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Lowering of the Kinetic Energy in Interacting Quantum Systems

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Interactions never lower the ground state kinetic energy of a quantum system. However, at nonzero temperature, where the system occupies a thermal distribution of states, interactions can reduce the kinetic energy below the noninteracting value. This can be demonstrated from a first order weak coupling expansion. Simulations (both variational and restricted path integral Monte Carlo) of the electron gas model and dense hydrogen confirm this and show that in contrast to the ground state case, at nonzero temperature the population of low momentum states can be increased relative to the free Fermi distribution. This effect is not seen in simulations of liquid ^{3}He.

INTRODUCTION

It is a common assumption that the addition of interactions to a noninteracting quantum system will broaden the momentum distribution and increase the kinetic energy (proportional to the second moment of the momentum distribution). An intuitive understanding of this follows from perhaps the first example encountered in studying quantum mechanics, the particle in a box, where the kinetic energy scales as the box size L^{-2}. More generally the kinetic energy, given by the average curvature of the wavefunction, is expected to scale as the "localization length"$^{-2}$. Since interactions lead to a nonuniform density, i.e. increased "localization", the kinetic energy is expected to increase.

For condensed matter scientists, two well ingrained many body examples of this, illustrated in Fig. 1, are the broadening of the free Fermi ground state momentum distribution due to electron repulsion and the depletion of the zero momentum condensate in a strongly interacting Bose system such as ^{4}He [1]. For the homogeneous electron gas, Fig. 1a shows the promotion of low momentum states to higher momentum and the reduction in the step discontinuity at the Fermi surface [2]. Similarly Fig. 1b shows that the 100% condensation into the zero momentum ground state of a noninteracting Bose system is reduced to roughly 8% in ^{4}He with the rest going into an almost Gaussian distribution [3].

The proof of this assumption for systems at zero temperature is an immediate consequence of the ground state variational principle applied to the free particle Hamiltonian, H_0, which states that $K_0 = \langle\Psi_0|H_0|\Psi_0\rangle$ is minimized by Ψ_0, the true ground state wavefunction of H_0. Using any other wavefunction, such as the ground state, Ψ_G, for an interacting system, $H = H_0 + U$, leads to

$$K = \langle\Psi_G|H_0|\Psi_G\rangle \ \geq K_0 \ , \qquad (1)$$

demonstrating that the kinetic energy, K, of the interacting system is never lower than the free particle kinetic energy, K_0.

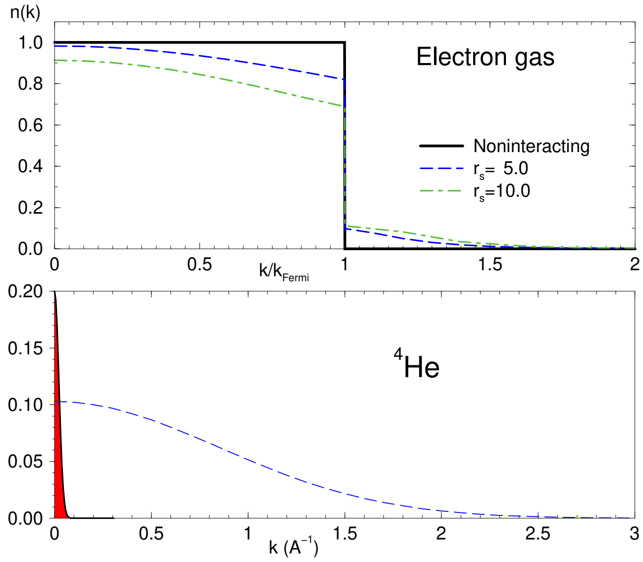

FIG. 1: Top figure: Broadening of the ground state electron gas momentum distribution at $r_s = 5$ (dashed line) and $r_s = 10$ (dot-dashed line) caused by interactions. r_s is the radius, in units of the Bohr radius, of a sphere containing one electron and in metallic elements at atmospheric pressure ranges from roughly 2 to 6. The unit discontinuity of the momentum distribution for the noninteracting system (solid line) at the Fermi surface is reduced by 28% and 42% respectively. Corresponding increases in the kinetic energy over the noninteracting case are 30% and 60%. Bottom figure: For ^{4}He at $T = 0$ and $P \approx 0$ roughly 92% of the zero momentum condensate (black vertical bar along y axis) in the noninteracting Bose system is promoted to higher momentum states (distribution given by dashed line) leading to a kinetic energy increase of over 14 K per particle.

