Improved Estimate on the Number of Bound States of Negatively Charged Bosonic Atoms

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Abstract

It is shown that the number of bound states of an atom whose "electrons" satisfy bosonic symmetry conditions is bounded above by $C_\beta(\log Z)^\kappa$ where, κ and C_β are constants, the nuclear charge $Z > Z_\beta$ for some constant Z_β and the number of "electrons" N satisifies $N > (1+\beta)Z + 1$ with $\beta > 0$. The constant κ is universal, but Z_β depends upon β and C_β is inversely proportional to a power of β.

1 Introduction

In a recent paper, Bach, Lewis, Lieb, and Siedentop [2] studied the number of bound states, i.e. discrete eigenvalues, of the Hamiltonian for an atom consisting of a nucleus with infinite mass and charge Z and N negatively charged spinless bosons interacting with a Coulomb potential. This system is described by the Hamiltonian

$$H = \sum_{i=1}^{N} \left(-\Delta_i - \frac{Z}{|x_i|} \right) + \sum_{i<j} \frac{1}{|x_i - x_j|} \tag{1}$$

restricted to the symmetric subspace of $\otimes[L_2(\mathbf{R}^3]^N$, i.e., the eigenfunctions of H are required to be symmetric under interchange of coordinates of any two particles. If the number of bound states of such a system is denoted as $\nu_b(N,Z)$, they showed that when $(1+\beta)Z + 1 < N < (1+\beta')Z$, then $\nu_b(N,Z) < CZ^k$ where the constants C and k may depend upon β and β'. Although their estimates are neither optimal nor easily extended to fermions, this result is significant because it is the first explicit

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bound on the actual number of bound states of a multi-particle atomic system. The only previous results gave conditions on N and Z for which the number of bound states was zero, finite, or infinite. (See [9] for references.)

The main result of Section 3 of [2] can be stated as follows.

Theorem 1 *If, the Hamiltonian $H(N,Z)$ has no bound states supported outside a ball of radius R, then $\nu_b(N,Z) < Cn^k$ where $n = \int_{|x|<R}(c_1 Z^2 + Z/|x|)^{3/2} d^3\mathbf{x}$ and c_1 and C are constants.*

The expression "Ψ has support outside a ball of radius R", means that at least one "electron" is outside the ball, i.e. $\text{supp}(\Psi) \subset \{\mathbf{x} : \|\mathbf{x}\|_\infty > R\}$, where $\mathbf{x}$ denotes $(x_1, x_2, \ldots x_n)$. If we write $R = f(Z)/Z$ and $f(Z) > 1$, then

$$\int_{|x|<R}(c_1 Z^2 + Z/|x|)^{3/2} d^3\mathbf{x} \leq [f(Z)]^3 \int_{|x|<1}(c_1 + 1/|x|)^{3/2} d^3\mathbf{x}$$

so that Theorem 1 can be restated as

Theorem 2 *If, the Hamiltonian $H(N,Z)$ has no bound states supported outside a ball of radius $R = f(Z)/Z$, then $\nu_b(N,Z) < C[f(Z)]^{3k}$ for some constant C.*

In [2] it was shown that the hypotheses of the theorem could be satisifed for N in the range $(1+\beta)Z + 1 < N < (1+\beta')Z$ and sufficiently large Z with $R = cZ^{-1/2} = c\sqrt{Z}/Z$ which yields $\nu_b(N,Z) < CZ^{3k/2}$. In this note we show that it is possible to find constants C_β and Z_β such that for $Z > Z_\beta$, $H(N,Z)$ has no bound states supported outside a ball of radius $R = C_\beta \log Z/Z$ which yields $\nu_b(N,Z) < C_\beta(\log Z)^{3k}$. Moreover, we show that this holds provided $N > (1+\beta)Z + 1$, i.e. we show that the upper limit on N can be removed, and discuss the dependence of $\nu_b(N,Z)$ on β. Our final result can be stated as follows.

Theorem 3 *For all $\beta > 0$ there exists Z_β such that whenever $Z > Z_\beta$, and $N > \beta Z$, then $\nu_b(N,Z) < C(\log Z)^{4\kappa}/\beta^{3\kappa}$ where C and κ are constants.*

2 General Remarks on Localization Error

We now discuss some heuristics about localization error. Except for Simon's enhancement of the "Sigal-Simon localization trick" the contents of this section are well-known. However, because computing the localization error precisely is rather tedious, it is useful to review some aspects of its general behavior. Since details are available in the literature (and one can always check a specific case explicitly by differentiation), we concentrate on heuristics here and refer the reader to [3, 7, 12] for further details.

