Explicit Bound States for Certain N–Body Hamiltonians

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We construct explicit bound state wave functions and bound state energies for certain N–body Hamiltonians in one dimension that are analogous to N–electron Hamiltonians for (three-dimensional) atoms and monatomic ions.

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The usual non–relativistic electronic Hamiltonian for an N–electron atom or monatomic ion with nuclear charge Z is

$$\widetilde{H}_N^Z \;=\; -\,\frac{1}{2}\,\sum_{j=1}^{N}\Delta_{x_j}\;-\;\sum_{j=1}^{N}\frac{Z}{|x_j|}\;+\;\sum_{j<k\le N}\frac{1}{|x_j-x_k|},$$

acting on the N–fold antisymmetric tensor product of $L^2(\mathbb{R}^3,\,dx_j,\,\mathbb{C}^2)$. Explicit eigenfunctions of these operators are only known for the case of $N=1$.

In this paper we consider a one–dimensional analog of atoms, with Hamiltonian $\widetilde{H}_N^Z$ modified as follows:

1. We take the ambient space to be $\mathbb{R}$ instead of $\mathbb{R}^3$.
2. We replace the Coulomb potentials by Dirac deltas. This is not unreasonable, because in many ways, Dirac deltas are one–dimensional analogs of the three–dimensional Coulomb potentials.
3. We drop the antisymmetry requirement. This is necessary to have any bound states at all when $N\ge 3$. The bound states we construct are symmetric with respect to interchange of the identical particles, so one could think of the particles as distinguishable or as identical spin-0 bosons.
4. We "symmetrize" the repulsions between pairs of particles. Explicitly, this amounts to replacing $\delta(x_j-x_k)$ by $\frac{1}{2}\left(\delta(x_j-x_k)+\delta(x_j+x_k)\right)=\frac{1}{2}\,\delta(|x_j|-|x_k|)$ for every $j\ne k$. Without this symmetrization, we do not know how to solve the eigenvalue problem explicitly.

These alterations yield the N–body Hamiltonian

$$H_N^Z=-\,\frac{1}{2}\,\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2}\,-\,Z\,\sum_{j=1}^{N}\delta(x_j)\,+\,\frac{1}{2}\sum_{j<k}^{N}\delta(|x_j|-|x_k|),$$

acting on $L^2(\mathbb{R}^N,\,dx)$. To construct these self–adjoint operators rigorously, one must use the technique of quadratic forms [10, 13] because the potentials are so singular.

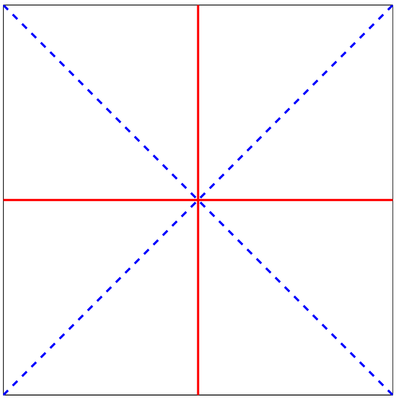

FIG. 1: A plot of the potential when $Z=N=2$. The solid red lines indicate attractions and the dashed blue lines indicate repulsions.

For $N\le 2$, it is easy to see that H_N^Z has at most

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one bound state. If we drop all the repulsion terms, the resulting operator is the sum of the N operators

$$h_j^Z \;=\; -\,\frac{1}{2}\,\frac{\partial^2}{\partial x_j^2} \;-\; Z\,\delta(x_j).$$

It is well-known that h_j^Z has exactly one bound state $\propto e^{-Z|x_j|}$, with energy $-Z^2/2$. Thus, with the repulsion removed, the full operator has one bound state $\propto \prod_{j=1}^{N} e^{-Z|x_j|}$ and has energy $-N\,Z^2/2$. When we add the repulsion terms, the number of bound states cannot increase because the repulsion potential is non-negative and the bottom of the continuous spectrum does not depend on the repulsion. Thus, H_N^Z has at most one bound state if $N \leq 2$. For $N \geq 3$, this argument fails because the bottom of the continuous spectrum does depend on the repulsion strength. Nevertheless, we can prove that when $N = 2Z + 1$, there is no discrete spectrum [8].

We have realized that it is possible to write down the ground state of H_N^Z explicitly for any $N \leq 2Z$:

$$\Psi_N^Z(x_1, \dots x_N) \;\propto\; \exp\left(-\sum_{k=1}^{N} \frac{2Z - j + 1}{2}\,|x_{j_k}|\right)$$

in the region where $|x_{j_1}| \leq |x_{j_2}| \leq \cdots \leq |x_{j_N}|$. As we consider all the permutations of the variables x_j, these regions cover all of $\mathbb{R}^n$, and on the (measure zero) overlaps of these regions, the various definitions all agree with one another.

