On the spectroscopic structure of two interacting electrons in a quantum dot

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Abstract

The shifted 1/N expansion technique used by El-Said (Phys. Rev. B 61, 13026 (2000)), to study the relative Hamiltonian of two interacting electrons confined in a quantum dot, is investigated. El-Said’s results from SLNT are revised and results from an alternative method are also reported. The distinctive role of the central spike term, \((m^2 - 1/4)/q^2\), in determining spectral properties of the above problem is shown, moreover.
In his paper (Phys. Rev. B 61, 13026 (2000)) El-Said [1] used the shifted 1/N expansion technique to study spectroscopic structure of the two - dimensional (flat land) motion of two electrons (with effective mass \( m^\ast \)), confined by a harmonic potential of characteristic length \( l_o = \sqrt{\hbar/(m^\ast \omega_o)} \) in the xy-plane.

The Hamiltonian of this problem is known to decouple into two quasi - particle Hamiltonians: the center of mass and relative motion ones [1-5]. The center of mass Hamiltonian is exactly soluble and the relative motion one

\[
\left[ -\frac{d^2}{dq^2} + \frac{(m^2 - 1/4)}{q^2} + \frac{\lambda}{q} + q^2 \right] U_{k,m}(q) = \Xi_{k,m} U_{k,m}(q),
\]

( with \( q = r/\sqrt{2}l_o \), \( \Xi_{k,m} = 2E_{k,m}/(\hbar \omega_o) \), \( \lambda = \sqrt{2}l_o/a^\ast \), and \( k \) is the radial quantum number) is known to belong to non-exactly soluble Hamiltonians. Therefore, one has to resort to approximation methods like SLNT, used by El-Said [1].

In fact, the up-normal performance of SLNT, reported in table I of [1], attracted our attention and inspired the current report. It is well known that because of the additive complexity in handling large - order corrections of the standard Rayleigh - Schrödinger perturbation theory, only low - order corrections (up to the third - order) have been reported for SLNT [6-9]. Eventually, the results of SLNT are not as accurate and reliable as sought after (documented by Mustafa and Odeh [10], Fernandez et al. [11], Maluendez et al. [12], and others [13]).

The actual results of SLNT (following SLNT procedure in [1,6-9]) are listed in table I, along with those reported by El-Said [1] and the exact numerical integration ones [2]. Obviously, sever deviations (underlined) from the exact ones occur for \( k \geq 1 \) results. Moreover, a level - ordering change is clearly manifested for the (1,3) and (2,0) states. Evidently, the results from SLNT [1] can not address the sensitive spectral properties of the attendant problem, especially when levels - ordering, energy - crossings, spin- oscillations, magnetic - fingerprints [5], · · · etc, are in point. Nevertheless, results from perturbation...
theory are limited to the case where $\lambda \ll 1$ \cite{14,15} and those from WKB treatments \cite{2} lead to dubious accuracies (in connection with level ordering and energy crossings).

In numerous methodical predecessors of a subset of papers \cite{5,13,16-18}, an alternative possibility has been sought in the power-law asymptotic expansions using some small parameter. It has been noticed that the presence of the central spike, e.g. $(m^2 - 1/4)/q^2$ in (1), just copies the effect of the centrifugal and/or centripetal force and immediately inspires the use of small shifted inverse angular momentum quantum number (PSLET). An exhaustive description of the necessary formulae of PSLET accompanied by the persuasive verifications of their numerical usefulness (by immediate comparisons of its results with available brute force numerical data) could be found in ref.s \cite{5,13,16-18}.

Following PSLET procedure we compare our results, in table II, with the exact numerical ones (obtained by direct numerical integrations, DNI) \cite{2} for $\lambda = 1$ and $\lambda = 10$. To avoid exhaustive numbers of tables we do not list Garcia-Castelan et. al’s results \cite{2} from WKB, WKB single-parabola (WKB-SP), and WKB double-parabola (WKB-DP). In contrast with the WKB, WKB-SP, WKB-DP \cite{2} and SLNT \cite{1} results, the comparison between PSLET and DNI results implies excellent agreement.

In order to make remediable analysis on the effect of $\lambda$, hence of the characteristic length $l_o (\lambda \sim l_o)$, we list (in tables III-V) PSLET results for $k = 0, 1, 2$ and $\lambda = 0, 1, 2, 4, 6, 8, 10, 12$ at different values of $|m|$. They are also plotted in figure I.