In many problems one wants to break up configuration space into pieces, i.e. one wants to consider

$$\langle \Psi, H\Psi \rangle = \int_{\mathbf{R}^{3N}} \Psi H \Psi d^3\mathbf{x} = \sum_k \int_{\Omega_k} \Psi H \Psi d^3\mathbf{x}. \tag{2}$$

However, this leads to technical difficulties unless $\Psi = 0$ on the boundary of each Ω_k. In order to achieve this one needs a set of localizing functions F_k such that $0 \leq F_k \leq 1$, $\mathrm{supp}(F_k) \subset \Omega_k$ and $\sum_k F_k^2 = 1$. Then instead of (2), one has

$$\langle \Psi, H\Psi \rangle = \sum_k \langle \, (F_k \Psi) H (F_k \Psi) \, \rangle - \sum_k \sum_i \mu_i \int_{\mathbf{R}^{3N}} |\nabla_i F_k|^2 |\Psi|^2 \tag{3}$$

The quantity $LE = \sum_k \sum_i \mu_i \int_{\mathbf{R}^{3N}} |\nabla_i F_k|^2 |\Psi|^2$ is called the localization error and there is term containing μ_i and ∇_i for each Laplacian $-\Delta_i$ with coefficient μ_i in the Hamiltonian H. Now suppose there are M localizing functions F_k (i.e. $k = 1...M$) and N gradient terms (i.e. $i = 1...N$). If one is dealing with a problem with permutational symmetry, one expects each of these terms to be roughly the same size (except possibly for a few exceptional terms which will not affect the large M, N behavior) so that one would expect the total localization error (LE) to be propertional to MN. Therefore, it is somewhat surprising that, at least for atomic problems, it is often possible to choose F_k so that LE grows only like $(\log M)^2$!

Beforing sketching the construction which yields this behavior, we review a few other facts. By a simple scaling argument, it is clear that LE is proportional to $1/(\mathrm{distance})^2$. Since F_k is usually chosen so that $F_k = 1$ on most of Ω_k, 0 outside Ω_k, and decreases smoothly from 1 to 0 near the boundary of Ω_k, it will have a non-zero derivative only near the boundary. Now one typically chooses the localization so that the boundaries of Ω_k are precisely the places where certain critical distances are equal, or at least comparable in a well-specified sense. Therefore, one has a natural parameter r so that $|\nabla_i F_k|^2$ is proportional to $1/r^2$.

It is often easier to first find functions G_k with $0 \leq G_k \leq 1$, $\mathrm{supp}(G_k) \subset \Omega_k$ and $\sum_k G_k^2 \geq 1$. One then defines $F_k = G_k / \sqrt{\sum_j G_j^2}$ and easily verifies that

$$LE \leq \frac{\sum_k \sum_i \mu_i \int_{\mathbf{R}^{3N}} |\nabla_i G_k|^2 |\Psi|^2}{\sum_k G_k^2} \tag{4}$$

Now one typically chooses G_K to have the form $G_k(x) = \chi(|x_k| / \|\mathbf{x}\|_p)$, where, $\mathbf{x}$ is often replaced by a specified subset of $x_1, x_2, ...x_n$; $\chi(t) : \mathbf{R}^+ \mapsto [0,1]$, $\chi(t) = 1$ if $t \geq 1$, and $\chi(t) = 0$ if $t \leq t_o$ for some chosen value of t_o.

We now show how to remove the dependence of LE on N. Since $\nabla_i \|\mathbf{x}\|_p = x_i^{p-1} / \|\mathbf{x}\|_p^{p-1}$, it follows that if G_k has the above form, then for $i \neq k$

$$|\nabla_i G_k|^2 \leq \frac{C}{r^2} \frac{x_i^{2p-2}}{\|\mathbf{x}\|_p^{2p-2}} \leq \frac{C}{r^2} \frac{x_i^p}{\|\mathbf{x}\|_p^p} \tag{5}$$

