Calculating energy shifts in terms of phase shifts

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Abstract

We clarify the relation in interacting systems, and in particular ultracold atomic gases, between energy shifts arising from interparticle interactions and scattering phase shifts. A principle result of this paper is an expression for the energy levels of an atom in a container of arbitrary shape in the presence of a short-range scatterer, generalizing the result of Lüscher to containers of shapes other than cubic. We show that, while the energy shifts for a spherical container are under many conditions proportional to the phase shift, those for a cubic container have a more complicated structure. The general relation is extended to problems of particles in traps with smoothly varying potentials, including, e.g., the interaction of a small neutral atom with a Rydberg atom. Finally, we discuss why, even though individual energy levels are very sensitive to boundary conditions, the energies of many-body systems are not.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Feshbach resonances in dilute atomic gases allow unprecedented control of the low-energy pairwise scattering amplitude [1]. Most recently, interest has focussed on strong interaction effects in broad and narrow resonances [2], in which energy shifts are analysed in terms of two-body scattering phase shifts [3]. Such interaction effects are described by theoretical analysis at the two-body level, in which the relative motion of two atoms is contained in a sphere, and the energy change of the system due to interactions is calculated by tracing the change of the energy levels as the s-wave phase shift \( \delta \) varies. A similar analysis has been applied to understand the equation of state of fermion gases on the ‘upper branch’ on the BEC side of a Feshbach resonance [4]. However, questions remain: e.g., what is the explicit relation between energy shifts and phase shifts; and how does the relation depend on boundary conditions? Modern cold atom physics enables these questions to be explored in considerable theoretical and experimental details.
length between the particles [12, 13]. From a quite different perspective, Lüscher [14] derived a formula for the energies of bound states of two particles in a box (with periodic boundary conditions) that is enjoying use in particle physics to extract scattering properties of elementary particles from lattice calculations of energies [15].

We derive a general result for the energy eigenvalues of a particle in a container of arbitrary shape in the presence of a short-range scattering centre in terms of the s-wave scattering phase shift and the eigenstates in the absence of the scatterer. The result, a generalization of a result of Lüscher [14] for the case of a cubic container, clarifies the relation between energy shifts arising from interparticle interactions and the corresponding scattering phase shifts. For simplicity, we focus on energies low enough that only s-wave scattering from the scatterer need be taken into account. In the presence of a short-range scatterer, the energy shifts for a particle in a spherical box are linear in the s-wave phase shift, \( \delta \), and not a trigonometric function of \( \delta \), such as the real part of the scattering amplitude. However, in the case of a particle in a more generally shaped container, with more complicated boundary conditions on the wavefunctions, we find that the energy shifts depend implicitly on \( \tan \delta \) (see equation (15)). In particular, as we will see explicitly for a particle in a cubic container, while the energy shifts are approximately linear in \( \delta \) for small \( \delta \), the slope of the shift varies from state to state. In the many-body problem, the energy shift is linear in an effective scattering phase shift that takes into account effects of the medium [16]; we comment on the reason for such simple behaviour.

We begin, in section 2, by reviewing the energy shifts of a particle in a spherical container. We then go on to derive a general expression for the energy of a single particle moving in a container of arbitrary shape in the presence of a scattering centre. The energy is obtained as an implicit function of the s-wave phase shift of the scatterer and the eigenfunctions of the one-particle problem in the absence of the scatterer. In section 3, we discuss the applications of our result to situations such as atoms in traps and Rydberg atoms in which the particle moves in a potential that varies smoothly in space, rather than in a container with infinitely repulsive walls. We point out that the effects of the boundary conditions result in the difference between the single-particle case and many-body systems. We take \( \hbar = 1 \) throughout.

