Analytic Results for N Particles with $1/r^2$ Interaction in Two Dimensions and an External Magnetic Field

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The $2N$-dimensional quantum problem of N particles (e.g., electrons) with interaction β/r^2 in a two-dimensional parabolic potential ω_0 (e.g., quantum dot), and magnetic field B, reduces exactly to solving a $(2N-4)$-dimensional problem which is *independent* of B and ω_0. An exact, infinite set of relative mode excitations are obtained for any N. The $N=3$ problem reduces to that of a fictitious particle in a two-dimensional, nonlinear potential of strength β, subject to a fictitious magnetic field $B_{\text{fic}} \propto J$, the relative angular momentum.

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Few-body problems have always attracted interest in the fields of atomic and nuclear physics. Recent work on laser-cooled ions in Paul traps [1] has heightened their importance in atomic physics. In condensed matter physics, such problems have been used indirectly as cluster calculations for understanding many-electron systems such as the two-dimensional (2D) electron gas in a magnetic field. A famous example is Laughlin's numerical calculation for $N=3$ electrons in a 2D parabolic potential used for investigating the fractional quantum Hall effect [2]. Few-body problems have recently taken on more direct relevance in semiconductor physics due to rapid advances in fabrication of quantum dots containing few electrons [3–6]. In lateral quantum dot structures, the electrons are typically free to move in only two spatial dimensions, and the confining potential is approximately parabolic [3,4]. A complete description of this few-electron system is complicated since the confinement energy, the electron-electron repulsion, and the cyclotron energy due to applied magnetic fields are typically comparable in magnitude. Numerical perturbative approaches employing a basis of noninteracting single-particle states become computationally intensive in the strongly interacting (Wigner solid) regime. Analytic simplifications of the exact N-particle Hamiltonian or exact solutions of model N-particle Hamiltonians can therefore be useful.

Few-body Hamiltonians are rarely solvable analytically. Exceptions include N particles in 1D with β/r^2 interaction [7] and $N=2$ electrons in 2D with β/r^2 interaction [8] and magnetic field. Here we show that the $2N$-dimensional problem of N particles (e.g., electrons) with β/r^2 interaction in a 2D parabolic potential ω_0 (e.g., quantum dot) and magnetic field B reduces exactly to solving a $(2N-4)$-dimensional problem which is *independent* of B and ω_0. An exact set of relative mode excitations are obtained. The $N=3$ particle problem reduces to that of a particle moving in a 2D nonlinear potential of strength β, subject to a *fictitious* magnetic field $B_{\text{fic}} \propto J$, the total relative angular momentum. The ground state J (i.e., magic number) transitions for $N=3$ are quantitatively consistent with numerical calculations for the Coulomb interaction [6]. Analytic results are given in the Wigner solid regime. The present work implicitly includes mixing with all Landau levels.

The exact Schrödinger equation for N particles, with repulsive interaction β/r^2 moving in a 2D parabolic potential subject to a magnetic field B (symmetric gauge) along the z axis, is given by $(H_{\text{space}} + H_{\text{spin}})\Psi = E\Psi$;

$$H_{\text{space}} = \sum_{i=1}^{N}\left(\frac{\mathbf{p}_i^2}{2m^*} + \frac{1}{2}m^*\omega_0^2(B)|\mathbf{r}_i|^2 + \frac{\omega_c}{2}l_i\right) + \sum_{i<j}\frac{\beta}{|\mathbf{r}_i - \mathbf{r}_j|^2}, \tag{1}$$

