II. TWO-BODY INTERACTION (GASES) AND SHORT-RANGE UNIVERSALITY

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In the following, we will look at the problem of interacting Bosons, mainly with the aim to describe the experimens of Bose-Einstein condensation of alcaline atoms in trapped systems, focusing on the dilute gas system. Let us assume that the mean particle distance, $n^{-1/3}$ (in three dimensions, n is the number density), is large compared to the range, R_e, of the interparticle interaction $nR_e^3 \ll 1$. Let us assume a typical situation of a gas where the distance of all particles remains of order $n^{-1/3} \gg R_e$. Let us consider the many-body ground-state wave function for this configuration, $\Psi_0(\mathbf{r}_1, \ldots, \mathbf{r}_N)$, and approach the two particles labeled by 1 and 2 arbitrarily close to each other, $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2| \to 0$. For distances smaller than $\mathbf{R}_e$, the particles enter the region where the interparticle interaction is non-vanishing. Since our wave function has to satisfy the Schrödinger equation, we write [1]

$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \ldots, \mathbf{r}_N) \to \phi(\mathbf{r}_1, \mathbf{r}_2)\widetilde{\Psi}_0(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4, \ldots, \mathbf{R}_N), \quad r_{12} \to 0, \quad r_{ij} \gg R_e \text{ for } i, j > 2 \tag{1}$$

where $\phi(\mathbf{r}_1, \mathbf{r}_2)$ is a solution of the two-body problem such that $\widetilde{\Psi}_0$ remains a smooth function when $\mathbf{r}_1 \to \mathbf{r}_2$ on the scale of $n^{-1/3}$, e.g. independent of R_e. As long as processes involving 3 particle collisions (whose probability is very small due to the reduced phase-space density) can be neglected, our N body problem should be entirely described in terms of the solution of the two-body problem.

Some time will therefore be spend with the two-body problem. Many properties of Bose condensates can be quantitatively explained by a simple non-linear Schrödinger equation, the Gross-Pitaevskii equation. However, in the non-linearity enters the scattering length, and not the bare potential. For analytical calculations, zero-range pseudo-potentials are quite useful.

Outline

- Problem of scales in an interacting gas:
  typical range of interaction much smaller than mean interparticle distance ($a \ll n^{-1/d}$)
  two-particle collisions almost "separate" from N-body problem
- How to characterize collisions without knowing the explicit interparticle potential, $v(r)$?
  discuss scattering cross section, scattering amplitude, phase shifts
- calculation of phase shifts for given potential, discussion of scattering properties
- (short-range) universal behavior of many-body systems
- inverse problem: pseudopotential for simplified calculations, given the asymptotic scattering properties (phase shifts) what is the simplest/best adapted potential for our calculations?

A. Interacting Particles: the two-body problem

1. *Formal solution*

In order to understand the N-body problem, we need some basic concepts and results from quantum scattering theory concerning simple two-body collisions. Quite generally, we can assume that the interaction potential between two particles, $V(\mathbf{r}_1, \mathbf{r}_2) = V(|\mathbf{r}|)$, depends only on the relative coordinate, $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$. We further assume, that the external potential also seperates in relative, and center-of-mass coordinates, so that the complete Hamiltonian of the two particles writes

$$H_{12} = H_{cm} + H_0 + V(|\mathbf{r}|) \tag{2}$$

$$H_0 = -\frac{\hbar^2}{2m_r}\Delta_{\mathbf{r}} \tag{3}$$

where $m_r = m/2$ and H_{cm} depends only on the center-of-mass coordinates $\mathbf{r}_{cm} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, e.g. a homogeneous system, or a system in an external harmonic potential. The wavefunction therefore separates

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_{cm}(\mathbf{r}_{cm})\phi(\mathbf{r}) \tag{4}$$

and we will concentrate on $\phi(\mathbf{r})$ in the following, which contains all collisional properties and is determined by

$$(H_0 + V)|\phi\rangle = E|\phi\rangle \tag{5}$$

together with the boundary conditions on $|\phi\rangle$.

