \tag{5.34}$$

In the estimate (5.34) we recognize the convex function (3.22). Thus,

$$\begin{aligned}|F_{\phi,\psi}(\zeta)| &\leqslant \|\phi\|_2\, \|\psi\|_2 \left\{\int \mathbf{dx} \int \mathbf{dy}\, [h(\mathbf{x})]^{-4}\, [|\rho_T|(\mathbf{x}, \mathbf{y})]^2\right\}^{1/2} \\ &= \|\phi\|_2\, \|\psi\|_2\, \|h^{-2}\, |\rho_T|\, \|_2 = \|\phi\|_2\, \|\psi\|_2\, \|h^{-2}\rho_T\|_2\end{aligned} \tag{5.35}$$

As argued after (3.22), this is finite. Therefore the integral (5.29) is uniformly convergent, implying that $F_{\phi,\psi}(\zeta)$ is analytic and bounded in the strip $0 \leqslant \operatorname{Re} \zeta \leqslant 1$.

Now we can apply Lemma 5.3 to show that at high density (5.17) holds for the cell model, and thus there are no eigenvalues. For this we compute the two terms on the right-hand side of inequality (5.21) and show that they tend to zero as the density tends to infinity. We recall that the density is

$$\rho = \frac{z}{1+z} \frac{1}{|\Delta|} \qquad (|\Delta| = a^3)$$

We will be interested in the limit where $z/(1+z)$ is sufficiently close to 1 and $|\Delta| = a^3$ is sufficiently small.

Estimate of the First Term of the r.h.s. of (5.21). Estimating the bracket in (2.11) simply by $A(\beta)(z^{-1}+a)$ $[A(\beta) = A\beta e^{\beta \sup |V|}$; see (3.9)], and using the translation invariance, we deduce

$$\begin{aligned} \int \mathbf{dy}\, |\rho_T(\mathbf{x}, \mathbf{y})| &\leqslant A(\beta)(z^{-1}+a) \frac{\rho}{N(\rho, \beta)} \int \mathbf{dy} \frac{\exp[-(\mathbf{y})^2/2\beta]}{(2\pi\beta)^{3/2}} \int \mathbf{D\alpha} \frac{1}{|\Delta|} \\ &\quad \times \int_\Delta \mathbf{d}\tau \exp\left[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{0}, \mathbf{y}, \alpha)\right] \\ &= A(\beta)(z^{-1}+a)\, \rho \tilde{\rho}_1(\mathbf{0}) \end{aligned} \tag{5.36}$$

Thus we have obtained $(m_0/\Sigma) \leqslant A(\beta)(z^{-1}+a)$, which can be made arbitrarily small for large z and small a.

The estimation of $\max(m_1, m_2)/\Sigma$ and of $\tilde{\rho}_1(\mathbf{k})$ is more complicated; it requires the computation of functional integrals by the Laplace method.

Estimate of the Second Term of the r.h.s. of (5.21). All the quantities of interest will involve the integrals over $(2\pi\beta)^{-3/2} e^{-\mathbf{x}^2/2\beta}\, \mathbf{dx}\, \mathbf{D}\alpha$ of the exponential of the functional

$$\begin{aligned} &\sum_{\mathbf{j}} C_{\mathbf{j},\tau a}(\mathbf{0}, \mathbf{x}, \alpha) \\ &\quad = \sum_{\mathbf{j}} \ln\left(1 + \frac{z}{1+z} \int_Q \mathbf{dr} \right. \\ &\quad \left. \times \left\{\exp\left[-\beta \int_0^1 ds\, V(s\mathbf{x} + \sqrt{\beta}\,\alpha(s) - \mathbf{j}a - \mathbf{r}a - \tau a)\right] - 1\right\}\right) \end{aligned} \tag{5.37}$$

where Q is the unit cube $Q=\{\mathbf{x} \mid |x_n| \leqslant 1/2,\ n=1,2,3\}$. For a given size of the cells a, we take z sufficiently large such that $1/(1+z)=O(a^3)$, as stated in III. One can perform a Taylor expansion for small a with respect to $\mathbf{r}a+\tau a$ (here $\tau \in Q$) and $1/(1+z)$. Then we approximate the sums over $\mathbf{j}$ by Riemann integrals. Carrying out these calculations (see Appendix E) leads to the result

$$\sum_{\mathbf{j}} C_{\mathbf{j},\tau a}(\mathbf{0},\mathbf{x},\alpha) = -\frac{\beta}{a^3}\int d\mathbf{r}\; V(\mathbf{r}) + \frac{\beta^2}{24a} G(\mathbf{x},\alpha) + O(1) \tag{5.38}$$

where

$$G(\mathbf{x},\alpha) \equiv \int d\mathbf{r} \left| \int_0^1 ds\, \nabla V(s\mathbf{x} + \sqrt{\beta}\,\alpha(s) - \mathbf{r}) \right|^2 \tag{5.39}$$

and $O(1)$ is a functional depending on $\mathbf{x}$, α, a, and z which is uniformly bounded with respect to all its arguments as $z^{-1}=O(a^3)$ and $a \to 0$. Thus, there exist constants C_1 and C_2 such that

$$\begin{aligned} C_1 \exp\left[\frac{\beta}{a^3}\int d\mathbf{r}\; V(\mathbf{r}) + \frac{\beta^2}{24a} G(\mathbf{x},\alpha)\right] &\leqslant \exp\left[\sum_{\mathbf{j}} C_{\mathbf{j},\tau a}(\mathbf{0},\mathbf{x},\alpha)\right] \\ &\leqslant C_2 \exp\left[\frac{\beta}{a^3}\int d\mathbf{r}\; V(\mathbf{r}) + \frac{\beta^2}{24a} G(\mathbf{x},\alpha)\right] \end{aligned} \tag{5.40}$$

In view of (5.40) we have to find the asymptotic behavior of functional integrals analogous to (5.1) with $\rho F(\mathbf{x},\alpha)$ replaced by $(\beta^2/24\mathrm{a})\, G(\mathbf{x},\alpha)$.