if $p \geq 2$. Since $\nabla_i G_k \neq 0 \Rightarrow \|\mathbf{x}\|_p \geq x_k \geq 2\|\mathbf{x}\|_p$, one can choose either $r = x_k$ or $r = \|\mathbf{x}\|_p$ as appropriate. In either case,

$$\sum_{i=1}^{N} |\nabla_i G_k|^2 \leq \frac{C}{r^2} \frac{1}{\|\mathbf{x}\|_p^p} \sum_{i \neq k} x_i^p = \frac{C}{r^2} \tag{6}$$

rather than NC/r^2. The reason for the apparent disappearance of the expected growth of LE with N is that, especially when p is large, only one derivative of the form $\nabla_i \|x\|_p (i = 1 \ldots N)$ dominates in any region of $\mathbf{R}^{3N}$. Localizations with p-norms (and $p \to \infty$) seems to have first been used in [7] (Zhislin [13] and others having previously used localizations with $p = 2$); Simon [3] subsequently advocated sacrificing some smoothness and using sup norms, for which it is somewhat clearer that, for a fixed k, the regions on which $\nabla_i G_k \ (i = 1 \ldots N)$ is non-zero do not overlap.

We now describe the"Sigal-Simon Localization Trick" for minimizing the dependence of LE on the number of localizing functions M. Let

$$\chi(t) = \begin{cases} 0 & 0 \le t < \frac{1}{2} \\ \frac{1}{2}\psi(t)^a = \frac{1}{2}(4t-2)^a & \frac{1}{2} \le t < \frac{3}{4} \\ 1 - \frac{1}{2}\psi(t)^a = 1 - \frac{1}{2}[4(1-t)]^a & \frac{3}{4} \le t < 1 \\ 1 & 1 \le t \end{cases} \tag{7}$$

where $a > 1$ and $\psi(t) = 1 - |4t - 3|$. [The precise form of ψ and the cut-off at $\frac{1}{2}$ are chosen for simplicity and are not essential. Moving the cutoff from $\frac{1}{2}$ to t_o closer to 1 may be desirable for some purposes but will increase the localization error by a factor of $1/(1-t_o)^2$.] With χ given by (7)

$$|\chi'(t)| = \begin{cases} 2a\psi(t)^{a-1} & \frac{1}{2} \le t \le 1 \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

Now consider (as a function of $\eta > 0$) the expression

$$\frac{|\chi'|^2}{\frac{1}{4}\psi^{2a}\eta^{-1} + \eta^{a-1}} = 16a^2\psi^{-2}\frac{\eta}{1 + 4\eta^a\psi^{-2a}}$$

which has its maximum when $\eta^a = \psi^{2a}/4(a-1)$ so that

$$|\chi'|^2 \le 16a^2(\chi^2\eta^{-1} + \eta^{a-1}) \ \ \forall \ \ a > 1 \ \text{ and } \ \eta > 0. \tag{9}$$

If one then uses this χ to construct a set of localizing functions F_k via G_k as above, one finds

$$\begin{aligned} \sum_k |\nabla_i F_k|^2 &\le 16a^2 \frac{\sum_k \eta^{-1} G_k^2 + \eta^{a-1}}{\sum_k G_k^2} \\ &\le 16a^2(\eta^{-1} + M\eta^{a-1}) \end{aligned} \tag{10}$$

If one now chooses $\eta = M^{-1/a}$ and combines this estimate with those above, one finds a net localization error satisfying $LE \le Ca^2 M^{1/a} \ \ \forall \ a > 1$. Writing $M = b^a$, or equivalently, choosing $a = (\log M)_b$ one gets the final estimate $LE \le C(\log M)^2$ for some constant C.

This trick was first used by Sigal [11, 12] in the special case $a = 2$, which yields a localization error proportional to $\sqrt{M}$ (and for which the bound in (9) can be obtained by a simple squaring argument). The idea of reducing this to M^σ with

$\sigma > 0$ arbitrarily small is due to Simon; it is sketched in [12] (see Sect. 5) and alluded to in [3] (see the remark on p. 47) and in [6, 9]; however, the details have not previously appeared in the literature and the reduction to $\log M$ seems new.

Finally it is worth remarking that this analysis is essentially unchanged if G_k is a product of a *fixed* number of χ. If however, one needs a product of N functions, as in [4, 8], this approach does not work.

