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Semi-classical estimation of ground state energies on a sphere

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Abstract We consider electrons confined to the surface of a sphere, and calculate the classical electrostatic energies for up to 32 electrons. Next, we introduce a magnetic field perpendicular to the surface of the sphere, by placing a magnetic monopole at the origin. The classical analysis can be extended by replacing the pair-potential by an effective potential, defined as the quantum mechanical energy of a pair of electrons at the appropriate distance. For the worst case of a filled Landau level, which can be calculated exactly, the approximated energies are correct within a few percent, and are considerably improved when the filling factor decreases. Further, we use the semiclassical energies to construct a simply parametrized function for extrapolating the ground state energy as a function of the filling factor, from finite particle numbers to an infinite number of particles.

1. Introduction

The fractional quantum Hall effect $(FQHE)$[1] is a remarkable many-body phenomenon that has attracted much attention[2,3] since its discovery. In $Al_{1-x}Ga_xAs - GaAs$ heterojunctions the electrons are confined to move in a two-dimensional plane. Geometrically, the electron gas is not two-dimensional, since the wavefunction has an extension of 10-50 Å in the third dimension. However, the gap up to the first excited state is of order 50 meV, much greater than the typical energies at the experimental temperatures of about 1 K $\simeq$ 0.1 meV or less. All degrees of freedom in the third direction are thus frozen, and the

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system is dynamically two-dimensional. In the two-dimensional plane, the motion remains nearly free, with extremely high mobilities. This very good realization of an idealized two-dimensional electron gas is achieved mainly due to the technique of modulated doping, which is available by molecular beam epitaxy. Hereby, one is able to remove the donor atoms from the carriers in the plane. Thus, scattering is highly reduced. Also the structural change by adding Al is small, giving rise to a very smooth interface.

In the presence of a strong magnetic field perpendicular to the plane, these high mobility samples show a quantization of the Hall conductivity $a_{xy} = \nu e^2/h$, where ν is a simple rational fraction, which equals the filling factor around which the quantization occurs (the first discovered and most pronounced case is the $\nu = 1/3$ state). At these values of ν the magnetotransport is dissipationless. The stability of a_{xy} suggests cusps in the ground state energy as a functions of ν, and corresponding gaps in the excitation spectrum. Experimentally one finds that the FQHE is more easily seen when the mobility of the sample is high, as opposed to the integer QHE' which can be stronger in samples with more disorder and lower mobility (above a certain limit below which the effect disappears). This supports the idea that the electron-electron interaction is the dominant cause of the effect. From studying a small number of particles, Laughlin[5] proposed a variational wavefunction of the Jastrow form which describes the situations very well when $\nu = 1/m$, m being a small, odd integer. Accordingly the electron gas condenses into a new state, which is a strongly correlated quantum fluid. This state is incompressible and is separated by a gap from its excitations. The excitations can be viewed as quasiparticles which are believed to carry a fractional charge $e^* = \nu e$, and may be considered to obey fractional statistics[6,7]. Extension to other filling factors of a more general form is due to Haldane[5]. According to his scheme, the quasiparticles condense into a new Laughlin state with its own set of new quasiparticle excitations. Repetition of this argument leads to a hierarchy of filling factors

$$\nu = \cfrac{1}{m + \cfrac{\alpha_1}{p_1 + \cfrac{\alpha_2}{p_2 + \ldots}}} \tag{1.1}$$

where α_i is 0 or ± 1, and $p_i = 2, 4, \ldots$.

To check the validity of Laughlin's theory, and to look for cusps in the ground state energy, finite-size calculations have been performed. Important contributions were made by Haldane and Rezayi . They modelled the system by mapping the two-dimensional planar electron gas onto a sphere, and diagonalized the Hamiltonian for small particle numbers. The calculations were done for particle numbers up to N = 7. Later, Fano et al.[10] did similar calculations for up to N = 10 particles in the $\nu = 1/3$ state. These calculations show that Laughlin's wavefunction is certainly very good for small particle numbers N. It is even exact for some model interactions of vanishingly short range, for arbitrary N. Whether this superiority still holds for higher particle numbers, and with more realistic interactions of longer range, is yet an open question. Thus, it is still of interest to push the study of the ground state towards higher particle numbers. And, even if exact calculations become inaccessible due to the matrix dimension of the Hamiltonian involved[11], one may search for approximative schemes[12].

