Schrödinger equation for the two-dimensional Coulomb potential

O. Atabek

Laboratoire de Photophysique Moléculaire, Université Paris XI, 91405, Orsay, France

C. Deutsch

Laboratoire de Physique des Plasmas, Université Paris XI, 91405, Orsay, France

M. Lavaud

Centre de Recherches des Hautes Températures, 45100 Orléans-La Source, France (Received 27 December 1973)

General properties of the Sturm-Liouville equation and numerical methods are used to determine the eigenquantities of the Schrödinger equation of a (+ -) pair interacting via the two-dimensional Coulomb potential $q^2 \ln r$. The spectrum is shown to be purely discrete and semibounded in its lower part with a density of levels of $dN(\lambda)/d\lambda \sim e^{2\lambda/q^2}$, while the wave functions behave like those of a harmonic oscillator. The spectrum is studied as a function of the coupling parameter q. Wave functions ψ and radial densities $r|\psi|^2$ are plotted against r and some matrix elements $\langle \psi | r^v | \psi \rangle$ are given. The q = 1 spectrum is used to evaluate the corresponding sum-over-states which allows us to give a clear meaning to the canonical thermodynamical functions of the two-dimensional Coulomb gas below the transition temperature $T_c = q^2/2k_B$.

I. INTRODUCTION

Recent investigations¹ in the statistical mechanics of the two-dimensional Coulomb gas have led us to consider quantum binary interactions in a pair of opposite charges, in order to set on a firm basis the canonical equilibrium at low temperature. This explains why we now address ourselves to solving the eigen-Schrödingerproblem for the two-dimensional Coulomb potential $q^2 \ln r$ solution of Poisson's equation

$$\Delta V = -(n-2)S_n\delta, \quad n \ge 3$$

= -S_n\delta, \quad n \le 2 (1.1)

with $S_n = 2\pi^{n/2}/\Gamma(n/2)$, *n* being the space dimensionality. This problem also deserves interest in its own right, by allowing us to gain some insight into the dimensionality dependence of the Coulomb interaction, the basic interaction upon which the real world is built.² The onedimensional Coulomb-Schrödinger problem is encountered in the quantum treatment of the linear Stark effect q^2r of a one-dimensional system.³ It is solved quasianalytically in terms of Airy functions. On the contrary, and in analogy with many other two-dimensional situations (see for instance the hard-disk problem in statistical mechanics), the present two-dimensional Schrödinger equation requires the introduction of numerical techniques nearly from the beginning. It must also be noticed that the solutions of the considered Schrödinger equation may have some connections with those obtained from similar problems with potentials $r^{-n} \ln r$ used in the

so-called peratization techniques in phenomenological quantum field theory.⁴ We shall first consider the general properties of the two-dimensional Schrödinger equation with a monotonic increasing potential in order to be able to draw semiquantitative conclusions about the spectrum behavior and obtain the minimum of information needed to support the numerical investigation considered further. Then, we study quantitatively the given discrete spectrum as a function of the coupling constant q. Furthermore, for q = 1, we graph some first-excited-state wave functions ψ together with corresponding radial densities, and indicate numerical values for matrix elements $\langle \psi | r^{\nu} | \psi \rangle$ ($\nu = 1, 2, 3$). The q = 1 spectrum is used to evaluate the pair (+ -) sum-overstates which gives access to the canonical thermodynamical functions of the two-dimensional Coulomb gas below the transition temperature $T_c = q^2/2k_B$. These results allow us to set on a firm basis preliminary conclusions drawn by Hauge and Hemmer⁵ from a perfect gas of noninteracting pairs (+ -) of hard disks.