where $\omega_0^2(B) = \omega_0^2 + \omega_c^2/4$, ω_c is the cyclotron frequency, and $H_{\text{spin}} = -g^*\mu_B B\sum_i s_{i,z}$. The momentum and position of the ith particle are given by 2D vectors $\mathbf{p}_i$ and $\mathbf{r}_i$, respectively; l_i is the z component of the angular momentum. The exact eigenstates are written in terms of products of spatial and spin eigenstates obtained from H_{space} and H_{spin}, respectively; eigenstates of H_{spin} are just products of the spinors of the individual particles. We employ standard Jacobi coordinates $\mathbf{X}_i$ $(i=0,1,\ldots,N-1)$ where $\mathbf{X}_0 = (1/N)\sum_j \mathbf{r}_j$ (center-of-mass), $\mathbf{X}_1 = \sqrt{1/2}(\mathbf{r}_2 - \mathbf{r}_1)$, $\mathbf{X}_2 = \sqrt{2/3}[(\mathbf{r}_1 + \mathbf{r}_2)/2 - \mathbf{r}_3]$, etc. (see Fig. 1 for $N=3$) together with their conjugate momenta $\mathbf{P}_i$. The center-of-mass motion decouples, $H_{\text{space}} = H_{\text{CM}}(\mathbf{X}_0) + H_{\text{rel}}(\{\mathbf{X}_{i>0}\})$, hence $E_{\text{space}} = E_{\text{CM}} + E_{\text{rel}}$. The exact eigenstates of H_{CM} and energies E_{CM} are well known [9]. The nontrivial problem is to solve the relative motion equation $H_{\text{rel}}\psi = E_{\text{rel}}\psi$. We transform the relative coordinates $\{\mathbf{X}_{i>0}\}$ to standard hyperspherical coordinates: $\mathbf{X}_i = r(\prod_{j=i}^{N-2}\sin\alpha_{j+1})\cos\alpha_i e^{i\theta_i}$ with $r \geq 0$ and $0 \leq \alpha_i \leq \pi/2$ $(\alpha_1 = 0)$. Because J remains a good quantum number, we introduce a Jacobi transformation of the relative motion angles $\{\theta_i\}$: in particular, $\theta' = (N-1)^{-1}\sum_{i=1}^{N-1}\theta_i$, $\theta = \theta_1 - \theta_2$, etc. (see Fig. 1 for $N=3$). We hence have $(N-1)$ θ variables, $(N-2)$

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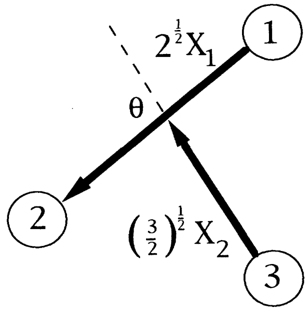

FIG. 1. The $N = 3$ system. Reading clockwise, classical configuration for three repulsive particles (132) corresponds to $(\alpha, \theta) = (\pi/4, \pi/2)$ [i.e., $(x, y) = (0, 0)$]; (123) corresponds to $(\alpha, \theta) = (\pi/4, -\pi/2)$ [i.e., $(x, y) = (0, \pi)$ or, equivalently, $(0, -\pi)$].

α variables, and a hyperradius r giving a total of $2(N - 1)$ variables as required for the relative motion. The exact eigenstates of $H_{\rm rel}$ have the form $\psi = e^{iJ\theta'}R(r)G(\Omega)$, where Ω denotes the $2N - 4$ remaining $\{\theta, \alpha\}$ variables excluding θ'; $R(r)$ and $G(\Omega)$ are solutions of the hyperradial and $(2N - 4)$-dimensional hyperangular equations, respectively. The hyperradial equation is

$$\left[\frac{d^2}{dr^2} + \frac{2N-3}{r}\frac{d}{dr} - \frac{\gamma(\gamma + 2N - 4)}{r^2} - \frac{r^2}{l_0^4} + \frac{2m^*(E_{\rm rel} - \hbar J\omega_c/2)}{\hbar^2}\right]R(r) = 0, \quad (2)$$

where $l_0^2 = \hbar[m^*\omega_0(B)]^{-1}$; the parameter $\gamma > 0$ and is related to the eigenvalue of the B and ω_0-independent hyperangular equation (see below). Equation (2) can be solved exactly yielding

$$E_{\rm rel} = \hbar\omega_0(B)(2n + \gamma + N - 1) + J\frac{\hbar\omega_c}{2}, \quad (3)$$

where n is any positive integer or zero and

$$R(r) = \left(\frac{r}{l_0}\right)^{\gamma} L_n^{\gamma+N-2}\left(\frac{r^2}{l_0^2}\right)e^{-r^2/2l_0^2}. \quad (4)$$