Extrapolation of finite-size results is a common method to gain insight into the thermodynamic limit, and results for a small number of electrons have boldly been extrapolated to an infinite number of particles. Strange to say, it seems that this extrapolation gives proper results for the Laughlin states, which may be due to the incompressibility of the ground state[13]. The main purpose of this paper is to investigate the extrapolation of the ground state energy, from a finite number of particles to an infinite number of particles, in the geometry of a spherical surface. This extrapolation is dependent on the filling factor. In section 2 we calculate the classical electrostatic energy for up to 32 electrons on a sphere, by placing electrons at the corners of the Platonian bodies and some rather natural extensions of these. These energies may serve as a lower bound for the quantum mechanical ground state energies. In section 3 we introduce a magnetic field by placing a magnetic

monopole at the center of the sphere. We use some of the properties of magnetic monopoles to show that the natural definition of the filling factor is somewhat different from the one used in the early papers investigating the FQHE in a spherical geometry. This definition of the filling factor leads to a better scaling behaviour for the classical energies, i.e. one where the leading $1/N$ correction is smaller. In section 4 we make a semi-classical extension of the classical analysis, in which some effects of the quantum mechanical spread of the wavefunction are taken into account, by replacing the true pair interaction potential by an effective pair-potential derived from the solution of the two-particle system. This method is exact for the three-particle system (in the $J = 0$ state), and also in the limit of low filling factors. It further gives a very good approximation to the ground state energy in the unfavorable case of a completely filled Landau level. We use the results of this semi-classical analysis to construct a function which extrapolates a (v dependent) finite N energy calculation towards inifinite N. The idea is that even though the semi-classical analysis gives a crude approximation to the ground state energies, which moreover smoothens out the cusplike behaviour which is believed to exist, the main part of the extrapolation function is a smooth function which is sufficiently well approximated by the semi-classical method.

2. The classical energies

We consider N electrons constrained to the surface of a sphere of radius R. The electrons interact with each other and with a positive neutralizing background through the $3D$ Coulomb potential $V(r) = 1/r$ (we choose units of energy such that $e^2/4\pi\epsilon = 1$). The interparticle distance is taken as the chord distance. This may not be the most realistic model for the particle interaction in the heterojunctions,but it has become fairly standard.

The self-energy of the background is $N^2/2R$, while the interaction energy between the electrons and the background is $-N^2/R$. The effect of the background is therefore merely to shift the energy by $-N^2/2R$.

The interaction energy of the electrons is

$$E_{ee} = \sum_{i<j} \frac{1}{r_{ij}} , \tag{2.1}$$

summing over all pairs, with r_{ij} being the distance between the particles. Classically, for a given configuration of particles, the problem is reduced to a geometrical problem of finding all the interparticle distances. We shall be interested in the total energy per particle $\epsilon_N = E/N$, which we measure in units of $1/R$.

For completeness we include the trivial cases N = 2 and N = 3 (where the three particles are placed at the corners of an equilateral triangle around a great circle), for which

$$\epsilon_2 = \frac{E_2}{2} = -\frac{3}{4R} ,$$

$$\epsilon_3 = \frac{E_3}{3} = -\frac{(9-2\sqrt{3})}{6R} \tag{2.2}$$

Furthermore, we shall consider the five Platonian bodies and locate the electrons at the corners of these. This will cover particle numbers $N = 4, 6, 8, 12$ and 20 (The last case was apparently overlooked by Fano et al.[14] who stated that there is no Platonic polyhedron beyond $N = 12$). The different electron-electron distance and the number of pairs with a given distance are shown in table 1.

We can extend this classical analysis. The case N = 5 amounts to three particles in a triangle around the equator and one particle at each pole. The distances are $\sqrt{2}, \sqrt{3}$ and 2 in units of R.

Further on, one may add particles on the sphere outside the midpoints of the faces of the Platonian bodies. This will only give back a new Platonian body except for two cases; the hexahedron and the dodecahedron. In these cases one achieves particle numbers 14 and 32 respectively.

The case $N = 14$ corresponds to an octahedron and a hexahedron put into each other. In addition to the internal distances in these bodies already given in table 1, one gets new distances r between one electron in the octahedron and one in the hexahedron. We find that these distances are given by

$$r^2 = 2\left(1 \pm \frac{\sqrt{3}}{3}\right) R^2 \ . \tag{2.3}$$

There are *24* connections for each sign.