This argument fails however, when generalized to nonzero temperature, T, where the system occupies a thermal distribution of energy eigenstates. From the Gibbs variational principle, the free energy functional,

$$F[\rho] = \mathrm{Tr}[H_0\rho] + k_B T \ \mathrm{Tr}[\rho \ln \rho] \ , \qquad (2)$$

takes its minimum value $F[\rho_0] = K_0 - TS_0$ for the equilibrium density operator $\rho_0 = e^{-\beta H_0}/\mathrm{Tr}[e^{-\beta H_0}]$ where $\beta = 1/k_B T$ and k_B is Boltzmann's constant. Any other normalized density operator, such as that for the interacting system, $\rho = e^{-\beta H}/\mathrm{Tr}[e^{-\beta H}]$, gives a higher value,

$$F[\rho] = K - TS \quad \geq \quad F[\rho_0] = K_0 - TS_0 \; . \tag{3}$$

The ground state inequality, Eq. 1, now generalizes to,

$$K \geq K_0 + T(S - S_0) \; . \tag{4}$$

Since interactions often increase order, the entropy S of the interacting system can be less than that of the noninteracting, S_0, and $S - S_0$ may be negative. This allows Eq. 4 to be satisfied while the ground state inequality, $K \geq K_0$, is not. In general, at nonzero temperature nothing forbids interactions from lowering the kinetic energy.

This kinetic energy lowering would only be observed in an intermediate range of temperatures since in the high temperature, classical limit, interactions only effect equilibration rates, not the final Maxwellian momentum distribution.

WEAK COUPLING LIMIT

Not only is this lowering theoretically possible, it can be shown to occur for a variety of weakly interacting physical systems using lowest order thermodynamic perturbation theory. The change in the Helmholtz free energy, F, to first order in the interaction potential is

$$F = F_0 + \langle U \rangle_0 \; , \tag{5}$$

where $\langle U \rangle_0$ is the potential averaged over the free particle configurations. Since the total energy is given by, $E = \partial(\beta F)/\partial\beta$, the first order change in the kinetic energy from Eq. 5 is

$$K_1 = \beta \frac{\partial \langle U \rangle_0}{\partial \beta} \; . \tag{6}$$

For a single component system of N particles with pair interaction, $V(r)$, the first order energy change reads,

$$\langle U \rangle_0 = N \frac{n}{2} \int g_0(r)\, V(r)\, dr^3 \tag{7}$$

where n is number density. The first order kinetic energy change

$$K_1 = -TN \frac{n}{2} \int \frac{\partial g_0(r)}{\partial T}\, V(r)\, dr^3 \tag{8}$$

depends on the temperature dependence of the free particle radial distribution function, $g_0(r)$.

As shown in Fig. 2, for both fermions and bosons $\partial g_0(r)/\partial T$ can be positive at all r leading to a kinetic energy decrease for repulsive interactions although for quite different reasons in the two cases. For fermions the increase of $g_0(r)$ with temperature is due to the filling in of the "Fermi hole", the region near the origin where due to the Pauli principle like spin particles are excluded. The size of this region is roughly the de Broglie thermal wavelength which is proportional to $1/\sqrt{T}$.

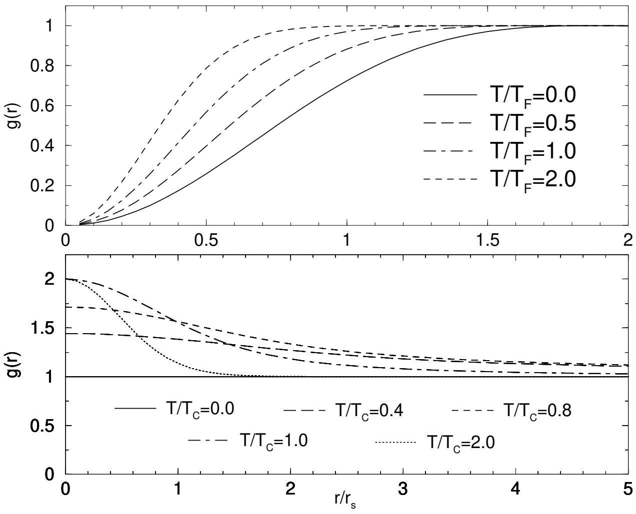

FIG. 2: Behavior of free fermion (top figure) and free boson (lower figure) radial distribution functions for indicated temperatures measured in terms of the Fermi temperature T_F or condensation temperature T_c respectively.

For noninteracting bosons at $T = 0$, all particles are in the zero momentum condensate and $g_0(r) = 1$. As the temperature increases particles are promoted from the condensate and $g_0(r)$ increases at all r for $T/T_c \leq (2/5)^{2/3}$, where T_c is the Bose condensation temperature, and thereafter at small r, reaching $g_0(0) = 2$ at $T = T_c$ [4, 5]. Since $T\partial g_0(r)/\partial T$ vanishes at $T = 0$, the ground state inequality, Eq. 1, is not violated.