2. Energy shifts

2.1. Spherical container

To set the stage, we first review the relation of the energy shifts and s-wave scattering phase shifts for the familiar problem of a particle of mass \( M \) interacting with a short-range potential \( v(r) \) at the centre of a hard-walled spherical container whose radius, \( R \), is much larger than the range, \( b \), of the potential. At low energies, scattering is predominantly s-wave, even if the potential is not spherically symmetric, and may be parametrized in terms of the s-wave phase shift, \( \delta \). Consequently, at low energies, eigenstates of the energy are also eigenstates of the angular momentum, and we characterize the states by the value of the angular momentum. In the low-energy limit, states other than s-wave are unaffected by the scatterer. For \( v(r) = 0 \), the single-particle eigenenergies for s-wave states are \( E_\nu = k_\nu^2/2M \), with \( k_\nu = v\pi/R \), and \( \nu = 1, 2, 3, \ldots \), with eigenfunctions

\[
\psi_\nu(r) = \frac{1}{\sqrt{2\pi R}} \sin(k_\nu r). \tag{1}
\]

In the presence of the scatterer, the eigenfunctions at points beyond the range of the potential become

\[
\psi_\nu'(r) = A_1 \frac{\sin(k_\nu' r + \delta(k_\nu'))}{r}, \tag{2}
\]

where \( A_1 \) is a normalization constant. The hard-wall boundary condition implies that

\[
k_\nu' R + \delta(k_\nu') = v\pi, \tag{3}
\]

or

\[
\cot(k_\nu' R) = -\cot(\delta(k_\nu')). \tag{4}
\]

The shift in the wavevector, \( \Delta k_\nu \equiv k_\nu' - k_\nu = -\delta(k_\nu')/R \), is linear in the phase shift. Without loss of generality, we may take \( \delta \) to lie in the range \( -\pi/2 \) to \( \pi/2 \), since an increase of \( \delta \) by \( \pi \) takes one from a given state in the sphere to the next higher state. Since beyond the range of the potential \( \psi_\nu'(r) \) is a solution of the Schrödinger equation with zero potential, the corresponding eigenenergies are \( E_\nu = k_\nu^2/2M \), and the shifts in the energies due to the interaction are

\[
\Delta E_\nu = \frac{k_\nu^2 - k_\nu'^2}{2M} = -\frac{2\pi \delta(k_\nu')}{Mk_\nu} \left( 1 - \frac{\delta(k_\nu')}{2k_\nu R} \right) |\psi_\nu(0)|^2. \tag{5}
\]

The term quadratic in \( \delta \) may be neglected if \( \delta \ll 1 \), since \( k_\nu R \gg 1 \). Even for resonant scattering, \( \delta \sim \pi/2 \), the quadratic term may be neglected for states with many nodes (\( k_\nu R \gg 1 \)). The energy shift is then given by

\[
\Delta E_\nu \approx -\frac{2\pi \delta(k_\nu')}{Mk_\nu} |\psi_\nu(0)|^2, \tag{6}
\]

which is linear in the phase shift\(^5\). The energy of the state \( \psi' \) must be determined self-consistently, since \( \delta \) depends on energy. But if \( R^{-1}(|d\delta/dk|) \ll 1 \) one may replace \( k_\nu' \) by the wave number of the state in the absence of the scatterer, \( k_\nu \).

In the limit \( k \to 0 \), away from a scattering resonance, \( \delta \to -k a_s \), with \( a_s \) the s-wave scattering length. Then equation (5) gives

\[
\Delta E(k) = \frac{2\pi a_s}{M} |\psi(0)|^2. \tag{7}
\]