Table 1 - The five Platonian bodies, with all interparticle distances and the number of pairs with a given interparticle distance.

PLATONIAN BODIES			
N	Name	r/R	Number
4	Tetrahedron	$2\sqrt{6}/3$	*6*
6	Octahedron	$\sqrt{2}$	12
		2	
8	Hexahedron	$2\sqrt{3}/3$	*12*
		$2\sqrt{6}/3$	*12*
		2	*4*
12	Icosahedron	$\sqrt{\frac{10 \pm 2\sqrt{5}}{5}}$	*30* of each
		2	*6*
20	Dodecahedron	$(\sqrt{5} \pm 1)/\sqrt{3}$	**30** of each
		$2\sqrt{3}/3$	*60*
		$2\sqrt{6}/3$	*60*
		2	*10*

In a similar way will the N = *32* body consist of an icosahedron and a dodecahedron placed inside each other. The new interbody distances are given by

$$r^2 = 2\left(1 \pm \sqrt{\frac{5 \pm 2\sqrt{5}}{15}}\right) R^2 \ , \tag{2.4}$$

where each of the four possible distances appears *60* times.

The total energy can now easily be calculated using eq.(2.1). The result is plotted in fig. **1.** Notice that we have plotted the energies in units of $\sqrt{4\pi\rho}$, where ρ is the areal density $\rho = N/4\pi R^2$. Thus, we have a constant density, while the radius ***R*** of the sphere is fixed by the number of particles to give this density. We have also marked the result given by Bonsall and Maradudin[15] for an infinite triangular

lattice in the plane. This seems to fit well to the extrapolation of our data. We see that the classical electron system prefers to arrange itself in equilateral triangles, which it achieves for particle numbers 4, *6* and 12. These have substantially lower energy than the others. For N = *32* the arrangement of the electrons is very close to this situation, being triangles with two equal sides, slightly different from the third. The ratio between the sides is 0.89799..., explaining the low energy. The variations when changing N can be explained by the ability to form triangular configurations.

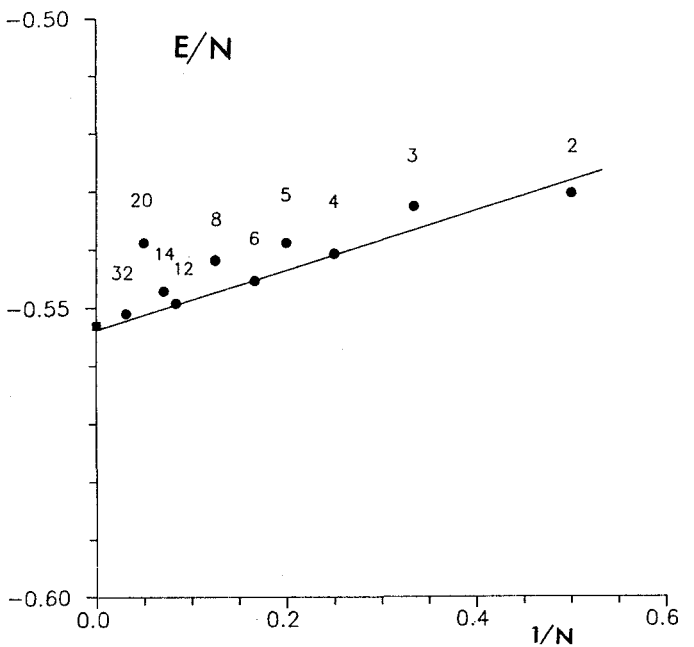

Fig.1 - The energy per particle as a function of $1/N$ in units $\sqrt{4\pi\rho}$.

We have fitted a straight line through the points N = 4,6 and *12.* The total energy per particle is thereby approximated as $\epsilon_N = -\alpha_0(1+\alpha_1/N)\sqrt{N}/R$, where the best fit is $\alpha_0 = 0.5537$ and $\alpha_1 = 0.09316$.