The mechanism for the narrowing of the electron gas momentum distribution can be seen from the first order shift in the free electron energy levels [6],

$$\Delta\epsilon(\mathbf{k}) = -\frac{4\pi e^2}{\Omega} \sum_{\mathbf{k}' \neq \mathbf{k}} \frac{n_0(\mathbf{k})}{|\mathbf{k} - \mathbf{k}'|^2} \; . \tag{9}$$

The decrease of $n_0(\mathbf{k})$ with k leads to a larger lowering of the energy levels at smaller k and thus to a population redistribution and momentum distribution narrowing as demonstrated in Fig. 3.

SIMULATION RESULTS

For the electron gas, this weak coupling expansion applies only at very high densities, $r_s \lesssim 0.5$, and is of little use for realistic condensed matter densities. It is necessary to use more powerful quantum many body simula-

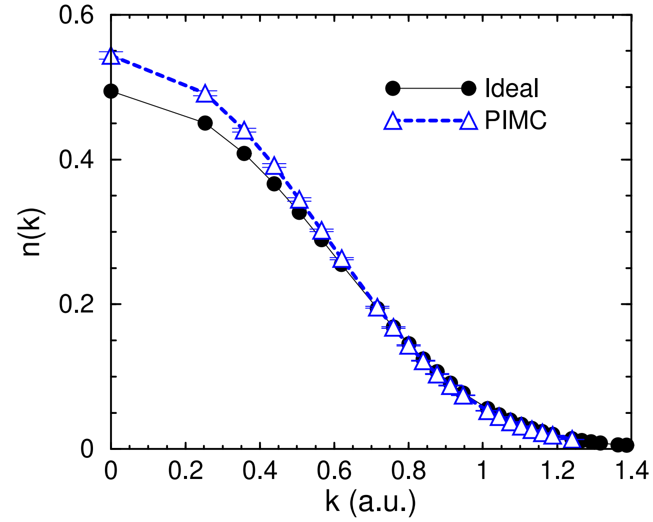

FIG. 3: Example of momentum distribution narrowing in the fully polarized electron gas at $r_s = 4$ and $T = T_{\mathrm{Fermi}}$ from simulations with 57 particles.

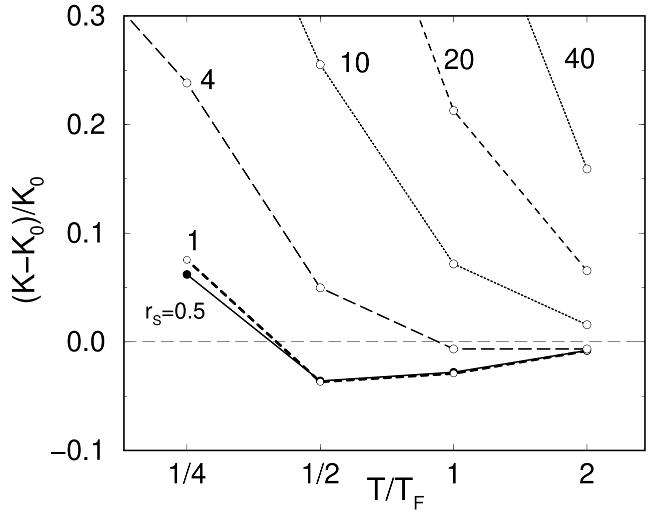

FIG. 4: Relative excess kinetic energy vs temperature for the unpolarized electron gas at indicated r_s values as calculated from PIMC simulations with 66 particles in the periodic cell.

tion methods. Two such methods, path integral Monte Carlo (PIMC) [7, 8] and a variational trial density matrix method (VDM) [9], have been used here to search for narrowing of the momentum distribution in a variety of fermion systems.

Liquid ^{3}He is a strongly coupled system. Due to its steeply repulsive short ranged interactions the weak coupling arguments of the preceding paragraphs do not apply. Restricted PIMC calculations using free particle nodes for ^{3}He at number density $n = 0.01636\text{Å}^{-3}$ and temperatures from 1 to 40 K show the kinetic energy to be more than 5 K above the noninteracting value. Narrowing of the momentum distribution is not found for this system.

For the electron gas model both restricted PIMC and VDM calculations find momentum distribution narrowing. The effect is small, with the relative decrease of the kinetic energy from its ideal value less than a few percent [10, 11], but well within the accuracy of the two methods. The computation of momentum distribution for fermions with PIMC (see Fig. 3) required extending the restricted path integral technique to simulations with open paths [12, 13].