Figure I (along with tables III-V) shows that the degeneracies associated with the harmonic oscillator confinement at $\lambda = 0$ are only partially lifted as $\lambda$ increases from zero (of course, such degeneracies would completely be lifted when a magnetic field is applied perpendicular to the plane of the dot). It also shows that the equidistance form of the energy levels at $\lambda = 0$ changes in the following manners; (i) for a given $k$, the spacing between two successive $|m|$ states decreases as $\lambda$ increases, and increases as $|m|$ increases for a given $\lambda$, whilst (ii) for a given $\lambda$, the spacing increases as the nodal quantum number $k$ increases. One should nevertheless notice that (iii) s-states (with $m = 0$) shift up more rapidly than states with $|m| \geq 1$, and for $|m| \geq 1$ states with lower $|m|$ shift up faster than states with
higher $|m|$ as $\lambda$ increases from zero.

The above mentioned features (i)-(iii), in fact, build up the sought after scenario for the change in level ordering, that manifests energy crossings and spin-singlet ($S_z = 0$) spin-triplet ($S_z = 1$) oscillations, and inspires the vital role of the central spike term in (1). More specifically, the twofold nature of the central spike term in the effective potential

$$V_{eff}(q) = \frac{m^2 - 1/4}{q^2} + q^2 + \frac{\lambda}{q}$$

(2)

explains the energy crossings as follows; (a) for $m = 0$ it represents an attractive core that strengthens the confinement $q^2$, whereas (b) for $|m| \geq 1$ it represents a repulsive core which renders, along with the Coulomb repulsion, the potential less potent. This is why, for a given $k$, the energy of a lower $|m|$ state increases much faster (more rapidly for $m = 0$) than that of a higher $|m|$, as $\lambda$ increases, and catches up with it (hence energy crossings and singlet-triplet spin oscillations occur, or, at most, energy levels clustering is manifested). On the physical sides, the two electrons are farther apart for higher $|m|$. Moreover, for a given $k$ energy crossings are not feasible between the corresponding states with different $|m|$. Whereas, states with a given $k$ and $|m|$ cross with states at lower $k$ and higher $|m|$. Therefore, the lowest three states $(0,0)$, $(0,1)$, and $(0,2)$ never cross any other state (i.e., they can never be depressed into a lower $k$-state).

The effect of correlation, between two interacting electrons in a harmonic QD, is therefore clear in the full energy spectrum for $\lambda > 0$ with all $(k,|m|)$-states for the relative motion as shown in figure I and documented in tables II-V. However, it should be noted that the level ordering reported by Garcia-Castelan et. al [2] is now changed, namely for the $(0,4)$ and $(1,1)$ states. Moreover, the $(1,4)$ and $(2,1)$ states seem to change order as $\lambda$ increases from 12.

To sum up, we have used SLNT [1,6-8] and revised the numerical results reported by El-Said [1], on the correlation energies for two interacting electrons in a parabolic QD. As an alternative, we have used a pseudo-perturbation recipe PSLET [5,13,16-18] and proved
PSLET persuasive numerical reliability in comparison with direct numerical integration method (in table II) for \( \lambda = 1, \) and 10. In contrast with perturbation theory results, which are limited to \( \lambda \ll 1 \) [14,15], we have obtained the correlation energies for \( \lambda = 2, 4, 6, 8, 12 \) and \( k = 0, 1, 2. \) We have documented (through figure I) that the level ordering reported by Garcia-Castelan et. al [2] is not absolute but bound to change as \( \lambda \) increases from zero. Herein, one should report that results from WKB treatments [2] lead to poor accuracy for states with \( k = 0 \) and/or \( m = 0. \) Moreover, the twofold effect of the central spike term, in the effective two-dimensional potential (2), is now clarified to inherit a major responsibility for energy crossings.
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TABLE I. Energies (in $\hbar \omega /2$ units) of two interacting electrons in a quantum dot.