II. GENERAL PROPERTIES OF THE STURM-LIOUVILLE EQUATION

Now, we follow quite closely a presentation due to Titchmarsh⁶ for the treatment of the twodimensional Schrödinger equation:

$$\Delta \psi + [\lambda - V(r)]\psi = 0 \tag{2.1}$$

with $V(r) = q^2 \ln r$ and atomic units $(\hbar = \mu = 1)$. The introduction of the usual polar coordinates in Eq. (2.1) through $\psi(r, \theta) = f(r)g(\theta)$ leads to

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$$\frac{g''(\theta)}{g(\theta)} = -m^2, \quad g(\theta) = \begin{cases} \sin m\theta \\ \cos m\theta \end{cases}$$
(2.2)

and

$$f''(r) + \frac{f'(r)}{r} + \left(\lambda - V(r) - \frac{m^2}{r}\right) f(r) = 0.$$
 (2.3)

Equation (2.2) could also result from the invariance under O(2) (the group of plane rotations) of Eq. (2.1). By inserting $f(r) = r^{-1/2} \chi(r)$ in Eq. (2.3), we get the required radial differential equation:

$$\chi''(r) + \left(\lambda - V(r) - \frac{m^2 - \frac{1}{4}}{r^2}\right)\chi(r) = 0, \qquad (2.4)$$

which looks like the corresponding hydrogen equation⁷ with $(m^2 - \frac{1}{4})$ instead of l(l + 1) in the centrifugal term, so that the fundamental state (m=0) retains the quadratic contribution $1/4r^2$ in the potential energy while it is known to vanish in three dimensions (l=0). This property is a very important one. It will be shown below to be responsible for the very large distance between the fundamental and the first excited state standing for all q values. The normalized eigenfunctions associated with the eigenvalues $\lambda_{m,n}$ may be written as

$$\psi_{\mathbf{m},\mathbf{n}} = \left(\frac{m}{2\pi}\right)^{1/2} r^{-1/2} \chi_{\mathbf{m},\mathbf{n}}(r) \begin{cases} \cos m\theta \\ \sin m\theta \end{cases}$$

$$(\epsilon_0 = 1, \quad \epsilon_1 = \epsilon_2 = \cdots = 2). \qquad (2.5)$$

The foregoing equations have been written with three-dimensional "atomic units," although the coupling constant q is not given a particular value by any physical constraint. However, in close analogy with the three-dimensional Coulomb problem, it appears possible⁸ to introduce twodimensional "atomic units." For this purpose, let us return to the radial hydrogen Schrödinger equation⁷ written as

$$\frac{1}{r}\frac{d^2}{dr^2}[rF_l(r)] = -\frac{2\mu}{\hbar^2}\left(\lambda + \frac{e^2}{r} - \frac{\hbar^2}{2\Gamma}\frac{l(l+1)}{r^2}\right)F_l \quad .$$
(2.6)

Then, the natural unit of length (e^2 in units of energy-length⁻¹) is the Bohr radius $a_0 = \hbar^2/\mu e^2$ with μ the reduced mass of the two-particle system, and the unit of energy is then the Rydberg $R_{\infty} = \mu e^4/2\hbar^2$. So, with $x = r/a_0$, Eq. (2.6) becomes

$$\frac{1}{x}\frac{d^2}{dx^2}\left(xF_l(x)\right) = -\left(\epsilon + \frac{2}{x} - \frac{l(l+1)}{x^2}\right)F_l(x)$$
(2.7)

with $\epsilon = E/R_{\infty}$. $F_l(x) = f_l(x)/x$ gives the expected

result

$$\frac{d^2}{dx^2}f_I(x) = -\left(\epsilon + \frac{2}{x} - \frac{l(l+1)}{x^2}\right)f_I(x) \quad .$$
 (2.8)

The same procedure may be duplicated in the two-dimensional situation with Eq. (2.3) written as

$$\begin{aligned} \left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}\right)F_m(r) \\ &= -\frac{2\mu}{\hbar^2}\left[\lambda - q^2\ln\left(\frac{r}{L}\right) - \frac{m^2}{r^2}\right]F_m(r) \quad . \end{aligned}$$

$$(2.9)$$

Now the natural unit of energy is q^2 with the corresponding "Bohr radius" $b = (2\mu q^2/\hbar^2)^{-1/2}$. In these units Eq. (2.9) becomes $(x = r/b, \epsilon = \lambda/q^2)$

$$\left(\frac{d^2}{dx^2} + \frac{1}{x}\frac{d}{dx}\right)F_m(x)$$
$$= -\left[\epsilon - \left(\ln x + \ln\frac{b}{L}\right) - \frac{m^2}{x^2}\right]F_m(x)$$
(2.10)