Equation (3) provides an exact (and infinite) set of relative mode excitations $2\hbar\omega_0(B)\Delta n$ for any N *regardless* of particle statistics and/or spin states. These are "breathing" modes, as shown below for $N = 3$; numerical Coulomb results have shown similar modes to this set of β-independent excitations [10]. All that remains is to solve the B and ω_0-independent hyperangular equation which resembles a (single-particle) Schrödinger-like equation in $(2N - 4)$-dimensional Ω space. The eigenvalue of the hyperangular equation

$$\epsilon = \frac{\hbar^2}{8}\left[\gamma(\gamma + 2N - 4) - J^2 - \left(\frac{V_{\rm class}}{\hbar\omega_0(B)}\right)^2\right], \quad (5)$$

where $V_{\rm class}$ is the potential energy of the classical, minimum-energy configuration (Wigner solid); $V_{\rm class} \propto \beta^{1/2}\omega_0(B)$, and hence ϵ (like γ) is independent of B and ω_0. The exact relative energy for any N

$$E_{\rm rel} = \hbar\omega_0(B)\left(2n + \left\{[N-2]^2 + J^2 + \left[\frac{V_{\rm class}}{\hbar\omega_0(B)}\right]^2 + \frac{8\epsilon}{\hbar^2}\right\}^{1/2} + 1\right) + J\frac{\hbar\omega_c}{2}. \quad (6)$$

$E_{\rm rel}$ only depends on particle statistics through ϵ. As $\hbar \to 0$, $E_{\rm rel} \to V_{\rm class}$ and $\epsilon \to 0$. Physically, ϵ accounts for the "zero-point energy" in Ω space associated with the quantum-mechanical spread of $G(\Omega)$ about the hyperangles Ω corresponding to the classical, minimum-energy configuration (Wigner solid); the actual spread in $G(\Omega)$ and hence ϵ will depend on total wave-function symmetry requirements (see below for $N = 3$). In general $\epsilon \geq 0$, $\epsilon \sim \beta^{\mu}$ where $\mu < 1$ [the dominant β dependence of $E_{\rm rel}$ lies in $(V_{\rm class})^2$] and $\epsilon \sim J^{\delta}$ where $\delta < 2$. Equation (6) implies that, for any N, the ground state J value will tend to become increasingly large and negative with increasing B field ($\omega_c > 0$, e.g., electrons). We now demonstrate these statements explicitly for $N = 3$.

For $N = 3$ we change variables from α, θ to x, y where $x = \ln(\tan\alpha)$ and $y = \theta - \pi/2$. Since $0 \leq \alpha \leq \pi/2$, hence $-\infty \leq x \leq \infty$ (N.B. $-\pi \leq y \leq \pi$). We define $p_x = (\hbar/i)\partial/\partial x$ and $p_y = (\hbar/i)\partial/\partial y$. The exact hyperrangular equation can be written in the form

$$\left\{\frac{p_x^2}{2} + \frac{[p_y + \hbar J\cos(2\tan^{-1}e^x)/2]^2}{2} + V(x, y; \epsilon)\right\}G(x, y) = \epsilon G(x, y), \quad (7)$$

where

$$V(x, y; \epsilon) = m^*\beta\left\{\frac{2 + \cos(2\tan^{-1}e^x)}{[\mathrm{cosec}(2\tan^{-1}e^x) + \cot(\tan^{-1}e^x)]^2 - 3\sin^2 y} - \frac{3}{4}\sin^2(2\tan^{-1}e^x) + \frac{1}{2}\cos^2(\tan^{-1}e^x) + \frac{\epsilon}{m^*\beta}\cos^2(2\tan^{-1}e^x)\right\}. \quad (8)$$

