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GROUND STATE AND ELEMENTARY EXCITATIONS OF SPIN-ALIGNED ATOMIC HYDROGEN

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Abstract. - Non parametrized, optimal Jastrow-HNC solutions have been obtained for condensed spin-aligned atomic hydrogen. Accurate values have been calculated for the energy, the pair correlation and the structure function as well as for the Bose condensate fraction. The elementary excitations and the stability of the system have been studied using methods adapted from the theory of liquid 4He.

Spin-aligned atomic hydrogen (H\textsuperscript{+}) has recently attracted considerable interest as a quantum system \cite{1,2}. If a collection of hydrogen atoms can be forced to a spin-aligned state by the application of a very large magnetic field at low temperatures, the pair interaction between the atoms is the triplet b\textsuperscript{3} P\textsuperscript{0} potential. This potential is accurately known from the variational calculation of Kolos and Woliniewicz \cite{3}, and is repulsive enough that H\textsuperscript{+} never forms a self-bound liquid state. The hydrogen atoms are very light bosons, and as the system is weakly interacting, H\textsuperscript{+} should exhibit even more extreme quantum behaviour than 4He. Unfortunately, it is certainly not easy to prepare this very exotic material. The main problem is containment, since interactions with vessel walls may cause spin-flips and thus very rapid recombination into the molecular state several eV/atom below the metastable H\textsuperscript{+} state.

We have calculated the ground state properties of H\textsuperscript{+} at zero temperature, starting from the Kolos-Woliniewicz-potential \cite{3} and a Jastrow many-body wavefunction. We use the optimal hypernetted chain (HNC) method \cite{4,5}, which requires no parametrization of any function and produces numerically accurate and asymptotically correct solutions without any imposed constraints. In the case of Bose statistics, the method has been successfully applied for liquid helium \cite{5} and the Bose Coulomb gas \cite{6}.

We have obtained optimal Jastrow solutions for H\textsuperscript{+} in the range of densities \( \rho = 1...10(10^{13})^{-1} \)Our energy values agree with those of Miller and Nosanow \cite{3}. We produce accurate values for the structure function \( S(k) \) and the pair correlation function \( g(r) \). The latter is of particular interest in studying the elementary excitations of H\textsuperscript{+} \cite{7} by generalizing the Feynman construction for 4He. A minimal stability condition is that the cost in the Zeeman energy of an electron spin flip is greater than the average gain in exchange energy, i.e.

\[ \mu_e H > \int \frac{1}{2} J(0), \]

where \( \mu_e \) is the electron magnetic moment, \( H \) the magnetic field and

\[ \int \frac{1}{2} J(k) = \rho \int J(r) g(r) e^{i k \cdot r} \, dr. \]

Above, \( J(r) \) is the triplet singlet potential difference \( V_T(r)-V_S(r) /3 \). The value of \( J(0) \) is very sensitive to the behaviour of \( g(r) \) near the origin. The present method of calculating the stabilizing field \( \int \frac{1}{2} J(0) \) is powerful, since the optimal HNC approximation yields essentially exact results for \( g(r) \) at small \( r \).

Also, the optimal HNC method gives an accurate structure function and a meaningful momentum distribution. We have obtained the one particle momentum distribution and the Bose condensate fraction by a recently developed summation technique \cite{8}. In this method one solves an integral equation analogous to the standard HNC-equation to obtain the one-particle density matrix.

Some of our results are summarized in Table I, where we give \( J(0) \) and the minimum stabilizing

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The mean exchange energy $J(0)$, the minimum stabilizing field $H_{min}$ and the Bose condensate fraction $\Delta \rho$ for spin-aligned atomic hydrogen at several densities. The density is in units $\sigma^{-3}$, with $\sigma$ the effective hard core radius of 3.69 Å.

<table>
<thead>
<tr>
<th>$\rho(\sigma^{-3})$</th>
<th>$J(0)$ (K)</th>
<th>$H_{min}$ (KG)</th>
<th>$\Delta \rho$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>5.149</td>
<td>38.3</td>
<td>82</td>
</tr>
<tr>
<td>0.10</td>
<td>12.32</td>
<td>91.7</td>
<td></td>
</tr>
<tr>
<td>0.20</td>
<td>34.30</td>
<td>255</td>
<td>44</td>
</tr>
<tr>
<td>0.30</td>
<td>68.93</td>
<td>513</td>
<td></td>
</tr>
<tr>
<td>0.40</td>
<td>119.4</td>
<td>889</td>
<td>19</td>
</tr>
</tbody>
</table>

In the spin-wave excitation spectrum there is a possibility of a soft mode instability /7/ at nonzero wavevector, but for all densities considered the "gap" instability (1) occurred first. To test our calculation routines, we have also calculated the condensate fraction in $^4$He as described by the Lennard-Jones potential. The result is $\Delta \rho = 12\%$ at the equilibrium density in excellent agreement with the best previous calculations /9/.

In conclusion, we have obtained several ground state and excitation characteristics of $^4$H$^+$ gas at 0 K, which allow us to map the quantum properties of this interesting system. More results and details will be presented elsewhere.

References

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