For a formal solution, we rearrange the Schrödinger equation

$$(E - H_0)|\phi\rangle = V|\phi\rangle \tag{6}$$

Starting from the known free solution, $|\phi_0(E)\rangle$, which satisfies the homogeneous equation,

$$(E - H_0)|\phi_0\rangle = 0 \tag{7}$$

we would like to obtain the full solution of Eq. (6) by inverting the operator $E - H_0$. However, since for a continuous, infinite system, scattering states will have the same energy than the free states, we cannot invert $(E - H_0)^{-1}$, but we introduce a small imaginary offset

$$|\phi^{\pm}(E)\rangle = |\phi_0(E)\rangle + \frac{1}{E - H_0 \pm i\epsilon} V|\phi^{\pm}(E)\rangle \tag{8}$$

with infinitesimal $\epsilon > 0$. As we will see, the wave functions $\phi^{\pm}$ describe different sets of solutions. Eq. (8) is called Lippmann-Schwinger equation.

2. Scattering amplitude and cross section (measurable quantities)

The interatomic (or molecular) potential is not necessarily known with high precision. Therefore, theoretical results on the N-particle problem should be expressed in terms of measurable quantities. Here we analyse the scattering problem in terms of quantities which may be obtained directly from scattering experiments, e.g the scattering amplitude and the cross section.

Let us start analyzing the Lippmann-Schwinger equation, Eq. (8), in position space, using plane waves.

$$\phi^{\pm}_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \int d^3\mathbf{r}' G^{\pm}(\mathbf{r} - \mathbf{r}'; E = k^2/2m_r) V(r') \phi^{\pm}_{\mathbf{k}}(\mathbf{r}') \tag{9}$$

where

$$G^{\pm}(\mathbf{r} - \mathbf{r}'; E) = \langle \mathbf{r}| \frac{1}{E - H_0 \pm i\epsilon} |\mathbf{r}'\rangle \tag{10}$$

Explicitly, in three dimensions, $d = 3$, we have

$$G^{\pm}(\mathbf{r} - \mathbf{r}'; E) = \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \frac{2m_r}{2m_r E - q^2 \pm i\epsilon} = \frac{2m_r}{(2\pi)^2} \int_0^{\infty} dq \, \frac{q^2}{2m_r E - q^2 \pm i\epsilon} \frac{e^{iq|\mathbf{r}-\mathbf{r}'|} - e^{-iq|\mathbf{r}-\mathbf{r}'|}}{iq|\mathbf{r} - \mathbf{r}'|} \tag{11}$$

$$= -\frac{2m_r}{(2\pi)^2} \int_0^{\infty} dq \, \frac{q^2}{q^2 - (\sqrt{2m_r E} \pm i\epsilon)^2} \frac{e^{iq|\mathbf{r}-\mathbf{r}'|} - e^{-iq|\mathbf{r}-\mathbf{r}'|}}{iq|\mathbf{r} - \mathbf{r}'|} \tag{12}$$

$$= -\frac{2m_r}{(2\pi)^2} \frac{1}{i|\mathbf{r} - \mathbf{r}'|} \int_{-\infty}^{\infty} dq \, \frac{q e^{iq|\mathbf{r}-\mathbf{r}'|}}{(q - \sqrt{2m_r E} \mp i\epsilon)(q + \sqrt{2m_r E} \pm i\epsilon)} = -\frac{2m_r}{4\pi} \frac{e^{\pm i\sqrt{2m_r E}|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \tag{13}$$

Inserting into Eq. (9), we get

$$\phi^{\pm}_{\mathbf{k}}(\mathbf{r}) \;\sim\; e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}', \mathbf{k}; k^2/2m_r \pm i\epsilon) \frac{e^{\pm ikr}}{r}, \quad \text{large } r \text{ with } \mathbf{k}' \equiv k\,\mathbf{r}/r \tag{14}$$

$$f(\mathbf{k}', \mathbf{k}; E = k^2/2m_r \pm i\epsilon) \;=\; -\frac{2m_r}{4\pi} \int d\mathbf{r}' e^{-i\mathbf{k}'\cdot\mathbf{r}'} V(r') \phi^{\pm}_{\mathbf{k}}(\mathbf{r}'), \tag{15}$$