3 Shrinking the Size of the Inner Ball

We now show how to apply these ideas to improve the estimates in [2]. Although this involves only the localization for the second partition in Section 2 of [2], which we will subsequently show (see Section 4 below) can actually be eliminated, the argument is simple and illustrates the power of the Sigal-Simon localization trick. Moreover, the final estimates obtained here will be slightly better than those in Section 4. Let $J_{kl} = \chi(|x_k|/\|\hat{\mathbf{x}}_k\|_\infty)\chi(|x_\ell|/\|\hat{\mathbf{x}}_{k\ell}\|_\infty)AJ_{n+1}$ where $\hat{\mathbf{x}}_k$ denotes $\mathbf{x}$ with x_k removed, etc., χ is as in (7) and the localizing functions A and J_{n+1} are defined in [2]. We need here only the facts that A and J_{n+1} make a contribution of $C/\delta^2 R^2$ to LE, and that AJ_{n+1} is supported on a region where at least two "electrons" are outside a ball of radius $R\delta$ so that

$$\text{supp} J_{k\ell} \subset \{\mathbf{x} : 4|x_k| > 2|x_\ell| > |x_i| \ \forall\ i \neq k, \ell \text{ and } |x_\ell| > R\delta\} \tag{11}$$

where $\delta < \beta$ and R will be chosen later. Now the number of $J_{k\ell}$ is $M = N(N-1)/2 \approx N^2/2$. As discussed in Section 2 above, one easily checks that the localization error from this partition satisifes $LE \leq C(\log N)^2/\delta^2 R^2$. Thus, eq. (10) of [2] now can be replaced by the following estimate which is valid on $\text{supp}(J_{k\ell})$

$$\begin{aligned} H(N,Z) - E_o(N-1,Z) \quad &\geq \\ &-\Delta_1 - \Delta_2 - \frac{Z}{|x_k|} - \frac{Z}{|x_\ell|} + I_o(N-1,Z) - \frac{C(\log N)^2}{\delta^2 R^2} \end{aligned} \tag{12}$$

where $I_o(N-1,Z) = E_o(N-2,Z) - E_o(N-1,Z)$ denotes the ionization potential of the $(N-1)-st$ "electron". If one now uses Bach's estimate [1] that $I_o(N,Z) \geq \mu Z^2$ for some constant μ, it is then evident that one can find constants C_β and Z_o such that the right side of (12) is positive if $R = C_\beta \log Z/Z$ and $Z \geq Z_o$. Using this in Theorem 2 gives the final bound of $\nu_b(N,Z) < C_\beta(\log Z)^{3k}$ as explained in the introduction. Note that the choice $R = C_\beta \log Z/Z$ implies that $-2Z/|x_k| > -2Z/\delta R > -(\text{constant})Z^2/\log Z$. Since the LE terms are also of the form $-Z^2/\log Z$, it will be necessary to choose either C_β or Z_o extremely large to ensure that they are dominated by μZ^2.

Thus far we, like BLLS [2], have ignored the question of how R and $\nu_(N,Z)$ depend upon the lower limit β. Using the fact that one must have $\delta < \beta$ and choosing $\delta = \beta/2$, one finds that the estimates above require $R > C\log Z/\beta Z$. However, the positivity of eq. (8) of [2] requires the stronger condition $R > C \log Z/\beta^3 Z$ so that $f(Z) = c \log Z/\beta^3$ which yields a net bound of

$$\nu_b(N,Z) < C\frac{(\log Z)^{3k}}{\beta^{9k}} \tag{13}$$

Since one must have $\beta < \beta_c \approx 0.21$ this estimate is large even near β_c (since $\beta_c^{-9} > 10^6$!) and becomes enormous as $\beta \to 0$.

4 Range of N — Removing the Upper Bound

The upper limit of $N < (1+\beta')Z$ in [2] arises because of the need for the bound on the ionization potential $E_o(N-1,Z) - E_o(N-2,Z) > \mu Z^2$, which requires that N be in the range where $H(N,Z)$ still has bound states. However, the number of bound states is expected to decrease as N approaches its upper limit of $\beta_c Z \approx 1.21Z$ so that this upper limit on N should not be necessary. We now show how to remove it.