3. Magnetic monopole field and the filling factor

To introduce a magnetic field perpendicular to the surface, we place a magnetic monopole of charge g at the center of the sphere. A magnetic monopole is the magnetic analog to an electric point charge, creating the magnetic field

$$\vec{B}(\vec{r}) = g\frac{\hat{r}}{r^2} \ . \tag{3.1}$$

A free electron moving in the field from the monopole will be described by the Hamiltonian $H_0 = (\vec{p} + e\vec{A})^2/2m$. The vector field $\vec{A}$ needed to produce the magnetic field in eq.(3.1) will have singularities, but these are not physical when the quantization rule[16]

$$q \equiv \frac{eg}{\hbar} = \frac{n}{2} \ , \quad n = 0, \pm 1, \pm 2, ..., \tag{3.2}$$

is fulfilled. The orbital angular momentum of the electron $\vec{L} = \vec{r} \times (\vec{p} + e\vec{A})/\hbar$ does not commute with the Hamiltonian, due to the non-vanishing momentum density which integrates up to qi. Thus, the proper angular momentum, measured in units of h, is $\vec{J} = \vec{r}$ x $(\vec{p} + e\vec{A})/\hbar + qf$. The square of the angular momentum is then $\vec{J}^2 = \vec{L}^2 + q^2$, and the Hamiltonian for one electron confined to the sphere of radius R is

$$H_0 = \frac{\hbar^2}{2mR^2}(\vec{J}^2 - q^2) \ , \tag{3.3}$$

with eigenvalues

$$\frac{\hbar^2}{2mR^2}\left(j(j+1) - q^2\right) \ , \quad j = |q|, \ |q| + 1, ...$$

There is no loss of generality in considering only q positive, since the energies are independent of the direction of the magnetic field. To keep the magnetic field constant on the surface of the sphere, the size of the sphere must scale as $R = \sqrt{q}\ell_B$, where $\ell_B = (\hbar/eB)^{1/2}$ is the magnetic length.

The n'th Landau level corresponds to $j = q + n$, where we start counting so that $n = 0$ is the lowest level. The energy is then

$$E_0 = \frac{\hbar^2 q}{mR^2}\left((n+\frac{1}{2}) + \frac{n(n+1)}{2q}\right) = \hbar\omega_c\left(n+\frac{1}{2}\right) + O(R^{-2}) \ , \quad (3.4)$$

where $\omega_c = eB/m$ is the cyclotron frequency.

Since the energy is independent of J_z, all the possible values $-j,\ldots,j$ will have the same energy. The degeneracy of the n'the Landau Ievel, will be finite on the sphere **and** equal to $2j+1 = 2q+2n+1$. We will confine our analysis to the lowest Landau level. Then there are $2q+1$ one-particle states available. When we have N electrons on the sphere, the filling factor will therefore be

$$\nu = \frac{N}{2q+1} \ . \quad (3.5)$$

This is different from the definition of the filling factor used previously by other authors[8]. They observe that the Laughlin states on a sphere exist when $2q = m(N-1)$. In the planar geometry, the filling factor is $1/m$, and generalising to the sphere one has $\nu_H = (N-1)/2q$. This filling factor is found to break the particle-hole symmetry at finite N [17].

The difference vanishes in the limit $N \to \infty$, but this is not enough, since one wants to extrapolate results from finite (and quite low) N. Thus, one should use the correct filling factor to have better control of the extrapolation process.

When we now let the electrons interact, we have a true many body problem which is not so easy tractable. But the static energies already calculated in chapter 2 will still hold as a lower bound for the interaction energy. They were all measured in units of $\sqrt{4\pi\rho}$. It is common now to calculate the energies for a fixed value of the filling fraction. We then have that

$$\rho = \frac{N}{4\pi R^2} = \frac{\nu}{2\pi\ell_B^2}\frac{1}{(1-\nu/N)} \quad (3.6)$$

The energy is now measured in units of ℓ_B^{-1} and is shown in fig. *2* for the particular case $\nu = 1/3$.

