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Higher Landau levels contribution to the energy of interacting electrons in a quantum dot

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Abstract

Properly regularized second-order degenerate perturbation theory is applied to compute the contribution of higher Landau levels to the low-energy spectrum of interacting electrons in a disk-shaped quantum dot. At "filling factor" near $\frac{1}{2}$, this contribution proves to be larger than energy differences between states with different spin polarizations. After checking convergence of the method in small systems, we show results for a 12-electron quantum dot, a system which is hardly tractable by means of exact diagonalization techniques.

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1. Introduction

The relevant energy scales entering the Hamiltonian of an N-electron system in a quantum dot (qdot) and a magnetic field are the following: the cyclotronic energy $\hbar\omega_c \sim B$, the dot confinement energy $\hbar\omega_0$, and the Coulomb characteristic energy $e^2/(\kappa l_B) \sim \sqrt{B}$. In strong enough fields, the spacing between Landau levels (LLs), given by $\hbar\omega_c$, is much greater than any other scale, and one can restrict the Hilbert space to functions built on one-particle states from the first LL. This is the 1LL approximation [1], which has been widely used to obtain exact solutions [2], to construct the famous $\nu = \frac{1}{3}$ FQHE functions [3], later extended to other filling factors by means of the Composite Fermion recipe [4] and, in general, has been used to numerically diagonalize the interacting Hamiltonian [1].

The inclusion of higher LLs in numerical calculations turns out to be prohibitive, even for relatively "small" systems. Consider, for example, $N = 12$ electrons in a qdot at "filling factor" near $\frac{1}{2}$, i.e. when the angular momentum of the electron droplet is $L = -132$. Out of only 78 one-particle states (orbitals) in the 1LL, one can construct 674 585 Slater determinants, which conform the truncated basis for the 12-particle system in the 1LL approximation. Taking 78 additional orbitals from each of the next two LLs causes the basis dimension to be raised to more than 172 millions, and the diagonalization of the Hamiltonian matrix becomes a very hard computational task.

In the present paper, we show that a way to circumvent the diagonalization of these large matrices is the use of properly renormalized degenerate perturbation theory (PT). We stress that, unlike Monte Carlo and other methods focusing on the properties of a particular state, by means of PT we obtain, in a single calculation, an approximation to the energy spectrum and the corresponding wave functions of the system.

The interest in computing the higher LL contribution to the energies relies on the fact that, for intermediate filling factors, this contribution may be even larger than energy differences between states with different spin polarizations

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[5]. Thus, a correct description of spin excitations in a system of interacting electrons should take account of higher LL effects. Recent work on the issue of spin excitations in qdots [6] has stressed the importance of the second LL at $\nu \approx 2$, but at lower ν the higher LL effects are commonly ignored.

The plan of the paper is as follows. In the next two sections a brief summary of PT and its regularization by means of Shank extrapolants [7] and the Principle of Minimal Sensitivity [8] is included for completeness. For simplicity, only spin-polarized systems will be studied, but any other spin-polarization sector may be treated as well. Section 4 is devoted to the results. The 2- and 6-electron dots are used as benchmarks where regularized second-order PT (PT2) is compared with exact or variational results. After validation, the method is applied to the 12-electron system mentioned above. Concluding remarks are given at the end of the paper.

2. Degenerate perturbation theory

The 1LL approximation can be seen, from another point of view, as first-order degenerate perturbation theory. In fact, writing the Hamiltonian in the form: $H = H_0 + V$, where H_0 describes free (spin-polarized) electrons in a magnetic field, and $V = V_{\rm conf} + V_{\rm coul}$ accounts for the external confinement and Coulomb interactions, the Hamiltonian matrix in the 1LL approximation,

$$H^{(1)}_{ij} = \langle S_i|H|S_j\rangle = E_0\delta_{ij} + \langle S_i|V|S_j\rangle, \tag{1}$$

where $E_0 = N\hbar\omega_{\rm c}/2$ and S_i, S_j are Slater determinants made up from 1LL orbitals, may be seen as the secular matrix of first-order degenerate perturbation theory [9]. The degeneracy subspace is spanned by the S_i.