Equation (7) represents the single-body Hamiltonian for a fictitious particle of energy ϵ and unit mass, moving in the x-y plane in a nonlinear (i.e., ϵ-dependent) potential $V(x, y; \epsilon)$, subject to a fictitious, nonuniform magnetic field in the z direction

$$B_{\rm fic} = \frac{\hbar Jc}{4e}\{1 - \cos[4(\tan^{-1}e^x)]\}. \quad (9)$$

B_{fic} is independent of B and has a maximum of $\hbar|J|c/2e$ at $x = 0$ for all y. For small x, $B_{\text{fic}} \approx (\hbar Jc/2e)(1 - x^2)$. As $x \to \pm\infty$, $B_{\text{fic}} \to 0$. Note we have here chosen to highlight the Schrödinger-like form of Eq. (7); a simple rearrangement of Eq. (7) shows it to be Hermitian with a weighting function $\sin^2(2\tan^{-1} e^x)$. Our results are exact so far.

Figure 2 shows the potential $V(x, y; \epsilon)$ in the (x, y) plane. $V(x, y; \epsilon) \geq 0$ everywhere. Minima occur at $(0, 0)$ and $(0, \pm\pi)$ where $V(x, y; \epsilon) = 0$ [N.B. $(0, \pi)$ is equivalent to $(0, -\pi)$]. Maxima occur at $(\ln\sqrt{3}, \pm\pi/2)$ in Fig. 2, where $V(x, y; \epsilon) \to \infty$. Since $\epsilon \geq 0$, these statements hold for any ϵ. We now discuss the physical significance of these features. The classical configurations of minimum energy (Wigner solid) correspond to the particles lying on a ring in the form of an equilateral triangle with $V_{\text{class}} = \omega_0(B)[6m^*\beta]^{1/2}$. There are two distinct configurations with clockwise orderings (132) and (123) corresponding to $(\alpha, \theta) = (\pi/4, \pm\pi/2)$. In (x, y) coordinates, these correspond to $(0, 0)$ and $(0, \pi)$ [equivalently $(0, -\pi)$]. Hence the classical configurations coincide with the minima in $V(x, y; \epsilon)$ in Fig. 2 and the maximum in B_{fic}. The formation of the Wigner solid should therefore be favored by both large B_{fic} (i.e., large $|J|$) and deep $V(x, y; \epsilon)$ minima (i.e., large β, strong electron-electron interactions).

Consider the limit of three electrons with very strong electron-electron interactions (i.e., $\beta \to \infty$). Since the tunnel barrier height between the two $V(x, y; \epsilon)$ minima $\sim \beta$, the fictitious particle sits at one of these minima and the system is locked in one of the two classical configurations, e.g., (132) at $(0, 0)$. The tunneling probability between the minima is zero. Tunneling between the two minima implies a mixture of configuration (123) into (132) and hence interchange of the original electrons; in many-body language exchange effects arising from wavefunction antisymmetry are therefore negligible. ϵ is small compared to $m^*\beta$ and Eq. (6) reduces to

$$E_{\text{rel}} = \hbar\omega_0(B)\left[2n + \left(1 + J^2 + \frac{6m^*\beta}{\hbar^2}\right)^{1/2} + 1\right] + J\,\frac{\hbar\omega_c}{2}. \tag{10}$$

The energy $E_{\text{rel}} \geq V_{\text{class}}$ since it includes the hyperradial zero-point energy (N.B. $\hbar \to 0$ yields $E_{\text{rel}} \to V_{\text{class}}$ and $B_{\text{fic}} \to 0$).