corresponding to Eq. (2.3). It is a direct analog of Eq. (2.7). Incidently the choice L = b drops out the constant term on the right-hand side. In three dimensions when one makes change $F_l(x) = f_l(x)x^{-1}$ nothing changes with the centrifugal term $l(l+1)r^{-2}$, but in two dimensions the analogous change $F_m(x) = f_m(x)x^{-1/2}$ modifies Eq. (2.10) to

$$\frac{d^2}{dx^2}f_m(x) = -\left(\epsilon - \ln x - \frac{m^2 - \frac{1}{4}}{x^2}\right)f_m(x), \qquad (2.11)$$

a direct analog of Eq. (2.4). It must also be noticed that the considered two-dimensional "atomic units" $\hbar = 1$, q = 1, and $\mu = \frac{1}{2}$ are compatible with the previous three-dimensional atomic units $\hbar = \mu = 1$. In the following most of an calculations will be performed with these two-dimensional "atomic units."

Before going on with the numerical task of evaluating $\lambda_{m,n}$ and $\psi_{m,n}$ it proves useful to invoke some general properties⁶ of the Sturm-Liouville equation (2.4). First, we obtain at once from the monotonic increasing behavior of V(r) that the eigenvalues spectrum $\lambda_{m,n}$ is a purely discrete one located between $-\infty$ and $+\infty$. Moreover, the number of eigenvalues smaller than an arbitrary λ is given by

$$N(\lambda) \sim \frac{1}{2} \int_{V(r) \leq \lambda} \left[\lambda - V(r) \right] r \, dr = \frac{1}{8} q^2 e^{2\lambda/q^2} ,$$
(2.12)

which is a very quickly increasing function of λ

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allowing the appearance of the very interesting property of lower semiboundedness.

A lower bound λ_a for the eigenvalues may be defined by

$$\int_{-\infty}^{\lambda_a} \frac{dN(\lambda)}{d\lambda} \, d\lambda < 1 \,. \tag{2.13}$$

From Eqs. (2.6) and (2.7) it follows that

$$\lambda_{o} < \frac{1}{2} q^{2} \ln |8/q^{2}|.$$
 (2.14)

Equation (2.14) makes it clear that the spectrum is void between $-\infty$ and λ_a . An immediate and important by-product of Eq. (2.14) will be the lower-semiboundedness of H_{2N} which is the first step toward the existence of the stability property for the two-dimensional Coulomb gas⁹ reached through the 2N-body Hamiltonian $(N = N_+ = N_-)$

$$H_{2N} = \sum_{1 \le i < j \le 2N} \left(-\frac{1}{2N-1} \left(\Delta_i + \Delta_j \right) - q_i q_j \ln |r_{ij}| \right)$$
$$= \sum_{1 \le i < j \le 2N} H_{ij}, \qquad (2.15)$$

where H_{ij} is the two-body Hamiltonian associated with Eq. (2.1) with the masses $m_i = m_j = 1$. We then have

$$\lambda_{\min} = \inf \langle \psi | H_{2N} | \psi \rangle \ge \sum_{1 \le i < j \le 2N} \inf \langle \psi | H_{ij} | \psi \rangle ,$$
(2.16)



FIG. 1. Variations of the lowest eigenvalue $\lambda_{0,0}$ (in three-dimensional atomic units) with the coupling constant q. Curve 1 gives the prediction formula (2.4). The numerical calculation is labeled as curve 2.

$$\inf \langle \psi | H_{2N} | \psi \rangle = \begin{cases} (2N-1)\lambda_a, & \text{for } q_i q_j < 0\\ 0, & \text{for } q_i q_j \ge 0 \end{cases}$$
(2.17)

which gives the required necessary condition $\lambda_{\min} \ge (2N-1)N^2 \mid \lambda_a \mid$ for the existence of stability.