By Schwartz's inequality applied to the s integral in (5.39) we find that $G(\mathbf{x},\alpha) \leqslant G(\mathbf{0},\mathbf{0}) = \int d\mathbf{r}\; |\nabla V(\mathbf{r})|^2$. Thus $(\mathbf{x}=\mathbf{0},\ \alpha=\mathbf{0})$ is an absolute maximum in the space Ω. Moreover, it is easy to check that it is also a stationary point. Thus we expand $G(\mathbf{x},\alpha)$ up to quadratic order around this stationary point and find the same quadratic form as (5.7) with $[K(\beta)]^2$ replaced by

$$[W(\beta)]^2 = \frac{1}{3}\int d\mathbf{r} \sum_{i=1}^{3} \left| \nabla \frac{\partial}{\partial y_i} V(\mathbf{y}) \right|^2 \tag{5.41}$$

Thus we have a formula analogous to (5.2), namely

$$J(a) \equiv \int \mathbf{dx} \frac{\exp[-(\mathbf{x})^2/2\beta]}{(2\pi\beta)^{3/2}} \mathbf{D}\alpha g(\mathbf{x}, \alpha) \exp\left[\frac{\beta^2}{24a} G(\mathbf{x}, \alpha)\right]$$

$$= [1+o(1)]\ g(\mathbf{0}, \mathbf{0}) \exp\left[\frac{\beta^2}{24a} \int \mathbf{dr}\ |\nabla V(\mathbf{r})|^2\right]$$

$$\times \int \mathbf{dx} \frac{\exp[-(\mathbf{x})^2/2\beta]}{(2\pi\beta)^{3/2}} \mathbf{D}\alpha$$

$$\times \exp\left\{-\frac{\beta^2}{24a} [W(\beta)]^2 \int_0^1 du \int_0^1 dv\right.$$

$$\left.\times [\delta(u-v)-1][\sqrt{\beta}\,\alpha(u)+u\mathbf{x}][\sqrt{\beta}\,\alpha(v)+v\mathbf{x}]\right\}$$

$$= [1+o(1)]\ g(\mathbf{0}, \mathbf{0})\ 2^{3/2} \left(\frac{2(3a)^{1/2}}{\beta^{3/2} W(\beta)}\right)^{1/2}$$

$$\times \exp\left(-\frac{\beta^{3/2} W(\beta)}{4(3a)^{1/2}}\right) \exp\left[\frac{\beta^2}{24a} \int \mathbf{dr}\ |\nabla V(\mathbf{r})|^2\right] \qquad (5.42)$$

Now we can readily estimate $\max(m_1, m_2)/\Sigma$. For this we use the inequality (3.9) and the translation invariance

$$m_1 = \sup_{\mathbf{y}} \int \mathbf{dx}\ [h(\mathbf{x})]^{-2}\ |\rho_T(\mathbf{y}, \mathbf{x})|$$

$$= \sup_{\mathbf{y}} \int \mathbf{dx}\ [h(\mathbf{x}+\mathbf{y})]^{-2}\ |\rho_T(\mathbf{y}, \mathbf{x}+\mathbf{y})|$$

$$\leqslant A(\beta)(z^{-1}+a) \frac{\rho}{N(\rho, \beta)} \sup_{\mathbf{y}} \int \mathbf{dx} \frac{\exp[-(\mathbf{x})^2/2\beta]}{(2\pi\beta)^{3/2}} \mathbf{D}\alpha$$

$$\times |h(\mathbf{x}+\mathbf{y})|^{-2} \int_0^1 ds\ [1+|\mathbf{y}+s\mathbf{x}+\sqrt{\beta}\,\alpha(s)|]^{-\eta/2}$$

$$\times \int_Q \mathbf{d}\tau \exp\left[\sum_{\mathbf{j}} C_{\mathbf{j}, \tau a}(\mathbf{0}, \mathbf{x}, \alpha)\right] \qquad (5.43)$$

We recall that

$$\Sigma = \rho \int \mathbf{dx}\ \rho(\mathbf{x}, \mathbf{0}) = \frac{\rho}{N(\rho, \beta)} \int \mathbf{dx} \frac{\exp[-(\mathbf{x})^2/2]}{(2\pi)^{3/2}} \mathbf{D}\alpha$$

$$\times \int_Q \mathbf{d}\tau \exp\left[\sum_{\mathbf{j}} C_{\mathbf{j}, \tau a}(\mathbf{0}, \sqrt{\beta}\,\mathbf{x}, \alpha)\right] \qquad (5.44)$$

In both (5.43) and (5.44), we replace the functional (5.37) by its continuous approximation (5.38) and use the asymptotic form of the integrals (5.42) with the suitable functions g. We get

$$\frac{m_1}{\Sigma} \leqslant \frac{C_2}{C_1} A(\beta)(z^{-1}+a)[1+o(1)] \sup_{\mathbf{y}}(|h(\mathbf{y})|^{-2}(1+|\mathbf{y}|^2)^{-\eta/2})$$
$$\leqslant B(\beta)(z^{-1}+a) \tag{5.45}$$

where $B(\beta)$ is finite, since we have $h(\mathbf{y})^{-2} = O(|\mathbf{y}|^3)$ and $\eta > 3$. Proceeding in the same way, one finds also that $m_2/\Sigma = O(z^{-1}+a)$.

Now it remains to compute $\rho\tilde{\rho}_1(\mathbf{k})/\Sigma$. We use again the continuous approximation (5.38) and the Gaussian approximation (5.42),

$$\frac{\rho\tilde{\rho}_1(\mathbf{k})}{\Sigma} = \frac{\int \mathbf{dx}\,[e^{-(\mathbf{x})^2/2\beta}/(2\pi\beta)^{3/2}]\,\mathbf{D}\alpha\, e^{i\mathbf{kx}} \int_\Delta \mathbf{d}\tau \exp[\sum_\mathbf{j} C_{\mathbf{j},\tau}(\mathbf{0},\mathbf{x},\alpha)]}{\int \mathbf{dx}\,[e^{-(\mathbf{x})^2/2\beta}/(2\pi\beta)^{3/2}]\,\mathbf{D}\alpha \int_\Delta \mathbf{d}\tau \exp[\sum_\mathbf{j} C_{\mathbf{j},\tau}(\mathbf{0},\mathbf{x},\alpha)]}$$
$$= [1+o(1)]\frac{\int \mathbf{dx}\,[e^{-(\mathbf{x})^2/2\beta}/(2\pi\beta)^{3/2}]\,\mathbf{D}\alpha\, e^{i\mathbf{kx}} \exp[-(\beta^2/24a)\,G(\mathbf{x},\alpha)]}{\int \mathbf{dx}\,[e^{-(\mathbf{x})^2/2\beta}/(2\pi\beta)^{3/2}]\,\mathbf{D}\alpha \exp[-(\beta^2/24a)\,G(\mathbf{x},\alpha)]}$$
$$= [1+o(1)]\exp\left(-\frac{2(3a)^{1/2}}{\sqrt{\beta}\,W(\beta)}|\mathbf{k}|^2\right) \tag{5.46}$$