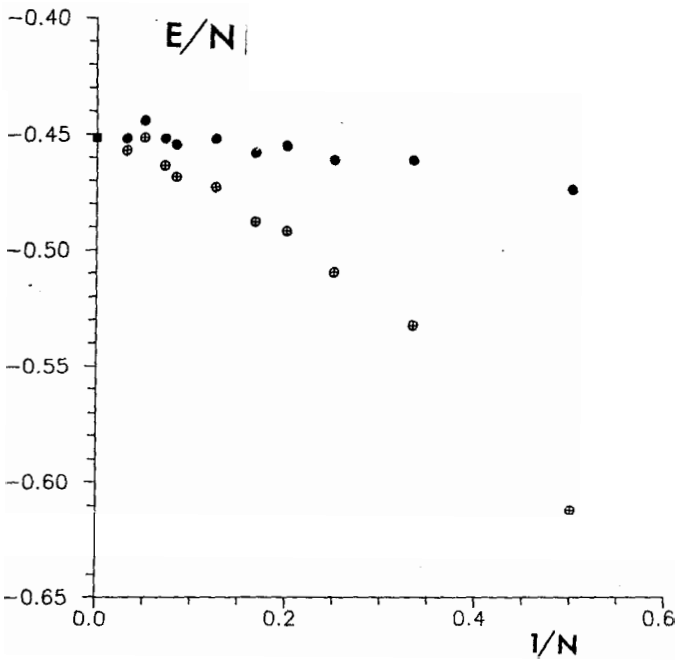

Fig.2 - The classical energy per particle (in units $e^2/4\pi\epsilon\ell_B$) as a function of $1/N$ when the filling is fixed (to 1/3). The filled circles use $\nu = N/(2q+1)$ and the crossed circles use $\nu_H = (N-1)/2q$.

This should be compared with the ones given in ref. **9.** We see that the correct definition of the filling factor **eq. (3.5)** significantly improves the scaling behavior. Let us demonstrate this. The radius of the sphere scales like $R = \sqrt{q}\ell_B$ to keep the magnetic constant on the surface. We can express the classical extrapolated energies with the two types of filling factors involved

$$\epsilon_H \approx -\alpha_0\sqrt{2\nu}\left(1+(\alpha_1+1/2)/N\right)\sqrt{N/q}$$
$$\epsilon \approx -\alpha_0\sqrt{2\nu}\left(1+(a,+\nu/2)/N\right)\sqrt{N/q}\,. \qquad (3.7)$$

Since $\alpha_1 > 0$, the $1/N$ correction is always smaller for the correct filling factor.

4. Semi-classical effective pair-interaction

We have seen in the previous section that electrons in the lowest Landau level have angular momentum $\vec{q}$. The interaction energy between two electrons coupled to a total angular momentum $\vec{L} = \vec{q} + \vec{q}$ can be written[17]

$$E_L^{(2)} = -\frac{2q+1}{2} \sum_j \begin{pmatrix} 4q+1 \\ 2q \end{pmatrix}^{-1} \begin{pmatrix} 4q+1 \\ 2q-J \end{pmatrix} \begin{Bmatrix} q & q & L \\ q & q & J \end{Bmatrix} \tag{4.1}$$

where the object in curly braces is a Wigner $6j$-symbol. In the classical limit $q \to \infty$, one can use the asymptotic expressions for the $6j$-symbols and find that the energy corresponds to a pair of electrons located with a relative angle ϑ_L,

$$E_L^{(2)} \approx V(\cos(\vartheta_L)) = \frac{1}{2\sin(\vartheta_L/2)} \tag{4.2}$$

for the Coulomb interaction eq.(2.1). The angle ϑ_L is

$$\cos\vartheta_L = \frac{L(L+1) - 2q(q+1)}{2q(q+1)} \tag{4.3}$$

Calculating the energies for a rotational symmetric state of three particles, one finds that

$$E_0^{(3)} = 3E_{L=1}^{(2)} , \tag{4.4}$$

which is precisely the classical result, but with the classical pair-interaction $V(\cos\vartheta)$ replaced by an effective interaction $E_L^{(2)}$. Note that the L-value via eq. (4.3) gives the spherical angle $\vartheta_1 = 2\pi/3$, precisely corresponding to the three particles being evenly distributed on a great circle, as far apart as possible.

We want to elaborate on this observation. By applying the geometrical results of the first section, we can calculate energies for higher particle numbers. To each interparticle distance there corresponds an angle ϑ, related to the pair-distance r_{ij} by $r_{ij} = 2\sin(\vartheta/2)$. The energy between two electrons separated by this distance can be approximated by $E_L^{(2)}$ where we now choose the value of L which gives the value of ϑ_L closest to ϑ. In fact, we will improve a little by interpolating linearly between the two closest values.

