How final-state effects were *really* calculated

The derivation of final-state broadening presented in the main text was physically intuitive but, like all heuristic arguments, involved a sleight of hand: The classical-trajectory concept was not derived from first principles. In practice. the theory of final-state effects is a very difficult many-body problem. Conventional perturbative expansion about the non-interacting ground state. a technique so successful in calculating the properties of' weakly interacting systems, is not a useful approach here because helium atoms interact at short distances through a steeply repulsive potential. However. alternatives to perturbation methods, such as the variational and Monte Carlo methods. are capable of handling strongly interacting systems and thus have been most successful in calculating ground-state properties of helium, including the momentum distribution *n(p)* and the pair-correlation function *g(r).*

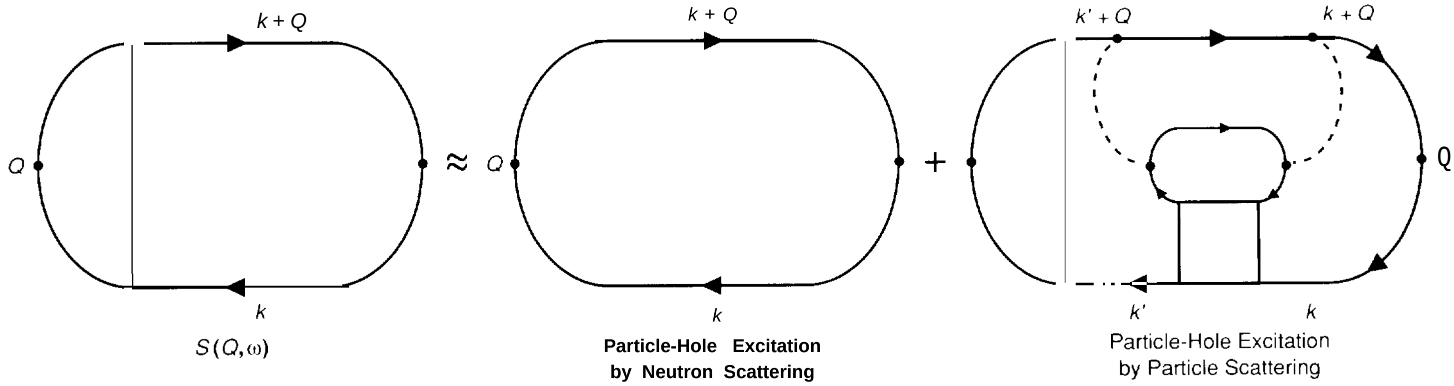
In order to test the ground-state results against neutron-scattering experiments, we need to calculate the dynamical response of the system to neutron scattering. Since we have an obvious interest in not repeating the considerable work involved in generating the ground-state results, we want to calculate the response by applying perturbation theory to the variational and Monte Carlo results for the ground state. However, conventional perturbation theory is again out of the question because the dynamical response also involves helium-helium interactions.

Before we present our solution to this problem, let's outline the starting point. We assume that neutron scattering at momentum transfer $h\,Q$ introduces, at time zero, a fluctuation about the ground state in the density of atoms with wave vector Q. By calculating the amplitude of that density fluctuation at a later time t and taking its Fourier transform, we can determine $S(Q, w)$, the observed scattering law. (Note that w is conjugate to t.) The density fluctuation is equal to a summation over all so-called particle-hole excitations about the ground state, that is, over all processes that add to the ground state an atom with wave vector $k + Q$ and remove from the ground state an atom with wave vector k.

In the impulse approximation we assume that the particle-hole excitations propagate freely without interacting with other atoms. Final-state effects, on the other hand, are due to interaction of the excitations with other atoms. Scattering of a particle and a hole creates more particle-hole excitations about the ground state. Although in principle an infinity of multiple scattering of a particle-hole pair can occur, the correlations in the ground-state wave function imply that only single additional particle-hole excitations need be considered. In effect, the correlations screen the steeply repulsive core interaction at short distances, rendering that interaction finite. After all, to minimize their energy in the ground state, the atoms tend to sit in the attractive part of the potential, far away from its steeply repulsive core. Thus the effective final-state interactions can be characterized by a small parameter. and perturbation theory can be used for systematic, controlled calculations.