Note that here we cannot replace $e^{i\mathbf{kx}}$ by 1, because this would not give the correct behavior for $|\mathbf{k}| \to +\infty$, which we need below. The computation of this Gaussian integral can be performed exactly and is explained in Appendix D. With (5.46) we find for small a

$$\int \mathbf{dk}\,\frac{\rho\tilde{\rho}_1(\mathbf{k})}{\Sigma - \rho\tilde{\rho}_1(\mathbf{k})} = O(a^{-3/4}) \tag{5.47}$$

Finally, gathering (5.47) and (5.45) for m_1/Σ and m_2/Σ and (5.21), we obtain (5.17) for z large enough and a small enough. We recall that the result is valid for $1/(1+z) < Ca^3$.

APPENDIX A. DERIVATION OF (2.7)–(2.10)

We sketch the derivation of the thermodynamic limit for the cell model. For the ideal gas and lattice models the arguments are similar. Using formulas (2.5) and (2.6), we can write the partition function of the cell model explicitly,

$$\Xi_\Lambda = (2\pi\beta)^{-3/2} \int \mathbf{dx} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau\, \chi_\Lambda(\alpha_{\mathbf{xx}}) \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{\mathbf{j}_1 \neq \cdots \neq \mathbf{j}_n}$$
$$\times \prod_{i=1}^{n} \left\{ \int_\Lambda \mathbf{dr} \frac{1}{|\Delta|} \chi_\Delta(\mathbf{r} - \mathbf{j}_i a - \tau) \right.$$
$$\left. \times \exp\left[-\beta \int_0^1 ds\, V(\mathbf{x} + \sqrt{\beta}\, \alpha(s) - \mathbf{r}) \right] \right\}$$
$$= (2\pi\beta)^{-3/2} \int \mathbf{dx} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau\, \chi_\Lambda(\alpha_{\mathbf{xx}})$$
$$\times \prod_{\mathbf{j} \in \mathbf{L}} \left\{ 1 + z \int_\Lambda \mathbf{dr} \frac{1}{|\Delta|} \chi_\Delta(\mathbf{r} - \mathbf{j}a - \tau) \right.$$
$$\left. \times \exp\left[-\beta \int_0^1 ds\, V(\mathbf{x} + \sqrt{\beta}\, \alpha(s) - \mathbf{r}) \right] \right\} \tag{A.1}$$

We choose a sequence of domains consisting of N cells, $|\Lambda| = N|\Delta|$, $N \to \infty$. If we set $V(\mathbf{r}) = 0$ in (A.1), we find the partition function of the classical fluid without the quantum particle: $(1+z)^N$. Thus the density is

$$\rho = \frac{1}{|\Lambda|} z \frac{\partial}{\partial z} \ln(1+z)^N = \frac{1}{|\Delta|} \frac{z}{1+z} \tag{A.2}$$

We can compute the thermodynamic limit of the ratio of (A.1) with the partition function of the classical gas

$$\lim_{|\Lambda|} \frac{\Xi_\Lambda}{|\Lambda|(1+z)^N}$$
$$= (2\pi\beta)^{-3/2} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau$$
$$\times \exp\left(\sum_j \ln \left\{ \frac{1}{1+z} + \frac{z}{1+z} \frac{1}{|\Delta|} \right. \right.$$
$$\left. \left. \times \int_\Delta \mathbf{dr} \exp\left[-\beta \int_0^1 ds\, V(\mathbf{x} + \sqrt{\beta}\, \alpha(s) - \mathbf{j}a - \tau - \mathbf{r}) \right] \right\} \right) \tag{A.3}$$

This is exactly the same as (2.9). In order to obtain (2.7) and (2.8) we divide the numerator and the denominator of (2.3) and (2.4) by $(1+z)^N$. The term corresponding to the denominator yields the normalization factor (2.9). Then one computes the thermodynamic limit of the term corresponding to the numerator. We sketch this computation for the case of the pair density matrix only. The modifications for the one-particle density matrix are obvious. We have

$$\begin{aligned}
&\sum_{n=0}^{\infty} \frac{z^n}{n!} \int_\Lambda \mathbf{dr}_1 \cdots \int_\Lambda \mathbf{dr}_n \, G_{n+1}(\mathbf{0}, \mathbf{r}_1, ..., \mathbf{r}_n) \\
&\qquad \times \exp(-\beta H_\Lambda[\mathbf{0}, \mathbf{r}_1, ..., \mathbf{r}_n])(\mathbf{x}, \mathbf{y}) \\
&= \frac{\exp[-(\mathbf{x}-\mathbf{y})^2/2\beta]}{(2\pi\beta)^{3/2}} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau \, \chi_\Lambda(\alpha_{\mathbf{xy}}) \\
&\qquad \times \sum_{n=0}^{\infty} \frac{z^n}{n!} \frac{1}{|\Delta|} \chi_\Delta(\tau) \exp\left[-\beta \int_0^1 ds \, V(\alpha_{\mathbf{xy}}(s))\right] \\
&\qquad \times \sum_{\mathbf{0} \neq \mathbf{j}_1 \neq \cdots \neq \mathbf{j}_n} \prod_{i=1}^{n} \left\{ \int_\Lambda \mathbf{dr} \frac{1}{|\Delta|} \chi_\Delta(\mathbf{r}-\mathbf{j}_i a - \tau) \right. \\
&\qquad \left. \times \exp\left[-\beta \int_0^1 ds \, V(\alpha_{\mathbf{xy}}(s)-\mathbf{r})\right]\right\} \\
&= \frac{\exp[-(\mathbf{x}-\mathbf{y})^2/2\beta]}{(2\pi\beta)^{3/2}} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau \, \chi_\Lambda(\alpha_{\mathbf{xy}}) \\
&\qquad \times \frac{1}{|\Delta|} \exp\left[-\beta \int_0^1 ds \, V(\alpha_{\mathbf{xy}}(s))\right] \\
&\qquad \times \prod_{\mathbf{j} \in \mathbf{L}/\{\mathbf{0}\}} \left\{ 1 + z \int_\Lambda \mathbf{dr} \frac{1}{|\Delta|} \chi_\Delta(\mathbf{r}-\mathbf{j}a-\tau) \right. \\
&\qquad \left. \times \exp\left[-\beta \int_0^1 ds \, V(\alpha_{\mathbf{xy}}(s)-\mathbf{r})\right]\right\} \\
&= \frac{1}{|\Delta|} \frac{\exp[-(\mathbf{x}-\mathbf{y})^2/2\beta]}{(2\pi\beta)^{3/2}} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau \, \chi_\Lambda(\alpha_{\mathbf{xy}}) \\
&\qquad \times \exp\left[-\beta \int_0^1 ds \, V(\alpha_{\mathbf{xy}}(s))\right] \\
&\qquad \times \exp\left(\sum_{\mathbf{j} \in \mathbf{L}/\{\mathbf{0}\}} \ln \left\{ 1 + z \frac{1}{|\Delta|} \int_{|\Delta|} \chi_\Delta(r) \right.\right. \\
&\qquad \left.\left. \times \exp\left[-\beta \int_0^1 ds \, V(\alpha_{\mathbf{xy}}(s)-\mathbf{r}-\mathbf{j}a-\tau)\right]\right\}\right) \qquad \text{(A.4)}
\end{aligned}$$