Next consider large but finite β. The fictitious particle now moves in the vicinity of the minimum [i.e., $(x, y) \approx (0, 0)$]. The electrons in the Wigner solid are effectively vibrating around their classical positions. Expanding the potential $V(x, y; \epsilon)$ about $(0, 0)$ to third order, the exact Eq. (7) becomes

$$\left[\frac{p_x^2}{2} + \frac{(p_y - \hbar Jx/2)^2}{2} + \frac{1}{2}\,\omega_x^2 x^2 + \frac{1}{2}\,\omega_y^2 y^2\right]G(x, y) = \epsilon G(x, y), \tag{11}$$

where $\omega_x^2 = 3m^*\beta/4 + 2\epsilon$ and $\omega_y^2 = 3m^*\beta/4$. This has the form of a single electron moving in an anisotropic parabolic potential, subject to a uniform magnetic field $B_{\text{fic}} = \hbar Jc/2e$. Equation (11) is exactly solvable for ϵ using a symmetric gauge [11] (the energies are independent of the choice of gauge for B_{fic}). A full discussion of the results for any ϵ will be presented elsewhere. As an illustration, we consider small ϵ hence $\omega_x \approx \omega_y$. Equation (6) becomes

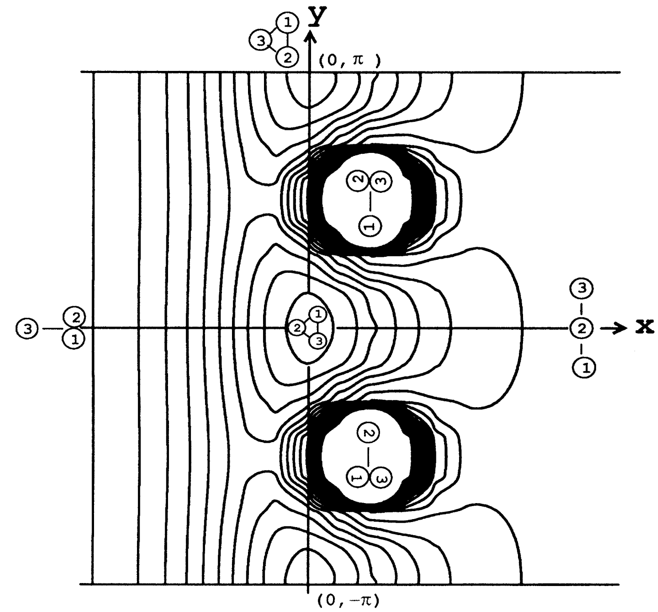

FIG. 2. Contour plot of fictitious potential $V(x, y; \epsilon)$ in the (x, y) plane for $N = 3$. Relevant corresponding configurations are shown. Minima in $V(x, y; \epsilon)$ occur at $(0, 0)$ and $(0, \pm\pi)$ (i.e., at classical configurations). Maxima occur at $(\ln\sqrt{3}, \pm\pi/2)$, where $V(x, y; \epsilon) \to \infty$ (i.e., particles 2 and 3 or 1 and 3 coincident). $V(x, y; \epsilon)$ is positive and finite everywhere else. The same qualitative features appear for all ϵ ($\epsilon/m^*\beta = 5$ for illustration).

$$E_{\text{rel}} = \hbar\omega_0(B)\left\{2n + \left[1 + J^2 + \frac{6m^*\beta}{\hbar^2} + 2(2n' + |l|' + 1)\left(J^2 + \frac{12m^*\beta}{\hbar^2}\right)^{1/2} 2l'J\right]^{1/2} + 1\right\} + J\,\frac{\hbar\omega_c}{2}. \tag{12}$$

The fictitious particle has its own set of Fock-Darwin (and hence Landau) levels [9] labeled by n' and a fictitious angular momentum l'. For large β and small n', l', and J, Eq. (12) yields an oscillator excitation spectrum with two characteristic frequencies $\sqrt{2}\,\hbar\omega_0(B)$ and $2\hbar\omega_0(B)$ representing "shear" and "breathing" modes of the Wigner solid.

