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Title: "The Kinetic Energy Functional of an N Particle System"

Quantum mechanical simulations of atoms are still too complex for today's modern computers to process. There are two approaches to this problem, either to develop a more capable computer or to further develop quantum mechanical theory itself. Working with Randall Jones, Ph.D. of the Loyola University Physics Department, I have made advancements to Electron Density Functional Theory and built upon the ground work done by two physicists in the late twentieth century, $Pierre\ Hohenberg\ and\ Walter\ Kohn^1$.

The many particle wavefunction solutions to Schrodinger's equation are difficult and nearly impossible to solve for atoms. In particular, one major challenge in determining the properties of nanoparticles is the calculation of the total energy of any particular configuration of the atoms. Due to the lack of exact wavefunction solutions, only approximations have been available to use in defining the total energy of a system. In current practice, the total energy depends on 3N variables, where N particles are free to move in the three dimensions, but the *Hohenberg-Kohn* theorem states it should be possible to determine the total energy of a system directly as a functional of the electron density. If the energy could be a function of only three coordinates, the problem would be greatly simplified! Reasonably good approximations exist for the functional representing electron-electron potential energy, but if we knew the kinetic energy, we could use that to determine the total energy and search for its relation to the electron density.

During the Hauber Summer Research Program, Dr. Jones and I have rediscovered a $model\ system^2$ consisting of N, interacting, spin ½ particles that can be solved exactly to obtain the many-particle wavefunction. This model system involves particles that interact via spring-like forces, therefore the Schrodinger equation can be completely solved to obtain its wavefunction, particle density, and exact energy. I am now working to determine the functional for this model system with an arbitrary number of particles that generates the kinetic energy density from the particle density where the potential is already defined. The form of this functional corresponding to this model system can provide insight and guide the development of the functional for a real electron system.

Each particle in this system is subject to two separate potentials. The first potential is a harmonic restoring potential that attracts each particle to the origin and is of the form $V(x) = \frac{1}{2} m \omega^2 x^2$. The second potential is a harmonic potential that governs particle interaction and is of the form $V_{int} = -\frac{1}{2} \beta \left(x_j - x_i\right)^2$ where β determines the strength of the particle interaction.

Using $Mathematica^3$ as the primary computational platform, I have found the complete wavefunction solution for the two particle case. Once it was discovered that the system could yield exact solutions, I then determined solutions for three, four, and five particles. After

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thoroughly analyzing the patterns and simplifying these solutions, the wavefunction solution for an arbitrary number of particles became evident.

The exact wavefunction solution for N particles in the model system is as follows:

$$\Psi(\{x_i\}) = \prod_{\substack{i=1 \\ j>i}}^{N} (x_i - x_j) Exp\left(-\frac{1}{2}\gamma \sum_{i=1}^{N} x_i^2 - \frac{1}{2}\alpha \sum_{\substack{i=1 \\ j>1}}^{N} x_i x_j\right)$$

With $\quad \gamma = \frac{1}{N}\left(1 + (N-1)\sqrt{1 - \frac{N\beta}{2}}\right) \quad$ and $\quad \alpha = \frac{2}{N}\left(1 - \sqrt{1 - \frac{N\beta}{2}}\right)$

The complete proof of the general case is still under development, but these solutions provide enough insight to proceed.

The next step was to obtain the exact particle density and kinetic energy density for the two-particle system so that we could begin to construct a functional. For two particles, we note that

$$\alpha = 2(1 - \gamma)$$

and the wavefunction can be written as a function of gamma alone.

$$\Psi(x_1, x_2) = (x_1 - x_2) Exp\left(-\frac{1}{2}\gamma(x_1 - x_2)^2 - x_1 x_2\right)$$

The (un-normalized) particle density and kinetic energy density are

$$\rho(x) = (2x^2 + \gamma) Exp\left(\frac{-2(\gamma - 1)}{\gamma}x^2\right)$$

$$k(x) = \left(4x^4(1 - 2\gamma)^2 + \gamma^2(3 - 2\gamma + 6\gamma^2) + 4x^2\gamma(3 + \gamma(-7 + 3\gamma))\right) Exp\left(\frac{-2(\gamma - 1)}{\gamma}x^2\right)$$

The goal is to write $k(x)$ as a function of $\rho(x)$ and its derivatives.

Dr. Jones and I first looked at the non-interacting system, in which $\alpha = 0$ and $\gamma = 1$, but even this is a difficult problem. After extensive trial and error with the various combinations, we discovered the following kinetic energy functional.

$$k[\rho(x)] = 3\rho(x) + \frac{1}{2}\rho''(x) - \frac{1}{2}f(\rho(x)) \text{ with } f(\rho(x)) = \frac{1}{4}\frac{\rho''(x)^2 - \rho(x)\rho''''(x)}{\rho(x)}$$

This process was repeated for the case where $\beta = \frac{3}{4}$, which also corresponds to $\gamma = \frac{3}{4}$, and a more elaborate functional was obtained.

$$k[\rho(x)] = \frac{3}{8}\rho(x) + \frac{7}{64}\rho''(x) - \frac{3}{256}f[\rho(x)]$$

with $\quad f[\rho(x)] = \dfrac{\rho''(x)^2 - \frac{3}{2}\rho'''(x)^2 + \rho'(x)\,\rho'''(x) + \frac{3}{2}\rho''(x)\,\rho'''''(x)}{\rho(x)}$

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This is an important result in that we have proved that such a functional can be obtained for a system with a non-zero particle interaction. Though the Hauber Summer Research Program has ended, the research is on-going; I am still working with Dr. Jones to determine the functional for arbitrary values of β. Ultimately, I hope to find the functional for 3, 4, and 5 particles with the goal to deduce the form for an arbitrary number of particles with a method similar to that which was used for obtaining the wavefunction solutions.

Once this system is completely understood, it will provide insights into the behavior of the kinetic energy functional corresponding to a real electron density function. Applying results from this research in electron density functional theory to real electron systems will allow for chemists to run accurate simulations with current computer processors and lead to better testing and understanding of particle interactions. This experience has created a strong interest in me to solve this problem that lies within quantum mechanical theory and has introduced me to the caliber of work done at the graduate level.

The results and methods of this research have been presented to multiple audiences at Loyola University Maryland and I have been selected to represent my university at the annual National Conference for Undergraduate Research (NCUR) in Memphis. Dr. Jones and I are currently in contact with the American Journal of Physics to publish our results regarding the further development of Electron Density Functional Theory.

References:
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[1]Hohenberg, P., and Kohn, W. (1964). Inhomogeneous electron gas. $Phys. Rev.$ **136**: B864 − B871.
[2]M. Moshinsky, Amer. J. Phys. **36**, 52 (1968).
[3]Wolfram Research, Inc., Mathematica, Version 10.4, Champaign, IL (2016)