BCS theory tested in an exactly solvable fermion fluid

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Remarkably the one-dimensional (1D) many-fermion fluid with pairwise-attractive δ -function interactions is exactly solvable in that one can determine the exact many-body ground-state energy and chemical potential for all values of the coupling strength and/or density. Bardeen-Cooper-Schrieffer (BCS) theory is tested in this model by numerically determining the BCS total ground-state energy and chemical potential as a function of the coupling strength and/or density, and comparing with the exact results. As is the case for 2D and 3D theories, two regimes are apparent: (a) a BCS-proper regime of weakly coupled, overlapping Cooper pairs and (b) a Bose-gas regime of strongly interacting fermions which pair to form an ideal Bose gas at low density. In the two extremes the BCS energy and chemical potential are identical to the exact values and are moderately close for intermediate coupling and/or density.

Recently the exactly solvable one-dimensional (1D) fermion fluid¹ with pairwise-attractive δ interactions has proved interesting for several reasons. For the case of two distinct fermion species, for example, electrons with spin up and down, there exist dynamical similiarities between the present 1D model and the 3D electron fluid jellium model, and one reproduces for weak coupling the essential singularity characteristic of standard 3D lowtemperature superconductivity.² Furthermore, the model displays a crossover transition³ from the strong-coupling extreme of tightly bound noninteracting local Bose pairs to the weak-coupling limit of large, overlapping Cooper pairs. Crossover transitions of this type are of interest in their own right and are also present in Fermi systems with attractive interactions both in two⁴ and three⁵ dimensions, and in the extended negative-U Hubbard model.⁶ Since Bardeen-Cooper-Schrieffer (BCS)-like⁷ theories are frequently applied, we wish to investigate and test the BCS theory in the present simple 1D model for which the exact results are also known. We stress that the BCS theory has been used in the context of providing a variational ansatz for the ground-state wave function and that weak coupling is not assumed.

Consider a system of $N \ (\gg 1)$ spin- $\frac{1}{2}$ fermions of mass m and degeneracy 2 in a box of length L interacting via a pairwise-attractive δ interaction of strength $v_0 > 0$. The Hamiltonian in dimensionless form is

$$H' \equiv mH / \hbar^2 \rho^2 = -\frac{1}{2} \sum_{i=1}^{N} \frac{d^2}{dx'_i^2} - \lambda \sum_{i < j} \delta(x'_i - x'_j) , \qquad (1)$$

where $\rho = N/L$ denotes the density, the dimensionless coordinates are $x'_i = \rho x_i$, and $\lambda \equiv m v_0 / \hbar^2 \rho$ is a dimensionless parameter ($0 \le \lambda < \infty$). This parameter then com-

pletely specifies the ground-state properties of the system. From the expression for λ , one can see that high (low) particle density is associated with weak (strong) coupling.

Using the Gaudin equations⁸ one can numerically determine² the exact ground-state energy E(N), i.e., the lowest eigenenergy of the N-fermion Schrödinger equation, as a function of λ . Table I gives the dimensionless ratio, $\epsilon(\lambda) \equiv E(N)/|E_0(N)|$, where $E_0(N)$ is the energy evaluated at $\rho=0$. One can also determine the chemical potential by

$$\mu = \frac{E(N)}{N} + \rho \frac{\partial [E(N)/N]}{\partial \rho} .$$
⁽²⁾

It has already been noted that the BCS approximation gives the exact results in the two extremes of λ ,² and we now present the results in the intermediate region of $0 < \lambda < \infty$. The appropriate equations are the BCS gap and number conservation equations,

$$\Delta = \frac{v_0}{4\pi} \int_{-\infty}^{+\infty} dk [\xi_k^2 + \Delta^2]^{-1/2} , \qquad (3)$$

$$N = \frac{L}{2\pi} \int_{-\infty}^{+\infty} dk \left[1 - \frac{5k}{\sqrt{\xi_k^2 + \Delta^2}} \right] ,$$

$$\xi_k = \frac{\hbar^2 k^2}{2m} - \frac{1}{2} \rho v_0 - \mu .$$
(4)

One should note that only in the limit of weak coupling is the chemical potential³ given by the Fermi energy, i.e., $\mu = E_F$. In general, one must solve for the chemical potential and the gap self-consistently for all values of the dimensionless constant λ .