Using (A.3) and (A.4), we get the formula (2.8) for the thermodynamic limit.

To check that the density matrices are translation invariant, one can use

$$\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x}+\mathbf{x}_0, \mathbf{y}+\mathbf{x}_0, \alpha) = \sum_{\mathbf{j}} C_{\mathbf{j},\tau-\mathbf{x}_0}(\mathbf{x}, \mathbf{y}, \alpha) \tag{A.5}$$

and

$$\frac{1}{|\Delta|}\int_\Delta \mathbf{d}\tau \exp \sum_{\mathbf{j}} C_{\mathbf{j},\tau-\mathbf{x}_0}(\mathbf{x}, \mathbf{y}, \alpha) = \frac{1}{|\Delta|}\int_\Delta \mathbf{d}\tau \exp \sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha) \tag{A.6}$$

Formula (A.6) follows from the periodicity of the integrand considered as a function of τ.

APPENDIX B. PROOF OF (3.15)

We differentiate (2.11) with respect to the components of the vector $\mathbf{x}$ and make the following observations.

(i) According to (2.10) and (3.2), one finds that the first and second derivatives of $\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x}, \mathbf{y}, \alpha)$ are bounded by Cst $\int \mathbf{dx}\, |\nabla V(\mathbf{x})|$ and Cst $\int \mathbf{dx}\, |\Delta V(\mathbf{x})|$ uniformly with respect to all the arguments.

(ii) In view of (2.2), the derivatives of the large bracket in (2.11) are majorized by

$$\text{Cst} \int_0^1 ds\, [1+|\alpha_{\mathbf{xy}}(s)|^2]^{-\eta/2}$$

(iii) Derivatives of the Gaussian $\exp(-|\mathbf{x}-\mathbf{y}|^2/2\beta)$ have Gaussian bounds.

Thus there exist constants C_1 and C_2 such that $\Delta\rho_T(\mathbf{x}, \mathbf{y})$ has a bound similar to (3.7),

$$|\Delta_{\mathbf{x}}\rho_T(\mathbf{x}, \mathbf{y})| \leqslant C_1 \exp(-C_2\, |\mathbf{x}-\mathbf{y}|^2) \int \mathbf{D}\alpha \int_0^1 ds\, [1+|\alpha_{\mathbf{xy}}(s)|^2]^{-\eta/2} \tag{B.1}$$

Using (B.1) and (3.7) together with the Schwartz inequality for the normalized measure $\mathbf{D}\alpha\, ds$, we obtain

$$\begin{aligned}
&|(-\Delta_{\mathbf{x}}+1)\,\rho_T(\mathbf{x}, \mathbf{y})|^2 \\
&\quad \leqslant 2[|\Delta_{\mathbf{x}}\rho_T(\mathbf{x}, \mathbf{y})|^2 + |\rho_T(\mathbf{x}, \mathbf{y})|^2] \\
&\quad \leqslant C_1' \exp(-C_2'\, |\mathbf{x}-\mathbf{y}|^2) \int \mathbf{D}\alpha \int_0^1 ds\, [1+|\alpha_{\mathbf{xy}}(s)|^2]^{-\eta/2}
\end{aligned} \tag{B.2}$$

With our choice of $h(\mathbf{x})$, we have $|h(\mathbf{x})|^{-2} \leqslant 1 + |\mathbf{x}|^{3+2\varepsilon}$; thus,

$$\int \mathbf{dx} \int \mathbf{dy}\, |h(\mathbf{x})|^{-2}\, |(-\Delta_{\mathbf{x}} + 1)\, \rho_T(\mathbf{x}, \mathbf{y})|^2$$

$$\leqslant C_1' \int \mathbf{D}\alpha \int_0^1 ds \int \mathbf{dx} \int \mathbf{dy}\, \exp(-C_2' \mathbf{y}^2) \left[\frac{1 + |\alpha_{\mathbf{xy}}(s)|^{3+2\varepsilon}}{(1 + |\mathbf{x}|^2)^{\eta/2}}\right] \tag{B.3}$$

Since $\eta > 6$, this last integral is finite provided that ε is small enough.

APPENDIX C. PROOF OF (4.10)

In this appendix we prove (4.10)–(4.11). Let ϕ be three times differentiable with bounded derivatives, and $\phi \in L^1(\mathbf{R}^3)$. We have the Taylor expansions

$$\phi(\mathbf{x} + \sqrt{\beta}\, \mathbf{y}) = \phi(\mathbf{x}) + \sqrt{\beta}\, \mathbf{y} \cdot \nabla\phi(\mathbf{x}) + \frac{1}{2}\beta(\mathbf{y} \cdot \nabla)^2\, \phi(\mathbf{x}) + \beta^{3/2} O(|\mathbf{y}|^3) \tag{C.1}$$

$$\exp\left\{-\beta \int_0^1 ds\, V(\mathbf{x} + \sqrt{\beta}[s\mathbf{y} + \alpha(s)])\right\}$$
$$= 1 - \beta V(\mathbf{x}) + \beta^{3/2} O(|\mathbf{y}| + \sup_s |\alpha(s)|) \tag{C.2}$$