In [2], their analysis of the outer region begins with a localization on which the effective potential of the k-th electron, $V_k^{\text{eff}} = -Z/r_k + \sum_{i\neq k} 1/r_{ik}$ is bounded below (see eq. (8) of [2]) as

$$V_k^{\text{eff}} \geq \frac{-Z + (N-1)/(1+\delta)}{r_k} \geq \frac{(\beta-\delta)Z}{(1+\delta)r_k} \tag{14}$$

which will be positive only if $\beta > \delta$. Since this is valid on a region on which $r_k\delta > r_i \ \forall \ \ i \neq k$, and since $\beta < 0.21$, such regions will not cover the outer region (which would requires $\delta \geq 1$) and the resulting localization will not give a partition of unity. In order to treat the remaining region they make an additional partition into regions on which $r_k > r_\ell > r_i \ \ \forall i \neq k, \ell$, as discussed in Section 3 above. In this region they need Bach's estimate of μZ^2 on th ionization potential which requires $N - Z < \beta' Z < \beta_c Z$

In order to eliminate the second partition, we replace the estimate (14) by a more refined electrostatic estimate used by Lieb, Sigal, Simon and Thirring [6] to give the first proof of asymptotic neutrality. They show that for any $\epsilon > 0$ there exist N_ϵ and regions Ω_k which cover $\mathbf{R}^{3N}$ when $N > N_\epsilon$ and on which

$$\sum_{i\neq k} \frac{1}{r_{ik}} \geq \frac{(1-\epsilon)N}{r_k} \tag{15}$$

They also showed that one can find a localization corresponding to these regions with $LE \leq C\sqrt{N}(\log N)^2/\epsilon^2 \|\mathbf{x}\|_\infty^2$. In the terminology of Section 2 above, the contribution of $1/\epsilon^2$ corresponds to $1/(1-t_o)^2$; the factor $\sqrt{N}$ corresponds to $M^{1/a}$ when $a = 2$ and can be replaced by $(\log N)^2$; and the $(\log N)^2$ already present is an additional factor that arises because of a cut-off parameter needed, as explained in [6]). Thus one can improve this bound (as already remarked in [6]) to $LE \leq C(\log N)^4/\epsilon^2\|\mathbf{x}\|_\infty^2$. Thus, on $\mathrm{supp}(\Omega_k)$, the effective potential and LE can be estimated as

$$V_k^{\mathrm{eff}} - LE \geq \frac{(1-\epsilon)N - Z}{r_k} - \frac{C(\log N)^4}{\epsilon^2 r_k^2} \tag{16}$$

$$\geq \frac{(\beta-\epsilon)Z}{r_k} - \frac{C'(\log Z)^4}{\epsilon^2 r_k R} \tag{17}$$

where we have used the fact [5] that $N < 2Z+1$ (but we really only need that $N < Z^m$ for some m to replace $\log N$ by $\log Z$). The first term will be positive if $\beta > \epsilon$. Choosing $\epsilon = \beta/2$, one can conclude that $V_k^{\mathrm{eff}} - LE > 0$ if $R > C(\log Z)^4/\beta^3 Z$. Using this in Theorem 2 with $f(Z) = C(\log Z)^4/\beta^3$ gives a final bound of

$$\nu_b(N,Z) \leq C\frac{(\log Z)^{12k}}{\beta^{9k}} \tag{18}$$

valid whenever $Z+1 > N - Z > \beta Z$ and $Z > Z_\beta$. The price one pays for removing the restriction $N - Z < \beta' Z < \beta_c Z \approx 0.21Z$ is a higher power of $(\log Z)$. A more serious price is that we do not have any information about how Z_β depends upon β. In addition, we have not been able to improve the dependence of $\nu_b(N,Z)$ on $1/\beta$, even for β near β_c.

In [2] the restriction that the particles are bosons was used in the outer region only to estimate the ionization potential as μZ^2. Since we have eliminated the need for this, the argument above should also work for fermions, and it does. Unfortunately, it only works for $N > \beta Z$ and we already know [4, 6, 10] that, because fermionic atoms are asymptotically neutral, $\nu_b(N,Z) = 0$ in this region, i.e. for fermions the only region of interest is the very delicate region $Z+1 < N < Z + cZ^\sigma$ with $\sigma < 1$. (By [10] $\sigma < 5/7$). Indeed, the estimates sketched in this section combined with the easily proved fact that no bound states have support such that *all* electrons lie within a ball of radius $O(N^{-1/3})$ suffice to prove asymptotic neutrality and this is essentially the argument in [6].

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