III. QUANTITATIVE DETERMINATION OF THE SPECTRUM

A. Eigenvalues

The FORTRAN computer program due to Cashion, Cooley, and Zare¹⁰ is used to calculate the eigenquantities $\lambda_{m,n}$ and $\psi_{m,n}$ attached to Eq. (2.4). The key quantity of importance in the numerical procedure is the number of nodes n of a given $\psi_{m,n}$, which is allowed to run over the whole spectrum by labeling the eigenvectors once a given $\lambda_{m,n}$ has been reached, through the essay and errors method. Keeping in mind further applications to the statistical mechanics of the two-dimensional Coulomb gas in Sec. IV, we first study the variations of the lowest eigenvalue $\lambda_{0,0}$ with q. It is shown in Fig. 1 together with the prediction (2.14). Note that at the limit q=0, Eq. (2.4) gives back the Bessel equation with $\lambda_{0,0} = 0$. The true variations being much less important than those due to Eq. (2.14). It then appears possible to let q = 1 in the following without introducing any significant restrictions. The expression (2.12) for the density of levels



FIG. 2. Density of levels ρ as a function of the magnetic quantum number m.

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is an average taken over the magnetic quantum number m. A sharper expression may be obtained by considering the number of levels per unit energy

$$\rho = \frac{21}{\lambda_{m, 20} - \lambda_{m, 0}} \tag{3.1}$$

plotted in Fig. 2. We restrict ourselves to the first twenty levels because the higher part of the spectrum appears as a very dense one for all q values, in accord with Eq. (2.12). The resulting curve is well fitted by

$$\begin{split} \rho &= 0.7787 \times 10^{-5} m^2 + 0.35302 \times 10^{-2} m + 4.525 , \\ &0 \leq m \leq 300 \\ &= 0.6421 \times 10^{-4} m^2 - 0.2413 \times 10^{-1} m + 7.795 , \\ &300 < m \leq 600 \\ &= 0.8938 e^{0.4385 \times 10^{-2} m} + 4.1237 , \\ &600 < m \leq 900 \\ &= 0.2912 e^{0.5626 \times 10^{-2} m} + 2.630 , \\ &900 < m \leq 1200 \\ &(3.2) \end{split}$$

with q = 1.

A straightforward localization of $\lambda_{m,n}$, with $m \ge 1$, may be obtained through the density of levels and the minimum of the potential curve:

$$U(r) = q^{2} \ln |r| + (m^{2} - \frac{1}{4})/r^{2}$$
(3.3)



FIG. 3. Lowest eigenvalues $\lambda_{m,0}$ (two-dimensional "atomic units" $\hbar = 2\mu = q = 1$) referenced to the minimum of the potential part (3.3) as a function of the magnetic quantum number m.

given as

$$U_{\min} = q^{2} \left\{ \frac{1}{2} + \ln \left| q^{-1} \left[2(m^{2} - \frac{1}{4}) \right]^{1/2} \right| \right\}, \quad m \ge 1$$
(3.4)

for $\mathcal{V}_{\min} = q^{-1} \left[2(m^2 - \frac{1}{4}) \right]^{1/2}$. $\lambda_{m,0}$ could be referenced to U_{\min} , as in Fig. 3, where the quantity $\Delta = \lambda_{m,0} - U_{\min} \cdot (q = 1, 1 \le m \le 80)$ is quite well fitted by

$$\Delta = 0.4473 \times 10^{-3} m + 5.4530 - U_{\min} \text{ for } 1 \le m \le 20$$

and

$$\Delta = -0.2416 \times 10^{-2} m + 5.5103 - U_{\min}$$

for 20 < m < 80. (3.5)

Then, the sharp decrease observed in the behavior of Δ allows us to write

$$\lambda_{m,n} = U_{\min} + \Delta + n\rho^{-1} \text{ for } 1 \le m \le 80$$

and

$$\lambda_{m, n} = U_{\min} + n\rho^{-1} \text{ for } m > 80.$$
 (3.6)