\(^5\) This result might be thought at first sight to contradict standard many-body theory for bulk systems, in which one commonly identifies excitation energies with zeroes of the real part of the inverse of the single-particle propagator, i.e. the solution \( E \) of the equation \( E - k^2/2m - \text{Re}\Sigma(k, E) = 0 \), where \( \Sigma \) is the self energy. This identification would imply that for small \( \Sigma \) the energy shift is proportional to \( \text{Re}\Sigma(k, k^2/2m) \). For example, for scattering by impurities the self-energy is given to first order in the impurity density \( n \), \( T(k, E) \) [17], where \( T \) is the scattering matrix for forward scattering, given in terms of the phase shift by \( \pi i e^{2im\delta}/1/mk \); therefore, one would conclude that the excitation energy is proportional to \( (\sin 2\delta)/k \). The difference with equation (5) can be traced to the fact that the excitation energies that naturally appear in expressions for thermodynamic quantities (the statistical quasiparticle energies) are different from those obtained from the poles of propagators [18].
When this result is used to write the interaction energy of two particles of mass \(m \), \(M \) becomes the reduced mass and the effective (pseudopotential) interaction between the particles becomes

\[
V_{\text{eff}}(\mathbf{r} - \mathbf{r}') = \frac{4\pi a_s}{m} \delta(\mathbf{r} - \mathbf{r}').
\]

(8)

2.2. Arbitrary container

We now turn to establishing, for a particle of mass \(M \) interacting with a short-range central potential in a container of arbitrary shape, the relation between the energy shifts of the particle and the s-wave scattering phase shift. We consider a particle interacting with a scatterer located at some point within the container, which we take to be \(r = 0 \). We assume that the potential \(v(\mathbf{r})\) due to the scatterer vanishes for \(r > b \), the range of the potential, and that the characteristic dimension of the container, \(\lambda \), is much larger than \(b \). We consider energies \(E \) sufficiently low that only s-wave scattering is important. We denote the eigenfunction \(\psi_s(\mathbf{r})\) for energy \(E = k^2/2M \) by \(\psi_s^r(\mathbf{r})\) for \(r < b \) and \(\psi_s^r(\mathbf{r})\) for \(r > b \). For \(r \ll \lambda \), \(\psi_s^r(\mathbf{r})\) may be expanded in terms of spherical waves as

\[
\psi_s^r(\mathbf{r}) = A_2 \left[ \frac{\sin(kr)}{kr} + \frac{\cos(kr)}{kr} + \sum_{l=1}^{\infty} \sum_{m=-l}^{l} a_{lm} j_l(kr) Y_{lm}(\theta, \phi) \right],
\]

(9)

where \(j_l\) is the spherical Bessel function, the \(a_{lm}\) are expansion coefficients and \(A_2\) is a normalization constant. In the final sum, terms proportional to spherical Neumann functions \(n_l\), which are singular for \(r \to 0\), have been omitted, since we assume that only s-wave scattering is important, and consequently the wavefunction for other partial waves must be finite for \(r \to 0\). Thus, asymptotically, in the region \(b < r \ll 1/k\),

\[
\psi_s^r(\mathbf{r}) = A_2 \left[ \frac{\tan \delta}{kr} + 1 + O(kr) \right].
\]

(10)

To derive the energy of the state \(\psi_s(\mathbf{r})\), we re-express the wavefunction in terms of the single-particle eigenstates \(\{\phi_n(\mathbf{r})\}\) for \(v(\mathbf{r}) = 0\), with energy \(E_n\), as follows. The single-particle Green function for \(v(\mathbf{r}) = 0\), describing propagation of a particle from the origin to \(\mathbf{r}\), is

\[
G_k(\mathbf{r}, 0) = \sum_n \frac{\phi_n(\mathbf{r})\phi_n^*(0)}{E_n - E};
\]

(11)

\(G_k(\mathbf{r}, 0)\) satisfies the equation

\[
\frac{1}{2M} (\nabla^2 + k^2) G_k(\mathbf{r}, 0) = -\delta(\mathbf{r}),
\]