| $\lambda$ | $(k, m)$ | exact [2] | El-Said [1] | SLNT   |
|-----------|----------|-----------|-------------|--------|
| 1         | (0, 0)   | 3.4952    | 3.4234      | 3.4220 |
|           | (0, 1)   | 4.8553    | 4.8524      | 4.8522 |
|           | (0, 2)   | 6.6538    | 6.6535      | 6.6534 |
|           | (1, 0)   | 7.2340    | 7.2339      | 6.9650 |
|           | (0, 3)   | 8.5485    | 8.5484      | 8.5483 |
|           | (1, 1)   | 8.7594    | 8.7197      | 8.7196 |
|           | (0, 4)   | 10.4814   | 10.4814     | 10.4814|
|           | (1, 2)   | 10.6024   | 10.6023     | 10.5908|
|           | (2, 0)   | 11.0848   | 10.0848     | 10.7663|
|           | (0, 5)   | 12.4340   | 12.4340     | 12.4340|
|           | (1, 3)   | 12.5154   | 12.5153     | 12.5109|
|           | (2, 1)   | 12.6961   | 12.6962     | 12.6268|
| 10        | (0, 0)   | 10.4816   | 10.4398     | 10.4382|
|           | (0, 1)   | 10.8495   | 10.8341     | 10.8339|
|           | (0, 2)   | 11.7903   | 11.7860     | 11.7859|
|           | (0, 3)   | 13.0720   | 13.0717     | 13.0706|
|           | (1, 0)   | 14.0379   | 14.0380     | 13.5107|
|           | (1, 1)   | 14.4622   | 14.4621     | 14.2554|
|           | (0, 4)   | 14.5546   | 14.5544     | 14.5541|
|           | (1, 2)   | 15.4916   | 15.4915     | 15.4077|
|           | (0, 5)   | 16.1628   | 16.1629     | 16.1626|
|           | (1, 3)   | 16.8431   | 16.8431     | 16.8054|
|           | (2, 0)   | 17.6671   | 17.6670     | 16.6258|
TABLE II. Comparison of PSLET energies (in $\hbar \omega_{\alpha}/2$ units) and the exact ones from direct numerical integration [2] for $\lambda=1$ and 10.

| $(k, |m|)$ | $\lambda=1$ Exact | PSLET | $\lambda=10$ Exact | PSLET |
|---------|-----------------|-------|-----------------|-------|
| (1,7)  | 20.3587         | 20.3587 | (1,7)  | 23.5040         | 23.5040 |
| (0,9)  | 20.3280         | 20.3280 | (0,9)  | 23.2188         | 23.2188 |
| (3,2)  | 18.5351         | 18.5351 | (3,2)  | 23.0339         | 23.0339 |
| (2,4)  | 18.4388         | 18.4388 | (2,4)  | 22.2217         | 22.2217 |
| (1,6)  | 18.3843         | 18.3843 | (3,1)  | 21.8715         | 21.8715 |
| (0,8)  | 18.3472         | 18.3472 | (1,6)  | 21.7355         | 21.7355 |
| (3,1)  | 16.6498         | 16.6498 | (0,8)  | 21.3954         | 21.3954 |
| (2,3)  | 16.4895         | 16.4895 | (3,0)  | 21.3140         | 21.3140 |
| (1,5)  | 16.4163         | 16.4163 | (2,3)  | 20.6504         | 20.6504 |
| (0,7)  | 16.3701         | 16.3701 | (1,5)  | 20.0186         | 20.0186 |
| (3,0)  | 14.9850         | 14.9881 | (0,7)  | 19.6037         | 19.6037 |
| (2,2)  | 14.5646         | 14.5646 | (2,2)  | 19.2438         | 19.2438 |
| (1,4)  | 14.4579         | 14.4579 | (1,4)  | 18.3753         | 18.3753 |
| (0,6)  | 14.3983         | 14.3983 | (2,1)  | 18.1420         | 18.1420 |
| (2,1)  | 12.6961         | 12.6961 | (0,6)  | 17.8543         | 17.8543 |
| (1,3)  | 12.5154         | 12.5154 | (0,5)  | 16.8431         | 16.8431 |
| (0,5)  | 12.4340         | 12.4340 | (2,0)  | 16.1628         | 16.1628 |
| (2,0)  | 11.0848         | 11.0883 | (0,5)  | 15.4916         | 15.4916 |
| (1,2)  | 10.6024         | 10.6024 | (1,2)  | 14.5547         | 14.5547 |
| (0,4)  | 10.4814         | 10.4814 | (1,1)  | 14.4622         | 14.4622 |
| (0,3)  | 8.5485          | 8.5485  | (1,0)  | 14.0379         | 14.0381 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| (1,0) | 7.2340 | 7.2362 | (0,3) | 13.0720 | 13.0720 |
| (0,2) | 6.6538 | 6.6538 | (0,2) | 11.7903 | 11.7903 |
| (0,1) | 4.8553 | 4.8553 | (0,1) | 10.8495 | 10.8496 |
| (0,0) | 3.4952 | 3.4968 | (0,0) | 10.4816 | 10.4816 |
TABLE III. PSLET correlation energies (in $\hbar\omega_o/2$ units) for $k=0$, $|m|=0,1,2,3,4,5$ and $\lambda=0,1,2,4,6,8,10,12$