B. Wave functions and matrix elements

A general idea of the properties of the first excited states may be gained from the data collected in Table I where some matrix elements $\langle \psi | r^{\nu} | \psi \rangle$ are given in two-dimensional "atomic units." A number of corresponding eigenfunctions $\psi_{m,n}$ with m = 0, 1, 2 and n = 0, 1, 2 may be seen in Fig. 4. Their general shape looks very similar to the harmonic-oscillator wave functions in two or three dimensions.¹¹ Their best maximum is always located just before the right-turningpoint solution of $\lambda_{m,n} - U(r) = 0$. Related radial densities $\gamma |\psi_{m,n}|^2$ are plotted in Fig. 5. They are of course sharply peaked around the maxima of $\psi_{n,m}$. An interesting feature to note is the increasing localization towards large distances, of wave functions $\psi_{m,n}$, with increasing values of m. This is nothing but a by-product of the

TABLE I. Some data concerning the first excited states for coupling constant q = 1. All energies and matrix elements are in two-dimensional "atomic units."

m	n	$\lambda_{m,n}$	$\langle \psi m{r} \psi angle$	$\langle \psi \boldsymbol{r}^1 \psi angle$	$egin{array}{c r^2 \psi} \end{array}$
0	0	0,24395	14.99	278.24	0.6063×10^{4}
0	1	5.71537	$0.26598\! imes\!10^{6}$	$0.265\ 98 imes 10^{6}$	0.1400×10^{9}
0	2	6.30121	$0.89787 imes 10^3$	$0.818\ 29 \times 10^{6}$	$0.75582\! imes 10^9$
1	0	5.4539	0.3839×10^{3}	$0.1496 imes 10^6$	$0.5912 imes 10^8$
1	1	5.7416	$0.5119 imes10^3$	0.2660×10^{6}	0.14010×10^{9}
1	2	6.3012	0.8980×10^{3}	0.8183×10^{6}	$0.7559 imes 10^9$
2	0	5.4546	$0.3846 imes 10^3$	0.1501×10^6	$0.5942 imes 10^8$
2	1	5.7420	$0.5120 imes 10^3$	0.2661×10^{6}	0.14018×10^9
2	2	6.3013	$0.8983 imes 10^{3}$	0.8189×10^{6}	0.7567×10^{9}



FIG. 4. First excited-states wave functions (two-dimensional "atomic units").



FIG. 5. First excited-states radial densities (two-dimensional "atomic units").

relative weakness of the logarithmic potential when compared to the centrifugal term $(m^2 - \frac{1}{4})r^{-2}$ in the origin vicinity.

IV. TWO-DIMENSIONAL COULOMB GAS AT LOW TEMPERATURE

Now, we intend to apply the foregoing results to the study of the corresponding sum-overstates, so that the low-temperature canonical equilibrium of the two-component two-dimensional Coulomb gas could be described in the approximation of a perfect gas of N noninteracting pairs^{1, 5, 13} through the canonical partition function

$$Q^{*}(V, T) = N! V^{N} \lim_{V \to \infty} [Q_{+}(V, T)]^{N}$$
(4.1)

with¹²

$$\lim_{V \to \infty} Q_{+-}(V, T) = \int d^2 \vec{\mathbf{r}} \sum_{\alpha} \psi_{\alpha}^{*}(1, 2) e^{-\beta H} \psi_{\alpha}(1, 2) ,$$
(4.2)

where $\psi_{\alpha}(1, 2)$ denotes the two-body eigenfunctions of $H = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + V(r_{12})$ written as

$$\psi_{\alpha}(1,2) = \left(e^{i\vec{P}\cdot\vec{R}}/\sqrt{V}\right)\psi_{m,n}(r) \qquad (4.3)$$

with $\alpha \equiv (\vec{\mathbf{P}}, m, n)$, $\vec{\mathbf{P}} = \vec{\mathbf{P}}_1 + \vec{\mathbf{P}}_2$, $\vec{\mathbf{R}} = (\vec{\mathbf{r}}_1 + \vec{\mathbf{r}}_2)2^{-1}$ and $E_{\alpha} = \frac{1}{4}P^2 + \lambda_{m,n}$. Equation (4.2) then becomes

$$\lim_{V \to \infty} Q_{+-}(V, T) = \int d^2 r \sum_{P,m,n} |\psi_{m,n}(r)|^2 e^{-\beta P^2/4} e^{-\beta \lambda_{m,n}}.$$
(4.4)