Using the asymptotic solution $\Psi^+_{\mathbf{k}}(\mathbf{r})$ in Eq. (14), we describe the scattering of an incident plane wave of wave vector $\mathbf{k}$ with a scattered outgoing spherical wave of amplitude $f(\mathbf{k}', \mathbf{k}; E = k^2/2m_r + i\epsilon)$ where $\mathbf{k}'$ points into the scattering direction. The flux of of scattered particles into direction $\mathbf{k}'$ is then proportional to the square of the scattering amplitude, and the differential cross section writes

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{k}', \mathbf{k}; E = k^2/2m_r + i\epsilon)|^2 \tag{16}$$

Note that we have $|\mathbf{k}| = |\mathbf{k}'| = \sqrt{2m_r E}$ in the scattering amplitude entering "on-shell" the differential cross section, Eq. (16); analytic continuation to unconstraint, arbitray values of $\mathbf{k}$, $\mathbf{k}'$, and E defines the scattering amplitude "off-shell".

3. Partial wave analysis: Relation between scattering amplitudes and phase shifts

For a detailed analysis of the scattering problem including explicit solutions, it is useful to adapt to the symmetry of the problem. Using rotational symmetry, we introduce angular coordinates (r, θ, φ) and we separate the angular part of the wavefunction using the eigenfunctions of angular momentum

$$\phi(\mathbf{r}) = \sum_{nlm} a_{nml} R_{nl}(r) Y_{lm}(\theta, \varphi) \tag{17}$$

where the spherical harmonics $Y_{lm}(\theta, \varphi) \propto P_l(\cos\theta) e^{im\varphi}$ can be expressed using the Legendre polynomials $P_l(x)$. In the following, we will relate the asymptotic behavior of $R_{nl}(r)$ for large r, to the scattering amplitude defined previously in the asymptotic expression, Eq. (14).

Since $|\mathbf{k}| = |\mathbf{k}'|$ in Eq. (15), we expand the scattering amplitude only depends on the angle θ between $\mathbf{k}$ and $\mathbf{k}' = k\mathbf{r}/r$,

$$f(\mathbf{k}', \mathbf{k}; k^2/2m_r + i\epsilon) = \sum_l (2l+1) f_l(k) P_l(\cos\theta) \tag{18}$$

Using now the asymptotic expansion of the plane wave in terms of spherical waves

$$e^{ikr\cos\theta} \sim \frac{1}{2ikr} \sum_l (2l+1) P_l(\cos\theta) \left[e^{ikr} - e^{-il\pi} e^{-ikr}\right], \quad kr \gg 1 \tag{19}$$

we get from Eq. (14) and Eq. (17) (with $n = k$ in the infinite system limit)

$$\phi^+(\mathbf{r}) \sim \frac{1}{2ikr} \sum_l (2l+1) P_l(\cos\theta) \left\{[1 + 2ikf_l(k)] e^{ikr} - e^{-il\pi} e^{-ikr}\right\}, \quad kr \gg 1 \tag{20}$$

Due to flux conservation in each partial wave, the absolute value of the amplitude of in-going waves e^{-ikr} must equal that of out-going waves e^{ikr} so that

$$[1 + 2ikf_l(k)] = e^{i2\delta_l(k)} \tag{21}$$

with real $\delta_l(k)$, the factor 2 in the definition of δ is introduced for convinience, see below. The total scattering amplitude then writes

$$f(\mathbf{k}', \mathbf{k}; k^2/2m_r + i\epsilon) = \frac{1}{2ik} \sum_l (2l+1) \left[e^{2i\delta_l(k)} - 1\right] P_l(\cos\theta) \tag{22}$$

in terms of the phase shifts, $\delta_l(k)$, and the radial wave function is asymtotically given by

$$R_{kl}(r) \sim \frac{1}{2ikr}(2l+1) \left[e^{i2\delta_l(k)} e^{ikr} - e^{-il\pi} e^{-ikr}\right] = (2l+1) e^{-i(l\pi/2 - \delta_l(k))} \frac{\sin\left[kr - l\pi/2 + \delta_l(k)\right]}{kr} \tag{23}$$

We see that the factor 2 in the definition of the phase shifts, Eq. (21), we choosen such that $R_{nl}(r \to \infty)$ is proportional to the unperturbed solution (see below) shifted by a phase.