For smaller β (i.e., weaker interactions) and/or larger ϵ (i.e., excited states), the tunneling probability between the $V(x,y;\epsilon)$ minima in Fig. 2 becomes significant; the Wigner solid begins to melt and wave-function antisymmetry (exchange) must be included. For three spin-polarized electrons, ψ must be antisymmetric under particle interchange $i \leftrightarrow j$. The hyperradial part $R(r)$ is invariant; particle permutation operations in $(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ become straightforward *space-group* operations in the (x,y) plane. For small (x,y), $1 \leftrightarrow 2$ is equivalent to $(x,y) \rightarrow (x, y+\pi)$ with $\theta' \rightarrow \theta' + \pi/2$; $1 \leftrightarrow 3$ is equivalent to $(x,y) \rightarrow (\bar{x}, \bar{y} - \pi)$ with $\theta' \rightarrow \theta' + \pi/6$ [$(\bar{x},\bar{y})$ represents (x,y) rotated by $4\pi/3$]; and $2 \leftrightarrow 3$ is equivalent to $(x,y) \rightarrow (\tilde{x}, \tilde{y} + \pi)$ with $\theta' \rightarrow \theta' - \pi/6$ [$(\tilde{x},\tilde{y})$ represents (x,y) rotated by $-4\pi/3$]. Single valuedness of ψ implies $e^{\pm iJ\pi} G(x, y \pm 2\pi) = G(x,y)$. Note that we have implicitly satisfied Bloch's theorem in this analysis; i.e., $G(x, y \pm 2\pi) = e^{\pm i2\pi k} G(x,y)$. The solutions $G(x,y)$ of Eq. (7) with the lowest possible ϵ (and hence lowest $E_{\rm rel}$ at a given ω_c) should be nodeless in the vicinity of $(0,0)$ [cf. ground state in the parabolic potential with $n' = 0 = l'$ in Eq. (12)]. However, the above symmetry requirements forbid such a nodeless solution *unless* $e^{i\pi 2J/3} = 1$. Therefore the only symmetry-allowed solutions $G(x,y)$ which are nodeless (i.e., smallest ϵ and hence lowest $E_{\rm rel}$ at a given ω_c) are those where J is a multiple of 3. Evaluating the simplified expression for $E_{\rm rel}$ in Eq. (12) ($n' = 0 = l'$), the following ground state J transitions are obtained with increasing ω_c for three spin-polarized electrons in a GaAs dot ($\hbar\omega_0 = 3.37$ meV as in Ref. [6]) [12]; $-3 \rightarrow -6$ at $B = 5.0$ T, $-6 \rightarrow -9$ at $B = 8.7$ T, and $-9 \rightarrow -12$ at $B = 12.2$ T (N.B. $J = 0$ is not allowed by symmetry). The numerically obtained values from Ref. [6] are $B \sim 5.5$, 8.4, and 12.4 T using a Coulomb interaction. Our analytic results therefore agree well with the numerical calculations despite the different interaction form (see below). A feature of these analytic results is that they become more accurate in the Wigner solid regime (e.g., large β or $|J|$) while the numerical calculations become more computationally demanding.

For general N, the hyperrangular equation [cf. Eq. (7)] becomes $2N - 4$ dimensional. However, in the Wigner solid regime (large β or $|J|$) the classical minimum-energy configurations will still be important in determining ϵ and hence $E_{\rm rel}$, just as for $N = 3$. The classical minimum-energy configurations (with $1/r$ interaction) for $N < 6$ all consist of N particles on a ring; for $N = 6$ additional minima occur [13]. Intriguingly it is at $N = 6$ that the magic number J sequence of $\Delta J = N$ is broken [14]. The present formalism which emphasizes classical configurations may shed light on a possible link here.

Finally we note that the β/r^2 interaction ($\beta > 0$) is not unrealistic in quantum dots due to the presence of image charges; in particular, it resembles the dipolelike form used successfully in Ref. [4]. Furthermore, recent quantitative comparisons [10,11,15] have shown that the $1/r^2$ and $1/r$ repulsive interactions yield energy spectra with very similar features [e.g., ground state J transitions, the relative excitation $2\hbar\omega_0(B)$ for $N = 2$ [10]]; the above results for $N = 3$ are consistent with this finding. Significant differences will only arise for the case of attractive forces $\beta < 0$ (e.g., between electrons and holes) because of the increased importance of the $r \rightarrow 0$ dynamics for that case.

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