The divergent terms in the perturbative expansion of $S(Q, w)$ involve all processes that transform a $(k + Q, k)$ particle-hole pair to a $(k' + Q, k')$ pair. To obtain finite results, those divergent terms must be explicitly resummed to all orders in the perturbation expansion. In practice. the summation is accomplished by defining a "projection superoperator." which acts in the Hilbert space of $(k + Q, k)$ particle-hole excitations about the ground state much as ordinary operators act in the Hilbert space

Neutron Scattering Law = Impulse Approximation + New Final-State-Effects Theory



NEW THEORY OF FINAL-STATE EFFECTS

The author approximates the neutron scattering law for helium as the sum of the impulse approximation and one additional scattering that accounts for final-state effects. Shown here are Feynman diagrams for that approximation. The Feynman diagram for the neutron scattering law represents the propagation of a particle-hole excitation that removes a particle of wave vector *k* from the ground state and adds to the ground state a particle of wave vector *k* + *Q*. Arrows denote the direction of momentum flow. Arrows pointing right denote particle lines; arrows pointing left denote hole lines. Only the particle lines carry high momentum. The hatched area denotes the exact result for *S(Q, w)* including all scattering of particles and holes. The Feynman diagram for the impulse approximation indicates that both particles and holes propagate without scattering. The Feynman diagram. for the final-state effects indicates that each particle scatters from another atom and creates a new particle-hole excitation. (Further scattering are possible but not included in the approximation.) The shaded square is the two-particle density matrix describing the correlations between the two holes in the ground state created by the two particle-hole excitations. The hole-hole correlations are related by sum rules to the pair-correlation function of the ground state. The dashed lines represent the two-particle t-matrix that describes particle scattering. Because the hatched area appears in the Feynman diagrams for both the neutron scattering law and the final-state effects, the scattering that transform a *(k + Q, k)* excitation to a $(k' + Q, k')$ excitation must be calculated self-consistently.

of quantum-mechanical states. The neutron scattering law then equals the expectation value of the projection superoperator, and calculations analogous to ordinary perturbation theory can be carried out in the superoperator Hilbert space. The effective interaction is the two-atom scattering matrix multiplied by a ground-state correlation function, which acts to screen the short-distance pathologies of the potential. Additional restrictions on the important scattering processes are obtained by noting that all *k* entering a two-particle density matrix must be characteristic of the ground-state wave function, as given by the momentum distribution, and that Q is much larger than those characteristic values.

After the above procedure is implemented, the neutron scattering law can be expressed as the sum of the impulse approximation and one additional scattering process. The accompanying figure shows the Feynman diagrams for the components of the sum. In the Feynman diagram for the one additional scattering process, the dashed line represents the t-matrix describing the scattering of two particles and the square represents the two-particle density matrix for the ground state. The latter matrix is a generalization of the correlation functions, such as g(r) and n(p), that characterize the ground-state wave function.

If we approximate the density matrix in terms of *g(r)* and *n(p)* in a way that satisfies sum rules and, since Q is large, use a semiclassical approximation for the *t*-matrix, then the final "Dyson" equation can be solved analytically. The result for the final-state broadening, *R(Y, Q),* is given by

$$R(Y, Q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \exp\left[iYx - \int_0^{|x|} \Gamma(x')dx' \right],$$

where

$$\Gamma(x) = \rho\pi \int_0^{\infty} db^2 \left(e^{2i\delta_b} - 1\right) g\left(\sqrt{x^2 + b^2}\right).$$

The phase shift δ_b is the semiclassical value for scattering at impact parameter b.

The above expression for *R(Y, Q),* which is somewhat more complicated than Eq. 14 in the main text, is the expression we have plotted in Fig. 11 of the main text and used in comparing theory with experiment. It is essentially the same as the familiar Wentzel-Kramers-Brillouin (WKB) classical-trajectory approximation taught in elementary quantum mechanics except that the potential, V (x), is replaced by an "optical potential," $\hbar^2 Q\Gamma(x)/m$ that accounts for all repeated scatterings from the same helium atom. The quantity $\hbar^2 Q\Gamma(\infty)/m$ is simply the forward scattering t-matrix for the scattering of two helium atoms. The approach taken here is required for helium, a strong scatterer, but it is satisfying that the result reduces to the WKB approximation in the limit of a weak scatterer. ■