Let us compute the ratio (2.22) with the aid of the Taylor expansions (C.1) and (C.2). To this end we set

$$\Sigma'' = \int \mathbf{dy}\, \frac{\exp[-(\mathbf{y})^2/2]}{(2\pi)^{3/2}} \int \mathbf{D}\alpha\, \frac{1}{|\Delta|} \int \mathbf{d}\tau\, \exp\left[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\sqrt{\beta}\, \mathbf{y}, \mathbf{0}, \alpha)\right] \tag{C.3}$$

Using (3.2) [with $v(\beta) = O(\beta)$], one checks by dominated convergence that $\Sigma'' = 1 + o(1)$ for small β. We have

$$\frac{(\phi, \rho_2 \phi)}{\Sigma} = \frac{1}{\Sigma''} \int \mathbf{dx}\, \phi(\mathbf{x}) \int \mathbf{dy}\, \frac{\exp[-(\mathbf{y})^2/2]}{(2\pi)^{3/2}} \int \mathbf{D}\alpha\, \phi(\mathbf{x} + \sqrt{\beta}\mathbf{y})$$

$$\times \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau\, \exp\left\{-\beta \int_0^1 dx\, V(\mathbf{x} + \sqrt{\beta}[s\mathbf{y} + \alpha(s)])\right\}$$

$$\times \exp\left[\sum_{\mathbf{j} = \mathbf{0}} C_{\mathbf{j},\tau}(\mathbf{x} + \sqrt{\beta}\mathbf{y}, \mathbf{x}, \alpha\right]$$

$$= \frac{1}{\Sigma''} \int \mathbf{dx}\, \phi(\mathbf{x}) \Bigg[\phi(\mathbf{x}) + \sqrt{\beta}\, \mathbf{y} \cdot \nabla\phi(\mathbf{x}) + \frac{1}{2} \beta (\mathbf{y} \cdot \nabla)^2 \phi(\mathbf{x}) - \beta V(\mathbf{x})\, \phi(\mathbf{x}) \Bigg] \times \frac{\exp[-(\mathbf{y})^2/2]}{(2\pi)^{3/2}} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau \times \exp\Bigg[\sum_{\mathbf{j} \neq \mathbf{0}} C_{\mathbf{j},\tau}(\mathbf{x} + \sqrt{\beta}\, \mathbf{y}, \mathbf{x}, \alpha) \Bigg] + O(\beta^{3/2}) \tag{C.4}$$

where the term $O(\beta^{3/2})$ comes from contributions involving the remainders in the Taylor expansions in (C.1), (C.2). One checks that these contributions are indeed of order $\beta^{3/2}$ with the help of (3.2) and $\int |\phi(\mathbf{x})| < \infty$. Let us also note that

$$\begin{aligned} &\exp\Bigg[\sum_{\mathbf{j} \neq \mathbf{0}} C_{\mathbf{j},\tau}(\mathbf{x} + \sqrt{\beta}\, \mathbf{y}, \mathbf{x}, \alpha) \Bigg] \\ &= \Bigg\{ \exp\Bigg[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x} + \sqrt{\beta}\, \mathbf{y}, \mathbf{x}, \alpha) \Bigg] \Bigg\} \\ &\quad \times \Bigg(1 + \frac{z}{1+z} \frac{1}{|\Delta|} \int_\Delta \mathbf{dr} \left\{ \exp\left[-\beta \int_0^1 ds\, V(\alpha_{\mathbf{xy}}(s) - \mathbf{r} - \tau) \right] - 1 \right\} \Bigg)^{-1} \\ &= \Bigg[1 - \beta \frac{z}{1+z} \frac{1}{|\Delta|} \int_\Delta \mathbf{dr}\, V(\mathbf{x} - \mathbf{r} - \tau) + \beta^{3/2} O(|\mathbf{y}| + \sup_s |\alpha(s)|) \Bigg] \\ &\quad \times \exp\Bigg[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x} + \sqrt{\beta}\, \mathbf{y}, \mathbf{x}, \alpha) \Bigg] \end{aligned} \tag{C.5}$$

We insert (C.5) in (C.4), keeping explicitly all the contributions up to order β,

$$\frac{(\phi, \rho_2 \phi)}{\Sigma} = \frac{1}{\Sigma''} \int \mathbf{dx} \int \mathbf{dy}\, \phi(\mathbf{x}) \Bigg[\phi(\mathbf{x}) + \sqrt{\beta}\, \mathbf{y} \cdot \nabla\phi(\mathbf{x}) + \frac{1}{2} \beta (\mathbf{y} \cdot \nabla)^2 \phi(\mathbf{x}) - \beta V(\mathbf{x})\, \phi(\mathbf{x}) \Bigg] \times \frac{\exp[-(\mathbf{y})^2/2]}{(2\pi)^{3/2}} \int \mathbf{D}\alpha \frac{1}{|\Delta|} \int_\Delta \mathbf{d}\tau \exp\Bigg[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\sqrt{\beta}\, \mathbf{y}, \mathbf{0}, \alpha) \Bigg]$$

$$+\frac{1}{\Sigma''}\beta\frac{z}{1+z}\int \mathbf{dx}\,|\phi(\mathbf{x})|^2\frac{1}{|\Delta|}\int_\Delta \mathbf{d}\tau\int_\Delta \mathbf{dr}\,V(\mathbf{x}-\mathbf{r}-\tau)$$
$$\times\int \mathbf{dy}\frac{\exp[-(\mathbf{y})^2/2]}{(2\pi)^{3/2}}\int \mathbf{D}\alpha\exp\left[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x}+\sqrt{\beta}\,\mathbf{y},\mathbf{x},\alpha)\right]$$
$$+O(\beta^{3/2}) \tag{C.6}$$