The kinetic-energy part is obtained through

$$V^{-1} \sum_{P} e^{-\beta P^{2}/4} = \frac{2\pi}{h^{2}} \int_{0}^{\infty} dP \ P e^{-\beta P^{2}/4} = \frac{2}{\Lambda^{2}}$$
(4.5)

where $\Lambda = h/(2\pi m k_B T)^{1/2}$ denotes the corresponding de Broglie wavelength; so we have

$$\lim_{V \to \infty} Q_{+-}(V, T)$$

$$= 2\left(\frac{V}{\Lambda^2}\right) \left(\sum_{n=0}^{n=\infty} e^{-\beta\lambda_{0,n}} + 2\sum_{m=1}^{m=\infty} \sum_{n=0}^{n=\infty} e^{-\beta\lambda_{m,n}}\right)$$
(4.6)

where *n* is the number of nodes in $\psi_{m,n}(r)$. The estimation of Q_{+-} requires some insight into the quantitative behavior of λ_{mn} . The fundamental state with m = 0 has been singled out in the fore-going expression because the numerical study of the eigenvalues of Eq. (2.4) shows that for all q^2 values, the inequality

$$||\lambda_{0,0}| - |\lambda_{n,m}|| \gg ||\lambda_{n',m'}| - |\lambda_{n,m}||,$$

all n,m,n',m' , (4.7)

remains fulfilled. Moreover, the density of levels deduced from Eq. (2.13) predicts a very dense quasicontinuum for increasing λ , so that the numerical evaluation of the eigenvalues is expected to become meaningless above a critical λ_{m_0, n_0} depending on q^2 . Therefore, it appears convenient to rewrite Eq. (4.6) in the form

$$\lim_{V \to \infty} Q_{+-}(V, T) \sim \beta^{-1} \left(\sum_{n=0}^{n_0} e^{-\beta\lambda_0, n} + 2 \sum_{m=1}^{m_0} \sum_{n=0}^{n_0} e^{-\beta\lambda_m, n} + 2 \int_{\lambda_{m_0, n_0}}^{\infty} \frac{dN(\lambda)}{d\lambda} e^{-\beta\lambda} d\lambda \right)$$

$$(4.8)$$

which remains finite only when $\int_a^{\infty} e^{(2/q^2-B)\lambda} d\lambda < +\infty$ with $k_B T < \frac{1}{2}q^2$, thus providing an important and independent confirmation of the discontinuity of Q^* at the transition temperature $T_c = q^2/2k_B$. It must be kept in mind that we are still considering a classical system with quantum binary interactions, in accord with the splitting of the Hamiltonian into kinetic and potential parts, respectively. However, the quantum treatment of the (+-) interaction allows us to consider point particles and derive meaningful thermodynamic functions for $T < T_c$. More precisely, in the vicinity of $T \rightarrow T_c^-$, we get

$$F = -\frac{1}{2}k_{B}T \ln Q_{+-}(V, T)$$

$$\simeq -\frac{1}{2}\beta^{-1}(2/q^{2} - \beta)\lambda_{m_{0}, n_{0}} - \ln(-2/q^{2} + \beta) \qquad (4.9)$$

 $C_{v} = 1 + \frac{\beta^{2}}{2} \frac{\partial^{2}}{\partial \beta^{2}} \ln Q_{+-} \simeq 1 + \frac{1}{2(1 - T/T_{c})^{2}}$ (4.10)

with $V \rightarrow \infty$ (F and C_V being referred to one particle) where use has been made of the inequality

$$\int_{\lambda_{m_0,n_0}}^{\infty} \frac{dN(\lambda)}{d\lambda} e^{-\beta\lambda} d\lambda \gg \sum_{n=0}^{n_0} e^{-\beta\lambda_{0,n}} + 2\sum_{m=1}^{m_0} \sum_{n=0}^{n_0} e^{-\beta\lambda_{m,n}}$$

$$(4.11)$$

valid for $T \sim T_c^-$. More complete F and C_V expressions valid in the $0 \leq T \leq T_c$ domain may be reached as explained below, through the discrete sums in Eq. (4.8). It must be noticed also that the partition function (4.1) gives back immediately the ideal gas equation of state $PV = Nk_BT$. The diverging behavior of the thermodynamic functions near T_c now arises from the infinite set of discrete levels accessible to the two-dimensional "molecule" when the temperature