Numerically, we have done the calculation for q ranging from 3 to 85, thereby covering a quite large area in the parameter space (N, v). In fig. 2 we compare the energies fore $N = 4$ with the exact ones as calculated by Sollie and Olaussen (ref. 17). As expected the deviations vanish for low filling factors, since the particles do not overlap much at these low densities. The Eaughlin states are realized on a sphere for 2q = m(N – 1), and we observe that at the corresponding fillings (marked with arrows) there is a particularly good agreement between the energies. We have also compared our results with the energies found by Fano et al.[10] for the 1/3 Laughin state up to 10 particles, and we see a remarkable agreement (cf. table 2).

Table 2 - Comparison of the semi-classical energy E_{sc} with the exact energies E_e, as calculated from eq. (4.5) for v = 1 and by ref. 10 for $\nu_H = 1/3$.

v	N	E_e	E_{sc}	$\Delta E(\%)$
1	4	-.74651	-.73256	1.8
	5	-.71833	-.71833	0
	6	-.70090	-.67764	3.3
	8	-.68047	-.68131	0.1
	12	-.66137	-.62651	5.3
	14	-.65614	-.62660	4.5
	20	-.64697	-.62406	3.5
	32	-.63918	-.61294	4.1
"1/3"	4	-.475024	-.473815	0.25
	5	-.459510	-.458928	0.13
	6	-.450173	-.450568	-0.09
	8	-.439096	-.437449	0.38

We may also test our approximation in a case where all the energies can be calculated exactly. We know that for a filled Landau level, the energy per particle is

$$\epsilon(1) = -2^{4q-1}\binom{4q+1}{2q}^{-1}\frac{1}{R}. \qquad (4.5)$$

The classical energies are again converted into units of ℓ_B^{-1} by using that $R = \sqrt{q}\ell_B$. We compare these energies with the ones calculated from eq. (4.1) in table

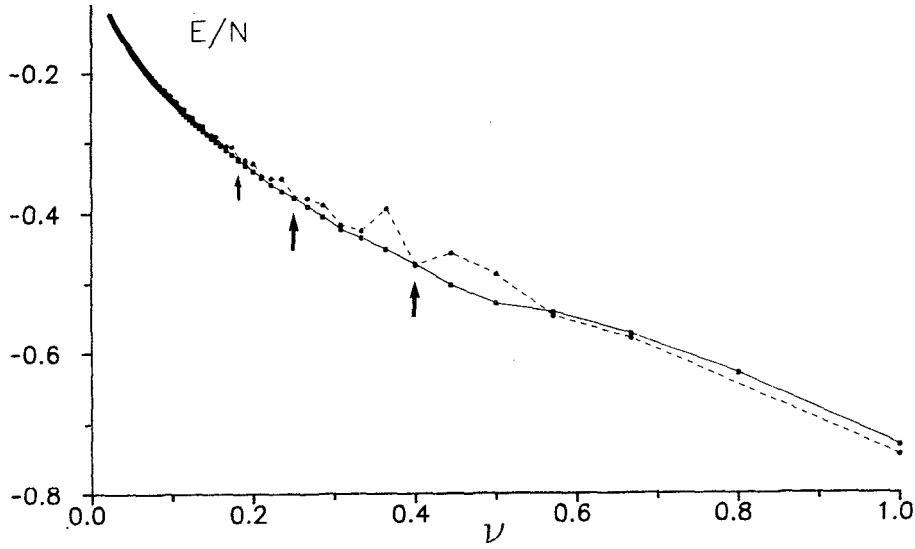

Fig.3 - The exact (dashed line) and approximated (solid line) energy for $N = 4$ particles. The Laughlin states $m = 3, 5$, and 7, are marked with arrows.

2. We see that the error is limited within a few per cent and that there is little systematics, but the error tencls do be larger for higher particle numbers. Note that this is a worst-case test, aince the overlap of the wavefunctions vanishes in the limit of small v, but is considerable for v = 1. We have also compared with the energies found by Fano et al. (ref. 10) for the Laughlin state up to N = 8 particles, and we see a remarkably good agreement, not only for the four-particle state.