Note that we have used (A.5)–(A.6). This is important because now we can exploit the symmetries of the cubic lattice to obtain

$$\frac{(\phi,\rho_2\phi)}{\Sigma}=1+\beta\frac{1}{2\bar{m}(\beta)}\int \mathbf{dx}\,\phi(\mathbf{x})\,\Delta\phi(\mathbf{x})-\beta\int \mathbf{dx}\,|\phi(\mathbf{x})|^2\,V(\mathbf{x})$$
$$+\beta\int \mathbf{dx}\,|\phi(\mathbf{x})|^2\,V_\beta(\mathbf{x})+O(\beta^{3/2}) \tag{C.7}$$

with

$$\bar{m}(\beta)=\frac{1}{\Sigma''}\int \mathbf{dy}\,|\mathbf{y}|^2\frac{\exp[-(\mathbf{y})^2/2]}{(2\pi)^{3/2}}\int \mathbf{D}\alpha\frac{1}{|\Delta|}$$
$$\times\int_\Delta \mathbf{d}\tau\exp\left[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\sqrt{\beta}\,\mathbf{y},\mathbf{0},\alpha)\right] \tag{C.8}$$

$$V_\beta(\mathbf{x})=\frac{z}{1+z}\frac{1}{|\Delta|^2}\int_\Delta \mathbf{d}\tau\int_\Delta \mathbf{dr}\,V(\mathbf{x}-\mathbf{r}-\tau)\frac{1}{\Sigma''}$$
$$\times\int \mathbf{dy}\frac{\exp[-(\mathbf{y})^2/2]}{(2\pi)^{3/2}}\int \mathbf{D}\alpha\exp\left[\sum_{\mathbf{j}} C_{\mathbf{j},\tau}(\mathbf{x}+\sqrt{\beta}\,\mathbf{y},\mathbf{x},\alpha)\right] \tag{C.9}$$

It is easy to show that

$$\left|\frac{z}{1+z}\frac{1}{|\Delta|^2}\int_\Delta \mathbf{d}\tau\int_\Delta \mathbf{dr}\,V(\mathbf{x}-\mathbf{r}-\tau)-V_\beta(\mathbf{x})\right|=o(1) \tag{C.10}$$

From (C.7) and (C.10) we deduce

$$\frac{(\phi,\rho_2\phi)}{\Sigma''}=1-\beta\left[\frac{1}{2\bar{m}(\beta)}\int \mathbf{dx}\,|\nabla\phi(\mathbf{x})|^2+\int \mathbf{dx}\,V^{\text{eff}}(\mathbf{x})\,|\phi(\mathbf{x})|^2\right]+O(\beta^{3/2}) \tag{C.11}$$

where V^{eff} is given by (4.11).

The eigenfunctions ϕ_ν of $H[\mathbf{0}]$ have an exponential decay,[16] so they belong to $L^1(\mathbf{R}^3)$, and they have the required differentiability properties as a consequence of the smoothness of the potential (2.2). Thus, (C.11) holds for $\phi = \phi_v$.

APPENDIX D. GAUSSIAN INTEGRALS

First, we show how to compute the general Gaussian integral

$$H_\gamma(\mathbf{k}) = \int \mathbf{dx} \frac{\exp[-(\mathbf{x})^2/2\beta]}{(2\pi\beta)^{3/2}} \mathbf{D}\alpha \exp(i\mathbf{kx}) \exp\left\{-\frac{\gamma^2}{2\beta}\int_0^1 du \int_0^1 dv \times [\delta(u-v)-1][\sqrt{\beta}\,\alpha(u)+u\mathbf{x}]\cdot[\sqrt{\beta}\,\alpha(v)+v\mathbf{x}]\right\} \tag{D.1}$$

where γ is a dimensionless parameter. It is convenient to define the normalized Gaussian measure

$$\mathbf{D}_\gamma \alpha = \mathbf{D}\alpha \frac{\exp\{-\frac{1}{2}\gamma^2 \int_0^1 du \int_0^1 dv\, [\delta(u-v)-1]\, \alpha(u)\cdot\alpha(v)\}}{\int \mathbf{D}\alpha \exp\{-\frac{1}{2}\gamma^2 \int_0^1 du \int_0^1 dv\, [\delta(u-v)-1]\, \alpha(u)\cdot\alpha(v)\}} \tag{D.2}$$

The normalization factor is equal to $[(2/\gamma)\sinh(\gamma/2)]^{-1}$ (see, for example, ref. 13). Since the covariance of the Brownian bridge is the inverse of $-d^2/ds^2$ on $[0, 1]$ with Dirichlet boundary conditions, the covariance $C_\gamma(s, t)$ of the measure (D.2) is the solution of

$$-\frac{d^2}{ds^2} C_\gamma(s, t) + \gamma^2\left[C_\gamma(s, t) - \int_0^1 ds\, C_\gamma(s, t)\right] = \delta(s-t) \tag{D.3}$$

with $s, t \in [0, 1]$, $C_\gamma(s, t) = C_\gamma(t, s)$, $C_\gamma(0, t) = C_\gamma(1, t) = 0$. One can check that

$$C_\gamma(s, t) = \left(\frac{\gamma}{2}\sinh\frac{\gamma}{2}\right)^{-1} \frac{1}{4}\left[\cosh\gamma\left(|s-t| - \frac{1}{2}\right) + \cosh\frac{\gamma}{2} - \cosh\gamma\left(t - \frac{1}{2}\right) - \cosh\gamma\left(s - \frac{1}{2}\right)\right] \tag{D.4}$$

We will also need the formulas

$$\int D_\gamma \alpha \exp\left[-\frac{\gamma^2}{2\beta}\int_0^1 du\, (2u-1)\sqrt{\beta}\,\alpha(u)\cdot\mathbf{x}\right] = \exp\left[\frac{\gamma^4}{8\beta}|\mathbf{x}|^2 \int_0^1 du \int_0^1 dv\, (2u-1)(2v-1)\, C_\gamma(u, v)\right] \tag{D.5}$$

and

$$\int_0^1 du \int_0^1 dv\,(2u-1)(2v-1)\,C_\gamma(u,v) = \frac{1}{3\gamma^2} - \frac{2}{\gamma^3}\coth\frac{\gamma}{2} + \frac{4}{\gamma^4} \qquad \text{(D.6)}$$

With the help of (D.5) and (D.6) the integral (D.1) can be computed as follows:

$$H_\gamma(\mathbf{k}) = \left(\frac{2}{\gamma}\sinh\frac{\gamma}{2}\right)^{-1} \int \mathbf{dx}\,\frac{\exp[-(\mathbf{x})^2/2\beta]}{(2\pi\beta)^{3/2}}\exp(i\mathbf{kx})$$

$$\times \int D_\gamma\alpha \exp\left\{-\frac{\gamma^2}{2\beta}\left[\frac{|\mathbf{x}|^2}{12} + \int_0^1 du\,(2u-1)\sqrt{\beta}\,\alpha(u)\cdot\mathbf{x}\right]\right\}$$

$$= \left(\frac{2}{\gamma}\sinh\frac{\gamma}{2}\right)^{-1} \frac{1}{(2\pi\beta)^{3/2}} \int \mathbf{dx}\exp(i\mathbf{kx})\exp\left[-\frac{|\mathbf{x}|^2}{2\beta}\left(\frac{\gamma}{2}\coth\frac{\gamma}{2}\right)\right]$$