(12)

which shows that \(G_k(\mathbf{r}, 0)\) satisfies the Schrödinger equation for \(\psi_s^r(\mathbf{r})\) when \(r \neq 0\). Thus, outside the range of the potential, \(G_k(\mathbf{r}, 0)\) satisfies the Schrödinger equation and in addition satisfies the same boundary conditions as the wavefunctions \(\phi_n\) at the walls of the container for any boundary condition that is linear in the wavefunction. Equation (12) implies that \(G_k(\mathbf{r}, 0) = M/2\pi k^2\) for \(kr \ll 1\). In fact for \(r > b\)

\[
\psi_s^r(\mathbf{r}) = \frac{2\pi A_2 \tan \delta}{Mk} G_k(\mathbf{r}, 0),
\]

(13) as we can see by the following argument [14]. The function

\[
\chi_s(\mathbf{r}) = \psi_s^r(\mathbf{r}) - \frac{2\pi A_2 \tan \delta}{Mk} G_k(\mathbf{r}, 0)
\]

(14)

is regular everywhere inside the container and according to the equations obeyed by \(\psi_s\) and \(G_k\) is an eigenfunction with eigenenergy \(E\) for \(v(\mathbf{r}) = 0\). But for \(v(\mathbf{r}) = 0\), \(\chi_s(\mathbf{r})\) must also be an eigenfunction of the unperturbed Hamiltonian \(H_0\); but if the shifted energy \(E\) is not part of the spectrum of \(H_0\), \(\chi_s(\mathbf{r})\) must vanish. (The more complicated case when \(E\) is also an eigenvalue of \(H_0\) is discussed in [14].)

Matching the singular and nonsingular parts in equations (10) and (13) for \(kr \ll 1\), we obtain an implicit expression for the energy of the state:

\[
\frac{k}{4\pi} \cot \delta(k) = \lim_{r \to 0} \left[ \sum_n \frac{1}{2M} \frac{\phi_n(\mathbf{r})\phi_n(0)}{E_n - E} - \frac{1}{4\pi r} \right],
\]

(15)

since non-s-wave contributions vanish in the limit \(r \to 0\). Equation (15) shows the eigenenergies in the presence of the potential, is one of the main results of this paper. When the potential strength tends to zero, \(E\) approaches an eigenvalue \(E\) of \(H_0\); accordingly, equations (11) and (13) imply that \(\psi_s(\mathbf{r})\) approaches the state

\[
\psi_s^r(\mathbf{r}) = C \sum_{E_n = E} \phi_n(\mathbf{r}) \phi_n^*(0),
\]

(16)

where the sum is over all possible degenerate states of energy \(E\), and \(C = (\sum_{E_n = E} |\phi_n(0)|^2)^{-1/2}\) is the normalization constant. By construction, \(\phi_s^r(\mathbf{r})\) has a nonzero s-wave component, i.e. \(\phi_s^r(0) \neq 0\) if not all \(\phi_s^r(0)\) equal zero. The remaining states \(\phi_s^r(\mathbf{r})\) in the subspace spanned by the states with \(E_n = E\) vanish at \(\mathbf{r} = 0\), as we now show. Since these states are energy eigenstates in the absence of the scatterer, we may write \(\phi_s^r(\mathbf{r}) = \sum_{E_n = E} c_n \phi_n(\mathbf{r})\). The integral \(\int d\mathbf{r} \phi_s^s(\mathbf{r}) \phi_s^s(\mathbf{r})\) by orthogonality is zero if \(s \neq \bar{s}\); inserting equation (16) and the expansion for \(\phi_s^r(\mathbf{r})\) in the integral, one finds \(\int d\mathbf{r} \phi_s^s(\mathbf{r}) \phi_s^s(\mathbf{r}) = C \sum_{E_n = E} c_n \phi_n(0) \phi_n(0) = C \phi_s^s(0) = 0\). Therefore, the \(\phi_s^s(\mathbf{r})\) for \(s \neq \bar{s}\) vanish at the origin and these states will be unaffected when the scatterer is introduced.