4. Calculation of phase shifts from potential, low energy scattering properties

Phase shifts for a given potential can be obtained by directly solving the Schrödinger equation using partial waves in a spherical box of infinite radius. The radial part satisfies a one-dimensional differential equation for each angular momentum l

$$-\frac{\hbar^2}{2m_r}\frac{1}{r}\frac{d^2[rR_{nl}(r)]}{dr^2}+\left[\frac{l(l+1)\hbar^2}{2mr^2}+V(r)\right]R_{nl}(r)=E_{nl}R_{nl}(r) \tag{24}$$

The interatomic potential V has a characteristic length scale R_e; for distances $r > R_e$ we can neglect the potential, $V(r > R_e) \equiv 0$. For vanishing potential correspoding to free particles, the solution of Eq. (24) are the spherical Bessel functions, $j_l(kr)$ and $n_l(kr)$, with $k = \sqrt{2m_rE_{nl}/\hbar^2}$. The solution of Eq. (24) for $r < R_e$ has to be calculated for any specific potential $V(r)$ and can then be matched at $r = R_e$ to the free solution, such that the wavefunction and its derivative are continuous functions at $r = R_e$. The outside solution is a superposition of j_l and n_l which is conviniently written as

$$R_l(kr) \equiv R_{nl}(r) = \cos\tilde{\delta}_l j_l(kr) - \sin\tilde{\delta}_l n_l(kr) \tag{25}$$

in terms of a so-far undetermined phase $\tilde{\delta}_l$. Considering the large distance asymptotic of the Bessel functions

$$j_l(x) \;\to\; \frac{\sin\left[x-l\frac{\pi}{2}\right]}{x}, \quad x\to\infty \tag{26}$$

$$n_l(x) \;\to\; -\frac{\cos\left[x-l\frac{\pi}{2}\right]}{x}, \quad x\to\infty \tag{27}$$

we get

$$R_l(kr) \to \frac{\sin\left[kr-l\frac{\pi}{2}+\tilde{\delta}_l\right]}{kr} \approx j_l(kr+\tilde{\delta}_l), \quad kr\to\infty \tag{28}$$

and, comparing with Eq. (23), we see that $\tilde{\delta}_k = \delta_k$ is the phase shift in terms of the scattering amplitude, Eq. (21).

Hard sphere scattering. Note that for small arguments, the Bessel functions behave as

$$j_l(x) \;\to\; \frac{x^l}{(2l+1)!!}, \quad x\to 0 \tag{29}$$

$$n_l(x) \;\to\; -\frac{(2l-1)!!}{x^{l+1}}, \quad x\to 0 \tag{30}$$

For hard spheres, the wavefunction has to vanish at $r = a$ where a is the diameter of one sphere, or $R_l(ka) \equiv 0$. Using the asymptotic expansion (30), valid for low-energy scattering, in the expression (25), we obtain for the phase-shift

$$\tan\delta_l \simeq -\frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!}, \quad ka\to 0 \tag{31}$$

In this low energy limit $ka \to 0$, the dominant contribution comes from $l = 0$, called s-wave scattering. Note that the s-wave phase shift $\delta_0 = -ka$ is negative for the repulsive potential.