Thus

$$H_\gamma(\mathbf{k}) = \left(\frac{2}{\gamma}\sinh\frac{\gamma}{2}\right)^{-1}\left(\coth\frac{\gamma}{2}\right)^{-3/2}\exp\left[-\beta\frac{|\mathbf{k}|^2}{2}\left(\frac{2}{\gamma}\tanh\frac{\gamma}{2}\right)\right] \qquad \text{(D.8)}$$

The asymptotic behavior for $\gamma \to \infty$ is

$$H_\gamma(\mathbf{k}) \sim 2^{3/2}\gamma^{-1/2}e^{-\gamma/2}e^{-\beta|\mathbf{k}|^2/\gamma} \qquad \text{(D.9)}$$

Application to (5.2), (5.42), and (5.46). To obtain (5.2), we set $|\mathbf{k}| = 0$ and $\gamma = \sqrt{\beta\rho}\,K(\beta)$ in (D.9). For (5.42) we set $|\mathbf{k}| = 0$ and $\gamma = \beta^{3/2}W(\beta)/2(3a)^{1/2}$. For this last value of γ the ratio in (5.46) is exactly $H_\gamma(\mathbf{k})/H_\gamma(\mathbf{0}) \sim \exp(-\beta\,|\mathbf{k}|^2/\gamma)$.

Application to Σ for the Ideal and Cell Models. For the ideal gas model we need to compute the asymptotic behavior of the normalization factor [see (2.9) and (2.12)]

$$N(\rho,\beta) = (2\pi\beta)^{-3/2}\int \mathbf{D}\alpha$$

$$\times \exp\left(\rho\int \mathbf{dr}\left\{\exp\left[-\beta\int_0^1 ds\,V(\sqrt{\beta}\,\alpha(s)-\mathbf{r})\right]-1\right\}\right) \qquad \text{(D.10)}$$

Applying the Laplace method to (D.10) as in (5.1)–(5.12), it is easy to see that the asymptotic behavior for $\rho \to \infty$ is given by

$$N(\rho, \beta) \sim (2\pi\beta)^{-3/2} \exp\left(\rho \int \mathbf{dr}\ \{\exp[-\beta V(\mathbf{r}) - 1\}\right)$$
$$\times \int \mathbf{D}\alpha \exp\left\{-\frac{\beta\rho}{2}[K(\beta)]^2 \int_0^1 du \int_0^1 dv\ [\delta(u-v)-1]\ \alpha(u)\cdot\alpha(v)\right\} \tag{D.11}$$

The Gaussian integral in (D.11) is simply the normalization factor of (D.2). Thus for $\rho \to \infty$

$$N(\rho, \beta) \sim (2\pi\beta)^{-3/2} (\beta\rho)^{1/2} K(\beta) \exp\left[-\frac{(\beta\rho)^{1/2}}{2} K(\beta)\right]$$
$$\times \exp\left(\rho \int \mathbf{dr}\ \{\exp[-\beta V(\mathbf{r})] - 1\}\right) \tag{D.12}$$

Finally we find from (5.2) with $g = 1$ and (D.12)

$$\Sigma = \rho \int \mathbf{dx}\ \rho_1(\mathbf{x}, \mathbf{0}) = \rho \frac{I(\rho)}{N(\rho, \beta)} = O(\rho^{1/4}) \tag{D.13}$$

For the cell model we need the asymptotic behavior of $N(\rho, \beta)$ given by (2.9). Repeating a similar analysis to that of Section 5, one finds as $a \to \infty$

$$N(\rho, \beta) \sim \exp\left[-\frac{\beta}{a^3}\int \mathbf{dr}\ V(\mathbf{r}) + \frac{\beta^2}{24a}\int \mathbf{dr}\ |\nabla V(\mathbf{r})|^2\right]$$
$$\times \int \mathbf{D}\alpha \exp\left\{-\frac{\beta^3}{24a}[W(\beta)]^2 \int_0^1 du \int_0^1 dv\ [\delta(u-v)-1]\ \alpha(u)\cdot\alpha(v)\right\}$$
$$\sim \frac{\beta^{3/2} W(\beta)}{2(3a)^{1/2}} \exp\left(-\frac{\beta^{3/2} W(\beta)}{4(3a)^{1/2}}\right)$$
$$\times \exp\left[-\frac{\beta}{a^3}\int \mathbf{dr}\ V(\mathbf{r}) + \frac{\beta^2}{24a}\int \mathbf{dr}\ |\nabla V(\mathbf{r})|^2\right] \tag{D.14}$$

Finally we find from (5.38), (5.42), and (D.14)

$$\Sigma = \rho \int \mathbf{dx}\ \rho_1(\mathbf{x}, \mathbf{0}) = O(\rho^{3/4}) \tag{D.15}$$

APPENDIX E. DERIVATION OF (5.38)–(5.39)

Setting $\omega_{\mathbf{j}}(s) = s\mathbf{x} + \sqrt{\beta}\,\alpha(s) - \mathbf{j}a$, a limited Taylor expansion with respect to $(\mathbf{r}+\tau)a$ up to order a^2 gives

$$\begin{aligned}\int_0^1 ds\, V(\omega_{\mathbf{j}}(s) - (\mathbf{r}+\tau)a) &= \int_0^1 ds\, V(\omega_{\mathbf{j}}(s)) - a(\mathbf{r}+\tau)_m \int_0^1 ds\, (\partial_m V)(\omega_{\mathbf{j}}(s)) \\ &\quad + \frac{a^2}{2}(\mathbf{r}+\tau)_m(\mathbf{r}+\tau)_n \int_0^1 ds\, (\partial^2_{mn} V)(\omega_{\mathbf{j}}(s)) + a^3 R(\omega_{\mathbf{j}}(s), \mathbf{r}a + \tau a)\end{aligned} \tag{E.1}$$

with summation on repeated indices $m, n = 1, 2, 3$.