For \(k \to 0\), away from a scattering resonance, the left-hand side of equation (15) becomes \(-1/4\pi a_s\), and so for \(a_s\) small compared with a characteristic dimension of the container, \(E\) must be very close to an unperturbed eigenenergy \(E\). Changing the order of the limit \(r \to 0\) and summation in equation (15), we obtain

\[
\Delta E = E - \mathcal{E} = \frac{2\pi a_s}{M} |\phi_s(0)|^2;
\]

(17)

thus, the result (7) found in a sphere holds for more general geometry.

More generally, for non-zero \(k\), the energy shift is not directly proportional to the phase shift. In the case of a spherical container, substitution of equation (1) into equation (15) yields \(\text{cot}(kr) = -\cot \delta(k)\), from which the linear result (5) between the energy shift and the phase shift follows. For an arbitrary container, however, equation (15) does not reduce to a simple relation between \(k\lambda\) and \(\delta(k)\); when \(\lambda \to \infty\),
\[ \Delta E_n = |\phi_0(0)|^2 f_n(\text{cot} \delta(k_n))/k_n \] with the dimensionless function \( f_n \) dependent on the level \( n \).

This behaviour is illustrated for the case of a cubic box of side \( L \), with periodic boundary conditions, the problem addressed by Lüscher [14]. The complications compared with the case of a spherical box arise because the rotational symmetry of the container is different from that of s-wave states which are affected by the scattering potential, and consequently different partial waves are mixed.

In the absence of the scatterer, the states are simply

\[
\phi_p(r) = \frac{1}{\sqrt{L^3}} e^{i p r}, \tag{18}
\]

where \( p = \{p_x, p_y, p_z\} = (2\pi/L)\{l_x, l_y, l_z\} \) with \( l_x, l_y, l_z = 0, \pm 1, \pm 2, \ldots \). As before, we consider only the s-wave contribution to the interaction, and from equation (15) find [14]

\[
\frac{k}{4\pi} \cot \delta(k) = \lim_{r \to 0} \left[ \frac{1}{L^3} \sum_p e^{i p r} \frac{p^2 - k^2}{L^3} - \frac{\Lambda}{4\pi} \right]. \tag{19}
\]

A relation similar to equation (19) is more useful for simulations on a lattice [15]:

\[
\frac{k}{4\pi} \cot \delta(k) = \frac{1}{L} \sum_{|p| < \Lambda} \frac{1}{p^2 - k^2} - \frac{\Lambda}{4\pi}, \tag{20}
\]

where \( \Lambda \) is the momentum cutoff on the lattice. To derive equation (20), we note that in the limit \( r \to 0 \) the terms in the sum in equation (19) for \( |p| > \Lambda \) and \( k \ll \Lambda \) can be written as

\[
\frac{1}{L^3} \sum_{|p| > \Lambda} e^{i p r} = \int_0^\Lambda \frac{d^3 p}{(2\pi)^3} \frac{\rho(r)}{p^2} = \frac{1}{4\pi} - \frac{\Lambda}{4\pi}, \tag{21}
\]

where \( \rho(r) = \frac{\sqrt{\frac{1}{2}}}{\sqrt{2\pi}} \frac{e^{-r^2/2}}{\sqrt{2\pi}} \) and the energy shift obeys equation (17). Whereas the shift in \( k \) for a sphere is linear in \( -\delta \), for a cube it is only approximately linear in \( -\delta \), as we see from figure 1, which gives a plot of \( k \) (panel (a)) and \( E \) (panel (b)) versus \( -\delta \) for the first few eigenstates, calculated from equation (20). When \( \delta \) is small (except in the ground state),

\[ k/L/2\pi \approx k_i L/2\pi - \alpha_i \delta, \tag{22} \]

where \( E = k_i^2/2M \) is the eigenenergy in the absence of the scatterer, and from equation (20), \( \alpha_i = D_i/(k_i L)^2 \), with \( D_i = \sum_p \delta_{p^2, k_i^2} \) the degeneracy of the level \( E \). Therefore, \( \Delta k'_i L/2\pi \approx -\delta D_i/(k_i L)^2 \) for small \( \delta \), where \( \Delta k'_i = k'_i - k_i \). The linear relation is valid only for small \( \delta \), but with a slope which varies with the eigenstate of the cubic box.