Corrections to (1) are computed in the standard form [9]. The second-order matrix is given by

$$H^{(2)}_{ij} = E_0\delta_{ij} + \left\langle S_i\left|V + \sum_Z \frac{V|Z\rangle\langle Z|V}{E_0 - E_0(Z)}\right|S_j\right\rangle, \tag{2}$$

where the sum runs over eigenfunctions of H_0 in the orthogonal subspace, $\langle Z|S_i\rangle = 0$, and $E_0(Z) = \langle Z|H_0|Z\rangle$.

We will use Eq. (2) to compute higher LLs contributions to the energy spectrum of an N-electron qdot. Note that the dimension of the secular equation is not increased by the inclusion of the second-order corrections. For the largest systems, an energy cutoff, $E_0(Z) - E_0 \leqslant K_{\rm cut}\hbar\omega_{\rm c}$, will be imposed to limit the number of states entering the sum. We will show results with $K_{\rm cut} = 2$, i.e. three LLs will be included.

2.1. The orthogonal subspace

One can explicitly use the fact that $V_{\rm conf}$ and $V_{\rm coul}$ are, respectively, one- and two-body operators, and exploit their symmetries (conservation of total angular momentum) in order to carry out the sum only over intermediate states, Z, having nonvanishing matrix elements with one of the external Slater functions, for example $\langle Z|V|S_j\rangle \neq 0$.

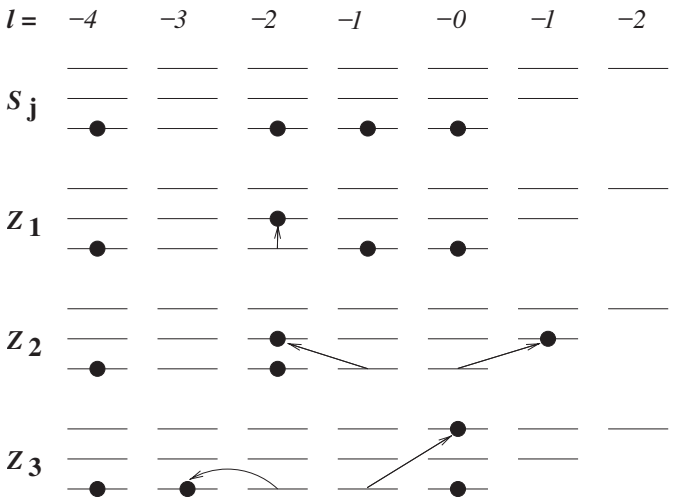

Fig. 1. Slater functions in the degeneracy subspace, S_j, and in the orthogonal subspace, Z, entering the sum in Eq. (2). The example is for a 4-electron system.

In Fig. 1, we have illustrated this statement for the simple 4-electron system. The top of the figure shows the occupation corresponding to a given S_j. Then, the sum will contain functions Z_1, where one occupied orbital of S_j is raised to an orbital in a higher LL (with the same angular momentum, l). The sum will also contain functions Z_2, where two occupied levels of S_j are moved to higher LLs. And, finally, functions Z_3 in which one occupied level of S_j is moved to an empty level in the 1LL and a second occupied orbital is moved to a higher LL shall also be included. In the first case, both the matrix elements of $V_{\rm conf}$ and $V_{\rm coul}$ could be nonzero, whereas in the later two cases only $V_{\rm coul}$ could have nonvanishing matrix elements.

3. Regularization of the perturbative series

To renormalize the perturbative series (usually an asymptotic series) many recipes have been invented. In the present paper, we will try Shank extrapolants [7] and the principle of minimal sensitivity (PMS) [8]. A variant of the later procedure has been recently applied to compute the correlation energy of the Coulomb gas [10].

3.1. Shank extrapolants

Shank extrapolants [7] are designed to accelerate the convergence of numerical series. For any three contiguous values, E_i, E_{i+1} and E_{i+2}, we define the extrapolant

$$F_i = \frac{E_iE_{i+2} - E^2_{i+1}}{E_i + E_{i+2} - 2E_{i+1}}. \tag{3}$$

From the series of extrapolants (which will be called first order) one can construct the second-order extrapolants, etc. In our case, we have only three values of energy, E_0, E_1