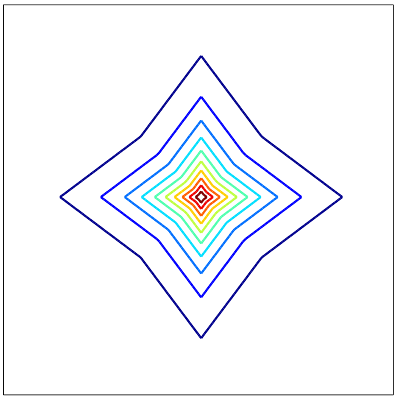

FIG. 2: A contour plot of the bound state probabilty density (computed numerically) when $N = Z = 2$.

The energy of this bound state is

$$\begin{aligned} E_N^Z \;&=\; -\sum_{j=1}^{N} \frac{(2Z - j + 1)^2}{8} \\ &=\; -\,\frac{N(N-1)(2N-1)}{48} + \frac{N(N-1)\,Z}{4} - \frac{N\,Z^2}{2}, \end{aligned}$$

which in the neutral case $Z = N$ yields

$$E_N^N \;=\; -\,\frac{N\,(1 + 9N + 14N^2)}{48}.$$

After discovering this result we learned that the explicit ground state for $Z = N = 2$ has been previously discovered by Gersch [5, 15]. However, we are not aware of prior results for Hamiltonian with $N \geq 3$. Since we have explicit formulas, it is not extremely hard to check that our results are correct. However, because the potentials are very singular, one must resort to quadratic form techniques to do this rigorously. In the language of the partial differential equations literature, we have weak solutions to the eigenvalue equations. Details of a proof that we have correctly solved the eigenvalue problem will be published elsewhere [8] (in the mathematical physics literature).

Our model joins the relatively short list of exactly-solvable many-body problems [7]. It strongly resembles the boson models in the one-dimensional continuum that recently became subject of intense interest due to the close connection to experiments, *e.g.*, on atomic traps [3]. McGuire showed that a system of identical N bosons in one dimension interacting via an *attractive*, finite strength delta-function potential is exactly soluble, with solution remarkably similar to ours [11]. The analogous model of N *repulsive* bosons can be solved exactly both in the hard-core (infinite repulsion) limit (the Tonks-Girardeau gas) [2, 6] and for finite interaction strength (the Lieb-Liniger model) [9] using the Bethe Ansatz [1, 4], Our model can be viewed as an extension of the Lieb-Liniger model to the case of a delta-function attractive "trap" at the origin, and with the associated symmetrization of the repulsion operator.

Remarks

1. From numerical computations, the coordinate symmetrization of the repulsion operator raises the energy typically by only about 1%, at least for small N and Z. It would be natural to view the unsymmetrized problem as a perturbation of the symmetrized problem. If we do this, the first order energy correction is zero.

2. One can also find the ionization energy by taking
$$E_{\text{Ionization}} \;=\; E_{N-1}^Z \;-\; E_N^Z \;=\; \frac{(2Z - N + 1)^2}{8}.$$
Thus, the ionization energy of the neutral N–electron "atom" is
$$E_{\text{Ionization}} \;=\; \frac{(N+1)^2}{8}.$$

3. Similarly, we can evaluate the second ionization energy. For a neutral N–electron "atom," it is
$$E_{\text{Second Ionization}} \;=\; \frac{(N+2)^2}{8}.$$

Thus, we easily see that the second ionization energy is greater than the first ionization energy, a fact that has not been proved starting from the Schrödinger equation for realistic atoms when $N \geq 3$.

4. Our model supports existence of negative "ions." Our formula yields an explicit discrete bound state as long as there are at most $N \leq 2Z$ electrons. We conjecture that this is the maximum number of electrons that can be bound with nuclear charge Z for these models.

5. For these models, one can also compute the Hartree energy. (Since our "electrons" are bosons instead of fermions, this is the appropriate analog of Hartree–Fock.) This has been done for $N = 2$ in [12], but their analysis generalizes to our situation. In general, the Hartree energy is

$$E^Z_{N,\,\mathrm{Hartree}} = -\,\frac{N\,\left((N-1)^2 - 6(N-1)Z + 12Z^2\right)}{24},$$

which, in the neutral case, becomes

$$E^N_{N,\,\mathrm{Hartree}} = -\,\frac{N\,(1 + 4N + 7N^2)}{24}.$$

This upper bound differs from the $O\left(N^3\right)$ exact energy by what in atomic and molecular physics is termed the correlation energy:

$$E_{N,\,\mathrm{correlation}} = \frac{N\,(N-1)}{48}.$$

It is rather remarkable that this correlation energy for $N = 2$ (the analog of the ground-state He atom) differs from the correlation energy of the physical helium atom, $\approx -2.903724 - (-2.861700) = -0.042024$, by only 0.000357, or less than 1%. However, our model predicts that the correlation energy for the two-electron series to be independent of Z, whereas the correlation energies of physical two-electron atoms decreases non-trivially (albeit slightly) with Z. [14]

Conclusion We have found an N-boson "atom" in one dimension for which the lowest bound state can be written explicitly. The Hamiltonian of our model strongly resembles to the electronic Hamiltonian of an atom. Several aspects of the solution have analogs in the real atoms. For example, first ionization potential is smaller than the second, and negative ions are stable. Notably, the correlation energy for $N = 2$ is within 1% of the exact correlation energy of the ground state helium atom.

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