The different dependences of \( k \) and \( E \) on \( \delta \) for cubic and spherical boxes are due solely to the different boundary conditions. The information on the boundary conditions is encoded in equation (15) through the unperturbed eigenvalues and eigenfunctions, while the effect of the short-range potential is taken into account via \( \delta \); in an arbitrary container, the energy change is a function of \( \cot \delta \) but the exact form of the function is determined by the boundary conditions.

We now summarize the salient results of this section. When the energies of states of a particle in the container in the absence of the scatterer are degenerate, one state, shown explicitly in equation (16), does not vanish at \( r = 0 \), while all other orthogonal states in the degenerate manifold vanish at \( r = 0 \). For weak scattering, \( |\delta(k)| \ll \pi \), the energy shift of the first state is given by equation (17) while the shift of the other states vanishes. For stronger scattering, it is necessary to solve equation (15) to derive the energy shift. The energy shift \( \Delta E \) given in equation (17) is reproduced by the expectation value of the effective interaction [19]:

\[
V_{\text{eff}}(r) = \frac{2\pi a_s}{M} \delta(r), \tag{23}
\]

in the unperturbed state, \( \phi_n \). The coefficient of the effective interaction of two particles of mass \( m \), is, as before, \( 4\pi a_s/m \).

One should note that the effective interaction (23) is not useful for calculating the perturbed wavefunction, \( \psi_r(r) \), outside the range of the potential in terms of a boundary condition at the origin. Here, one needs rather to employ the pseudopotential [7],

\[
V_p(r) = -\frac{2\pi}{Mk} \frac{\delta}{dr} \frac{\delta}{dr} r, \tag{24}
\]

in the Schrödinger equation

\[
\left(-\frac{\nabla^2}{2M} + V_p(r)\right) \psi_r(r) = \frac{k^2}{2M} \psi_r(r). \tag{25}
\]
The solution is clearly equation (9). The present discussion is readily generalized to higher angular momentum, with a pseudopotential involving higher derivatives of the wavefunction [20].

3. Discussion

3.1. External potentials that vary slowly in space

So far we have considered containers in which the potential is zero outside the range of the scatterer. The results may be extended to particles in a potential, \( V(r) \), such as in an atomic trap. If the scatterer is at point \( r_s \), the Green function for the particle in the potential satisfies the equation

\[
\left[ -\frac{1}{2M} \left( \nabla^2 + k^2 \right) + V(r) - V(r_s) \right] G_k(r) = \delta(r - r_s),
\]

where \( k^2 = 2M[E - V(r_s)] \). Provided \( V(r) - V(r_s) \) is small compared with other energy scales in equation (26) at distances from the scatterer of the order of the range of the potential, the arguments of section 2 still hold, with the origin shifted to \( r_s \). Explicitly, the condition is that \( |V(r) - V(r_s)| \ll M/b^2 \) for \( |r - r_s| \ll b \), in addition to the usual one \( kb \ll 1 \), where \( b \) is the range of the scattering potential (not \( V(r) \)). Equation (15) thus holds for this more general case, provided the \( \phi_n \) are taken to be the eigenfunctions including the effects of the potential \( V(r) \).

The general result (15) can be applied to calculate the effective potential between a Rydberg atom and a small neutral atom. In the absence of the neutral atom, the eigenstates \( \phi_n(r) \) for the outermost electron are hydrogenic wavefunctions for the Coulomb potential \( V_c(r) \) exerted by the ion, where we take the nucleus to be at the origin. We place the neutral atom at position \( r_s \), of magnitude much larger than \( a_0 \) (the Bohr radius). The eigenenergies \( E \) of the outermost electron of the Rydberg atom are functions of \( r_s \), and thus act as an effective potential between the neutral and Rydberg atoms.