Fig. 4 shows the difference in kinetic energy of the homogeneous electron gas for different densities and temperatures indicated by the degeneracy parameter T/T_{Fermi}. For densities corresponding to $r_s \lesssim 4$, a lowering of the kinetic energy with respect to the noninteracting value is found. The magnitude of the lowering increases with density (smaller r_s). The statistical uncertainty of these results was estimated at $r_s = 1$ and $T = T_{\mathrm{Fermi}}$ by a study of finite size effects (using 14, 38, 66, and 114 particles in the periodic simulation cell) and path discretization errors (using 16, 32, and 64 time steps) which gave $(K - K_0)/K_0 = 0.023 \pm 0.002$. The region of the effect, as predicted by PIMC simulations, is shown in the high temperature and density phase diagram in Fig. 5.

Simulations of dense hydrogen plasma [14] have also indicated kinetic energy lowering, which we confirmed and extended. We found a maximal lowering of $(K - K_0)/K_0 = 0.007 \pm 0.001$ for $r_s = 0.5$ and $T = T_{\mathrm{Fermi}}$. The magnitude is reduced compared to the electron gas because Coulomb interactions of electrons and protons counteract the entropic lowering. This also results in a reduction of the parameter region in the temperature and density plane for which the effect can be observed. However, in the limit of high density, the boundaries for the electron gas model and for hydrogen converge because interactions become weaker in the high density limit. Fig. 5 shows that the lowering region of hydrogen includes conditions near the core of the sun or other low mass stars [16] as well as on the compression path of inertial confinement fusion [15], indicating that hydrogen is a potential candidate for experimental verification of this effect.

CONCLUSIONS

Analytical and numerical arguments show that interactions can reduce the kinetic energy of a quantum system below the corresponding noninteracting value. The associated narrowing in the momentum distribution can potentially be verified experimentally. Prime examples are the Bose condensates in magnetic traps, in which the momentum distribution can be inferred by measuring the ex-

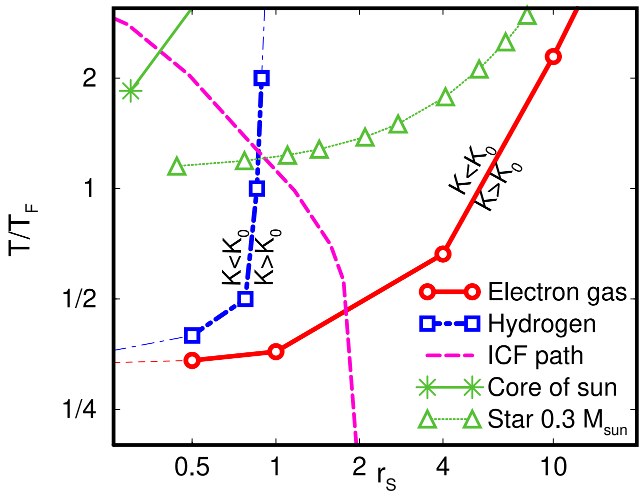

FIG. 5: Proposed region for momentum narrowing ($K < K_0$) in the unpolarized electron gas (area above the solid line) and in hydrogen plasma (area above the dot dashed line) as derived from PIMC simulations. The dashed line indicates the compression path of inertial confinement fusion [15]. The conditions near the core of the sun and a low mass star (0.3 solar masses) are also indicated [16].

pansion rates after the magnetic field has been switched off. Sufficiently accurate measurements of the momentum distribution could be used to provide information about the nature of the interactions of the trapped atoms.

Lowering of the kinetic energy was demonstrated in the homogeneous electron gas model, one of the fundamental models in condensed matter physics and a well studied example of a one-component plasma. Corrections to the noninteracting kinetic energy are always positive at zero temperature and vanish in the high temperature limit, which makes it counterintuitive to expect lowering at intermediate temperature. Research on the one-component plasma has focused more on the internal energy, pressure and correlation energy. However, the kinetic energy is relevant of our understanding of quantum systems and can be determined experimentally by measuring the momentum distribution.

The effect, previously indicated but left uninterpreted in dense hydrogen [14], is reconfirmed here. The arguments presented above suggest that the kinetic energy reduction should be present in weakly coupled systems with repulsive pair interactions. Simulation evidence for this effect was presented here only for Coulombic systems. More work is necessary to understand how these arguments apply to other systems and where the entropic reordering in the thermal population of states leading to a lower kinetic energy can best be observed experimentally.

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