The dimensionless energy per particle in the BCS ap-

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	$\widetilde{\mu}(\lambda)$			$\epsilon(\lambda)$		
λ^{-1}	Exact	BCS	PWHF	Exact	BCS	PWHF
0.05	-0.1242	-0.1120	-0.0219	-0.9978	-0.9488	-0.0918
0.10	-0.1215	-0.0979	-0.0377	-0.9909	-0.8947	-0.1671
0.15	-0.1165	-0.0825	-0.0472	-0.9784	-0.8374	-0.2260
0.20	-0.1088	-0.0657	-0.0507	-0.9595	-0.7766	-0.2684
0.25	-0.0978	-0.0470	-0.0479	-0.9333	-0.7117	-0.2944
0.30	-0.0832	-0.0262	-0.0390	-0.8989	-0.6421	-0.3039
0.35	-0.0643	-0.0030	-0.0239	-0.8551	-0.5674	-0.2970
0.40	-0.0407	0.0232	-0.0026	-0.8011	-0.4866	-0.2736
0.50	0.0220	0.0864	-0.0584	-0.6587	-0.3037	-0.1775
0.60	0.1075	0.1679	0.1441	-0.4652	-0.0858	-0.0156
0.70	0.2169	0.2716	0.2545	-0.2158	0.1753	0.2120
0.80	0.3510	0.4004	0.3900	0.0931	0.4872	0.5055
0.90	0.5100	0.5556	0.5493	0.4636	0.8560	0.8648
1.00	0.6938	0.7372	0.7337	0.8971	1.2858	1.2899
1.50	1.9848	2.0259	2.0258	4.0320	4.4021	4.2022
2.00	3.8934	3.9348	3.9348	8.7994	9.1594	9.5194
2.50	6.4191	6.4606	6.4606	15.2073	15.5617	15.5617
5.00	28.3010	28.3425	28.3425	71.9030	72.2467	72.2467

TABLE I. The dimensionless chemical potential $\tilde{\mu}(\lambda) = (\hbar^2 / m v_0^2) \mu$ and the dimensionless groundstate energy $\epsilon(\lambda)$ determined exactly, from BCS theory through (3) and (4), and from plane-wave Hartree-Fock theory, all as a function of the dimensionless parameter $\lambda^{-1} = \hbar^2 \rho / m v_0$.

proximation is given by

$$\epsilon(\lambda) = \frac{2\lambda}{\pi} \left[\frac{\hbar^2}{mv_0} \right]^3 \int_{-\infty}^{+\infty} dk \ k^2 \left[1 - \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta^2}} \right] -2\lambda^{-1} - 8\lambda \left[\frac{\hbar^2}{mv_0} \right]^2 \Delta^2 .$$
 (5)

This and the chemical potential were calculated numerically, the results being listed in Table I. One sees that although the BCS results are exact in the two extremes $\lambda \rightarrow 0$ and $\lambda \rightarrow \infty$, and interpolate smoothly between the two limits, there is a sizeable discrepancy in the intermediate range of λ , particularly for the strong-coupling interval $0 < \lambda^{-1} < 1$. This may have significant implications for calculations in 2D and 3D Fermi liquids and in the extended Hubbard model.

To better illustrate this discrepancy we consider the (low-density) expansion of $\tilde{\mu}(\lambda) = (\hbar^2/mv_0^2)\mu(\lambda)$ and $\epsilon(\lambda)$ in powers of λ^{-1} for small λ^{-1} . Using the Gaudin equations one can show² that

$$\epsilon(\lambda) = -1 + \frac{\pi^2}{12} \lambda^{-2} + O(\lambda^{-3}) \quad (\text{exact}) \tag{6}$$

and from (2) we have

$$\widetilde{\mu}(\lambda) = \frac{1}{8} [\epsilon(\lambda) - \lambda \epsilon'(\lambda)] = -\frac{1}{8} + \frac{\pi^2}{32} \lambda^{-2} + O(\lambda^{-3})$$
(exact). (7)

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For the BCS theory the corresponding limiting forms are

$$\widetilde{\mu}(\lambda) = -\frac{1}{8} + \frac{1}{4}\lambda^{-1} + O(\lambda^{-2}) \quad (\text{as } \lambda \to \infty) \text{ (BCS)} \quad (8)$$

and

$$\epsilon(\lambda) = -1 + \lambda^{-1} + \frac{1}{2}\lambda^{-2} + O(\lambda^{-3}) \quad (\text{as } \lambda \to \infty) \text{ (BCS)} .$$
(9)

These contain terms in λ^{-1} not present in the exact expansions (6) and (7). The results are, however, far better than those for other mean-field theories where pairing is not included, for example the most general Hartree-Fock result⁹ (not shown) and the plane-wave Hartree-Fock (PWHF) result.

In summary the BCS ground-state energy (which coincides with the exact ground-state energy for both zero and infinite coupling and/or density) is moderately close to the exact energy for intermediate values of the coupling/density. It is exponentially close to the planewave Hartree-Fock (PWHF) approximation for weak coupling and/or high density and notably superior to both PWHF and most general Hartree-Fock (HF) (Ref. 9) for strong coupling and/or low density.

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