What one really would like to find, is a better way to correct for the finite size of the sphere. Morf et al.[18] introduced their correction factor due to the N dependence of the areal density, by redefining the length unit such that the areal density is independent of N (for a fixed ν). We shall see what our semiclassical analysis gives. Let us write the energy as

$$E\ (\nu) = \epsilon_{N\,(V)} + \Delta\epsilon(\nu)/N + \ldots , \qquad (4.6)$$

where we shall not be interested in the higher order terms. We have our semiclassical data, and if we fix v and fit a straight line as a function of $1/N$, we are able to find the two quantities involved. We do this for filling factors $v = 2/m'$ with $m' = 2, 3, ..., 10$. The result for the correction factor $\Delta\epsilon$ is given in fig. 4. The solid line is the best fit of a power law, and the result is $\Delta\epsilon = a\nu^r$, with r = 1.9939 and a = 0.61874. This strongly suggests that the exact extrapolation function behaves quadratically as $v \to 0$.

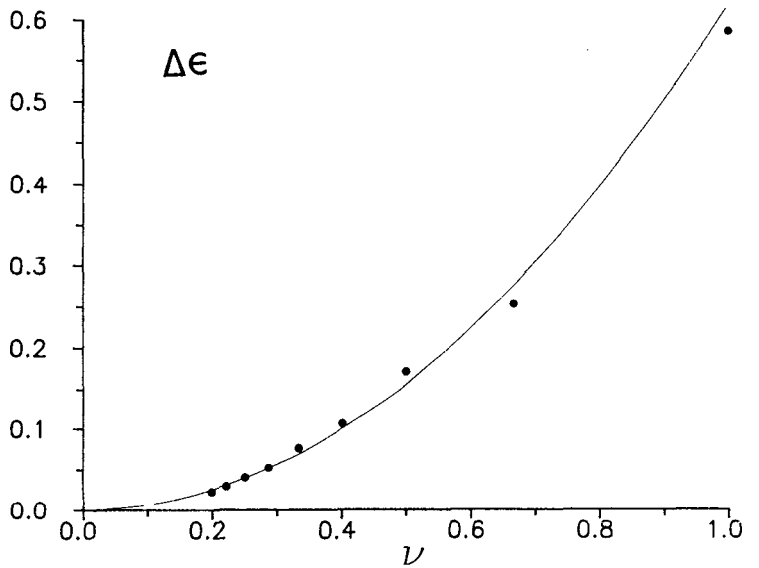

Fig.4 - The **first** $1/N$ correction $\Delta\epsilon$ as a function of ν.

5. Conclusion

We have studied the two-dimensional electron system on a sphere, and calculated the classical energies for electrons at the corners of the Platonian bodies and some simple extensions of them. Furthermore, we have introduced a magnetic field normal to the $2D$ surface created by a magnetic monopole, and found approximate energies by using the two-particle energies of all pairs. Thus, we model the

system by a classical system with an effective interaction between the particles. The effective interaction is to take into account the spread of the wavefunctiun.

In the limit of a vanishing filling of the Landau level, the electrons are well separated, with little overlap of the wavefunctions, and we recover the classical energies. We also use the data to find a parametrization of the extrapolation of energies from a finite number to the thermodynamic limit.

Naturally, these energies are merely approximations. Errors are introduced at several stages. First by the fact that the two-particle energies only exist for some discrete pair-distances, making an approximation to these discrete values necessary. (Of course, this enforcement of discretization in the pair distances may be the main cause of the $FQHE$). Next there is no reason for the axact quantum mechanical energies merely to be a sum over pair energies.

Despite these crudities, the results are quite good, and particularly for low filling factors. We are able to calculate the energies to within some percent, and even less than one percent for the $1/3$ Laughlin states.

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Resumo

Consideramos elétrons confinados à superfície de uma esfera e calculamos as energias eletrostáticas clássicas para até 32 elétrons. A seguir, introduzimos um campo magnético perpendicular à superfície da esfera, ao colocar um monopolo magnético na origem. A análise clássica pode ser estendida, substituindo o potencial de pares por um potencial efetivo, definido como a energia quântica de um par de elétrons à distância apropriada. Para o caso mais desfavordvel, de um nível de Landau completamente ocupado, o qual pode ser calculado exatamente, as energias aproximadas são corretas a menos de alguns poucos pontos percentuais, e são consideravelmente melhoradas quando o fator de enchimento diminui. Utilizamos ainda as energias semiclássicas para construir uma função simplesmente parametrizada para extrapolar a energia do estado fundamental como função do fator de enchimento, de números finitos de partículas até um número infinito.