and

rises from 0 to T_c . This feature complements in a certain way the high-temperature description underlying Eq. (1.7) of Ref. 1, so that we are faced with the unified picture of a transition temperature with divergent thermodynamic functions associated with the formation or destruction of low-lying internal states for the pairs of opposite charges. Nevertheless, we feel that the present low-temperature binary approach should be properly included in a many-body picture as the most important contribution in the vicinity of T_c . As stressed previously, the numerical resolution of the Schrödinger equation (2.4) could give access to well-defined canonical quantities for $T < T_c$. We have thus obtained

$$\ln\left(\sum_{n=0}^{n_0} e^{-\beta\lambda_{0,n}} + 2\sum_{m=1}^{m_0} \sum_{n=0}^{n_0} e^{-\beta\lambda_{m,n}}\right) \simeq a\beta + b \qquad (4.12)$$

in two-dimensional "atomic units" for q = 1, $2 < \beta < 11.50$ with a = -2.6093 and b = -0.5307, an estimate for the discrete sum particularly interesting when $\beta \rightarrow \infty$, which gives

$$\lim_{V \to \infty} Q_{+-} \simeq e^{a\beta+b} + \frac{2}{\beta} \frac{e^{(2-\beta)\lambda}m_0, n_0}{\beta-2}$$
(4.13)

with

$$\frac{2}{\beta(\beta-2)}\,\frac{e^{(2-\beta)\,\lambda_{m_0,\,n_0}}}{e^{a\beta+b}}\ll 1$$

- ¹C. Deutsch and M. Lavaud, preceding paper, Phys. Rev. A <u>9</u>, 2598 (1974).
- ²See, for instance, A. Lenard, *Lectures on the Coulomb stability problem*, Battelle Seatle 1971 Rencontres, (Springer-Verlag, Berlin, 1973), p. 114.
- ³E. C. Titchmarsh, *Eigenfunction Expansion* (Clarendon, Oxford, 1958), Part I, Chap. 4.
- ⁴W. M. Frank, D. J. Land, and R. M. Spector, Rev. Mod. Phys. 43, 36 (1971).
- ⁵E. M. Hauge and P. C. Hemmer, Physica Norvegica <u>5</u>, 209 (1971).
- ⁶Reference 3, Part II, Chaps. 15 and 16.

and $(m_0, n_0) \simeq (905, 0)$, so we get in that case $(q=1, \beta \gg 1)$

$$\lim_{V \to \infty} \ln Q_{+-} = -2.6093\beta - 0.5307 + 0.1575 \times 10^8 e^{-5.065\beta} / \beta(\beta - 2) ,$$

$$F = \frac{1}{2} \left(2.6093 + \frac{0.5307}{\beta} - \frac{0.1575 \times 10^8 e^{-5.065}}{\beta^2 (\beta - 2)} \right) ,$$
(4.15)

and

$$C_{\nu} = \frac{0.157 \times 10^8 e^{-5.063\beta}}{\beta(\beta - 2)^3} \left\{ 12.817\beta^4 - 41.142\beta^3 - 99.536\beta^2 + 14.252\beta + 14 \right\}.$$
(4.16)

Equation (4.15) shows a nonvanishing free energy at T = 0 corresponding to a residual interaction within each pair, while $\lim C_V = 0$ for $T \rightarrow 0$, as expected.

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- ⁷H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of* One- and Two-Electrons Atoms (Springer-Verlag, Berlin, 1957), p. 1.
- ⁸We are indebted to H. E. DeWitt for this suggestion.
- ⁹F. J. Dyson and A. Lenard, J. Math. Phys. <u>8</u>, 423 (1967).
- ¹⁰J. W. Cooley, Math. Comput. <u>15</u>, 363 (1961).
- ¹¹L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics* (McGraw-Hill, New York, 1935).
- ¹²K. Huang, Statistical Mechanics (Wiley, New York, 1963), Chap. 4.
- ¹³G. Knorr, Phys. Lett. A <u>28</u>, 166 (1968).