In view of the assumptions (2.2), the remainder in (E.1) is of order

$$R(\omega_{\mathbf{j}}(s), \mathbf{r}a + \tau a) = O\left(\int_0^1 ds\, [1 + |\omega_{\mathbf{j}}(s)|^2]^{-\eta/2}\right) \tag{E.2}$$

uniformly with respect to $\mathbf{r}$, τ, and a ($\mathbf{r}, \tau \in Q$, a small). Expanding the exponential in (5.37) gives

$$\begin{aligned}&\int_Q d\mathbf{r} \exp\left[-\beta \int_0^1 ds\, V(\omega_{\mathbf{j}}(s) - (\mathbf{r}+\tau)a)\right] \\ &= \left\{\exp\left[-\beta\int_0^1 ds\, V(\omega_{\mathbf{j}}(s))\right]\right\}\left\{1 + \beta a \tau_m \int_0^1 ds\, (\partial_m V)(\omega_{\mathbf{j}}(s))\right. \\ &\quad + \frac{1}{2}a^2\left(\frac{1}{12}\delta_{mn} + \tau_m\tau_n\right)\left[\beta^2 \int_0^1 ds \int_0^1 dt\, (\partial_m V)(\omega_{\mathbf{j}}(s))(\partial_n V)(\omega_{\mathbf{j}}(t))\right. \\ &\quad \left.\left. - \beta\int_0^1 ds\, \partial^2_{mn} V(\omega_{\mathbf{j}}(s))\right] + a^3 R(\omega_{\mathbf{j}}(s), \mathbf{r}a + \tau a)\right\}\end{aligned} \tag{E.3}$$

with a remainder, again denoted R, which satisfies the same estimates (E.2). We have used

$$\int_Q d\mathbf{r}\, \mathbf{r}_m = 0, \qquad \int_Q d\mathbf{r}\, \mathbf{r}_m \mathbf{r}_n = \frac{1}{12}\delta_{mn}$$

It is easy to see that the argument of the logarithm (5.37) can also be written in the form (E.3) with another remainder still satisfying (E.2). Indeed, writing $[1+A]$ for the bracket in (E.3), this argument equals

$$\exp\left[-\beta\int_0^1 ds\, V(\omega_{\mathbf{j}}(s))\right]\left(\left(1+\frac{z}{1+z}A\right)\right.$$
$$\left.-\frac{1}{1+z}\left\{1-\exp\left[\beta\int_0^1 ds\, V(\omega_{\mathbf{j}}(s))\right]\right\}\right) \tag{E.4}$$

With (2.2) and $1/(1+z)=O(a^3)$, the last term in (E.4) has a bound as in (E.2), so that (E.4) has the form (E.3).

Expanding now the logarithm of (E.3) gives

$$\sum_{\mathbf{j}} C_{\mathbf{j},\tau a}(\mathbf{0},\mathbf{x},\alpha)$$
$$=-\beta\int_0^1 ds\sum_{\mathbf{j}} V(\omega_{\mathbf{j}}(s))+\beta a\tau_m\int_0^1 ds\sum_{\mathbf{j}}(\partial_m V)(\omega_{\mathbf{j}}(s))$$
$$-\frac{1}{2}\beta a^2\left(\frac{1}{12}\delta_{mn}+\tau_m\tau_n\right)\int_0^1 ds\sum_{\mathbf{j}}(\partial^2_{mn}V)(\omega_{\mathbf{j}}(s))$$
$$+\frac{\beta^2a^2}{24}\sum_{\mathbf{j}}\left|\int_0^1 ds\,(\nabla V)(\omega_{\mathbf{j}}(s))\right|^2+a^3\sum_{\mathbf{j}}R(\omega_{\mathbf{j}}(s)\,\mathbf{r}a+\tau a) \tag{E.5}$$

where the remainder R satisfies (E.2).

It remains to approximate the lattice sums by the corresponding integrals. For this we use the Poisson summation formula for a smooth $\Phi(\mathbf{x})$ having the properties (2.2), i.e.,

$$\sum_{\mathbf{j}}\Phi(\mathbf{j}a)=a^{-3}\sum_{\mathbf{j}}\tilde{\Phi}\left(\frac{2\pi\mathbf{j}}{a}\right)=a^{-3}\left[\tilde{\Phi}(\mathbf{0})+\sum_{\mathbf{j}\neq\mathbf{0}}\tilde{\Phi}\left(\frac{2\pi\mathbf{j}}{a}\right)\right]$$
$$=a^{-3}\int d\mathbf{x}\,\Phi(\mathbf{x})+O(1) \tag{E.6}$$

If $\Phi(\mathbf{x})$ is four times continuously differentiable with integrable derivatives, $\tilde{\Phi}(\mathbf{k})=O(1/|k|^4)$ for large k and thus

$$\sum_{j\neq\mathbf{0}}\tilde{\Phi}\left(\frac{2\pi\mathbf{j}}{a}\right)=a^3O\left(\sum_{\mathbf{j}\neq\mathbf{0}}\frac{1}{|\mathbf{j}|^4}\right)$$

leading to (E.6).

If y is a fixed vector, we have the same result for the translates $\Phi(\mathbf{x}+\mathbf{y})$ and $e^{i\mathbf{k}\cdot\mathbf{y}}\tilde{\Phi}(\mathbf{k})$, i.e.,

$$\sum_{\mathbf{j}} \Phi(\mathbf{j}a+\mathbf{y}) = a^{-3} \int d\mathbf{x}\, \Phi(\mathbf{x}) + O(1) \tag{E.7}$$

uniformly with respect to $\mathbf{y}$.

We apply (E.7) to the terms of (E.5) with $\mathbf{y} = s\mathbf{x} + \sqrt{\beta}\,\alpha(s)$. The assumption (2.2) implies that (E.7) holds for V, $\partial_m V$, and $\partial^2_{mn} V$ (this is where we need V six times differentiable). The first and fourth terms in the r.h.s. of (E.5) give (5.38). Since $\int d\mathbf{r}\, \partial_m V(\mathbf{r}) = \int d\mathbf{r}\, \partial^2_{mn} V(\mathbf{r}) = 0$, the second and third terms are, respectively, $O(a)$ and $O(a^2)$. By (E.2) the last term is

$$\begin{aligned} a^3 O\left(\int_0^1 ds \sum_{\mathbf{j}} [1+|\omega_{\mathbf{j}}(s)|^2]^{-\eta/2}\right) \\ = O\left(\int d\mathbf{x}\,(1+|\mathbf{r}|^2)^{-\eta/2}\right) + O(a^3) = O(1) \end{aligned} \tag{E.8}$$

uniformly with respect to all arguments. This proves (5.38).

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