As a consequence of the electron’s interaction with the neutral atom, the wavefunction of the electron in the Rydberg atom acquires a form near \( r = r_s \) that corresponds to an s-wave phase shift \( \delta(k) \). Thus, from equation (15), the effective potential \( E(r_s) \) is determined by

\[
k = \frac{2\pi}{4\pi} \cot(\delta) = \lim_{r \to r_s} \frac{\phi_n(r)\phi_n^*(r_s)}{2m_e E_n - E(r_s)} - \frac{1}{4\pi |r - r_s|},
\]

where \( k = \sqrt{2m_e[E - V_c(r_s)]} \) is the scattering wavelength and \( m_e \) is the electron mass. The sum over \( n \) includes both discrete and continuum states. Solving this equation is an alternative route to the results of [9] for the interaction of a neutral atom with a Rydberg atom. When applied to the problem of two particles in a harmonic potential interacting via a short-range potential, equation (27) reproduces the result of [10].

3.2. Comparison with many-body systems

A striking feature of calculations of many-body systems is that energies of states and, more generally, thermodynamic quantities have a simple behaviour as a function of the phase shifts for two-body scattering, or of the generalization of the phase shift to allow for the effects of the medium [6, 18, 21]. As a simple example, we describe the interaction contribution \( \Omega_{int} \) to the thermodynamic potential of an interacting Fermi gas with two components in the ladder approximation, as in [22]. With effects of two-body bound states neglected, the result is [16]

\[
\Omega_{int} = V \int \frac{d^3p}{(2\pi\hbar)^3} \frac{d^3p'}{(2\pi\hbar)^3} f_p f_p' U_{eff}(p + p', \xi_p + \xi_{p'}),
\]

where \( f_p = 1/\exp(\xi_p/T) + 1 \) is the Fermi function, \( \xi_p = p^2/2m - \mu \), \( \mu \) is the chemical potential, \( V \) is the volume of the system and \( T \) is the temperature (we use units in which the Boltzmann constant is unity). Equation (28) has the form expected in the Hartree–Fock approximation for an effective two-body interaction \( U_{eff} \), which is given by

\[
U_{eff}(q, \omega) = \frac{\delta(q, \omega)}{\text{Im}\Pi(q, \omega)},
\]

where the phase shift in the medium is defined by

\[
\delta = \arctan \left( \frac{U_0 \text{Im} \Pi}{1 - U_0 \text{Re} \Pi} \right);
\]

in the absence of many-body effects this expression reduces to the usual result for a two-body system. Here, \( U_0 \) is an effective two-body contact interaction and

\[
\Pi(q, \omega) = \int \frac{d^3p}{(2\pi\hbar)^3} \left( \frac{1 - f_0/2 + f_{q/2} - f_{q/2} - f_{q/2}}{\omega - p^2/m - q^2/4m + 1} + \frac{1}{p^2/m} \right)
\]

is the regularized two-particle propagator. This result, and others like it [23]6, show that shifts of the energy and of thermodynamic potentials are linear in the phase shifts for many-particle systems.

The reason for the energy of many-body systems being relatively insensitive to the shape of the container, unlike in the single-particle problems discussed above, is that, even though individual single-particle energy levels may be sensitive to the boundary condition, the energy of a many-body system is a sum of the energies of many single-particle states. Repulsion between single-particle levels due to mixing via the scattering potential results in some levels being pushed up and others pushed down, but for a many-body system there is a large degree of cancellation between the individual contributions and the total energy turns out to be a rather smooth function of the interaction strength. This behaviour is exemplified by atomic nuclei, for which the total energy is given to a good approximation by the liquid drop model, with shell corrections, due to the finite size of the nucleus, being relatively small.

### Footnotes

6 Analogous results for particle–hole scattering were used in [24].
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