| $|m|$ | $\lambda=0$ | $\lambda=1$ | $\lambda=2$ | $\lambda=4$ |
|------|----------------|----------------|----------------|----------------|
| 0    | 2              | 3.4968         | 4.6391         | 6.4428         |
| 1    | 4              | 4.8553         | 5.6557         | 7.1251         |
| 2    | 6              | 6.6538         | 7.2872         | 8.4994         |
| 3    | 8              | 8.5485         | 9.0864         | 10.1331        |
| 4    | 10             | 10.4814        | 10.9564        | 11.8885        |
| 5    | 12             | 12.4340        | 12.8638        | 13.7112        |
|      | $\lambda=6$    | $\lambda=8$    | $\lambda=10$   | $\lambda=12$   |
| 0    | 7.9373         | 9.2644         | 10.4816        | 11.6184        |
| 1    | 8.4599         | 9.6938         | 10.8496        | 11.9425        |
| 2    | 9.6480         | 10.7425        | 11.7903        | 12.7975        |
| 3    | 11.1440        | 12.1226        | 13.0720        | 13.9947        |
| 4    | 12.7978        | 13.6861        | 14.5547        | 15.4049        |
| 5    | 14.5429        | 15.3599        | 16.1628        | 16.9525        |
TABLE IV. Same as table 3 for $k=1$.

| $|m|$ | $\lambda=0$ | $\lambda=1$ | $\lambda=2$ | $\lambda=4$ |
|-----|-------------|-------------|-------------|-------------|
| 0   | 6           | 7.2362      | 8.2945      | 10.0462     |
| 1   | 8           | 8.7594      | 9.4879      | 10.8608     |
| 2   | 10          | 10.6024     | 11.1913     | 12.3314     |
| 3   | 12          | 12.5154     | 13.0233     | 14.0173     |
| 4   | 14          | 14.4579     | 14.9110     | 15.8031     |
|     | $\lambda=6$ |             |             |             |
| 0   | 11.5189     | 12.8317     | 14.0381     | 15.1665     |
| 1   | 12.1368     | 13.3327     | 14.4622     | 15.5362     |
| 2   | 13.4252     | 14.4772     | 15.4916     | 16.4721     |
| 3   | 14.9840     | 15.9254     | 16.8431     | 17.7388     |
| 4   | 16.6773     | 17.5343     | 18.3753     | 19.2009     |
TABLE V. Same as table 3 for $k=2$.

| $|m|$ | $\lambda=0$ | $\lambda=1$ | $\lambda=2$ | $\lambda=4$ |
|-----|------------|------------|------------|------------|
| 0   | 10         | 11.0883    | 12.0757    | 13.7327    |
| 1   | 12         | 12.6961    | 13.3720    | 14.6650    |
| 2   | 14         | 14.5646    | 15.1195    | 16.2015    |
|     | $\lambda=6$ | $\lambda=8$ | $\lambda=10$ | $\lambda=12$ |
| 0   | 15.1801    | 16.4736    | 17.6660    | 18.7833    |
| 1   | 15.8856    | 17.0418    | 18.1420    | 19.1937    |
| 2   | 17.2480    | 18.2613    | 19.2438    | 20.1978    |
Figures captions

**Fig.1:** PSLET correlation energies for two interacting electrons in a harmonic quantum dot vs $\lambda = \sqrt{2} l_o / a^*$ (the ratio of the oscillator length $l_o$ and the effective Bohr radius $a^*$). The energies are normalized with the oscillator energy $\hbar \omega_o / 2$. The full lines represent states with $k = 0$, dashed lines for $k = 1$, and dashed dotted lines for $k = 2$. 