Scattering length, alcaline atoms. For low-energy scattering ($k \to 0$) one introduces the s-wave scattering length a_s for a general interaction potential writing

$$\frac{k}{\tan\delta_0} = -\frac{1}{a_s}+\frac{1}{2}r_{eff}k^2 \tag{32}$$

where r_{eff} is called effective range of the potential. The phase shift, and therefore also the scattering length can be measured. Let us consider alcaline atoms. The short range interactions at the range of the Bohr radius is dominated by the exchange energies of the overlapping electronic wavefunctions, and strongly repulsive. The long-range tail of the interaction can be described by a van-der-Waals interaction $V(r) = -C_6/r^6$ with characteristic distance $R_e = (4mC_6/\hbar^2)^{1/4}$ with $\hbar^2/(2\mu R_e^2) = C_6/R_e^6$. For alcalines R_e ranges from 20 Å for Li, 80 Å for Rb, up to 100 Å for Cs. For larger distances, the scattering properties are described by the phase shifts, corresponding to a scattering length of 55 Å for Rb, and −600 Å for Cs.

5. Universality and pseudo-potentials

If we consider properties where the distance between particles is large compared to the characteristic length scale of the interaction R_e, we expect that we can express all properties by the phase shifts. The properties which depend only on the phase shifts are universal with respect to different interactions. Since we can obtain the same phase-shifts for different microscopic interactions, we are free to choose the one which is best suited for our calculations. These potentials are called pseudo-potentials. In particular, at low energy, scattering is dominated by the s-wave (isotropic) contribution and further neglect effective rangle effects in the expansion Eq. (**??**). In the limit $a_s \to 0$, we have $\delta_0(k) = -ka_s$ (up to multiplies of 2π), and

$$f(\mathbf{k}, \mathbf{k}'; k^2/2m_r + i\epsilon) = -a_s, \quad k \to 0 \tag{33}$$

The scattering amplitude is minus the scattering length which is the only parameter needed to describe collisions. Note that we have $a_s = a$ in case of hard spheres.

The idea of pseudo-potentials is to replace the true scattering potentials by a model. The model is chosen to simplify the calculations still maintaining the scattering properties, e.g. we can use hard spheres in explicit calculations instead of a very complicated effective interaction for the "true" atom-atom collision.

B. Universality

Let us consider the situation of low energy scattering, $k \to 0$. From Eq. (14) we obtain the form of the two-body wave function (relative motion) in the asymptotic limit $r \to \infty$

$$\phi_0(\mathbf{r}) \sim 1 + \frac{f(0,0;i\epsilon)}{r} = 1 - \frac{a_s}{r} \tag{34}$$

In order to make best use of our simulation resources, we do not necessarily want to perform simulations with the exact two-body potential underlying the experiment addressed. It might not even be sufficiently well known. What is however frequently well determined are collision properties in terms of cross-sections or phase shifts. We therefore look for a generic potential which allows us to perform simulations for any a_s, avoiding possible unwanted instabilities, due to details of the potential, e.g. attractive potentials might lead to collapse to arbitrary high densities.

1. Interaction potential

For calculations explicitly involving the two-body interaction potential $v(r)$, let us consider the model of a short repulsive hard core of diameter σ with an attractive box potential of width r_0 and depth u_0

$$v(r) = \begin{cases} \infty & r \le \sigma \\ -u_0 & \sigma < r \le \sigma + r_0 \\ 0 & r > \sigma + r_0 \end{cases} \tag{35}$$

The s-wave solution of the scattering problem can be written down explicitly

$$R_{0k}(r) = \begin{cases} 0 & r \le \sigma \\ A\frac{\sin \mu(r-\sigma)}{r} & \sigma < r \le \sigma + r_0 \\ \sqrt{\frac{2}{\pi}}\frac{\sin[k(r-\sigma-r_0)+\phi_k]}{kr} & r > \sigma + r_0 \end{cases} \tag{36}$$

with

$$\tan\phi_k = \frac{k}{\mu}\tan\mu r_0, \quad A = \sqrt{\frac{2}{\pi}}\frac{1}{G}, \quad G^2 = k^2 + \frac{s^2}{r_0^2}\cos^2\mu r_0, \quad \mu^2 r_0^2 = k^2 r_0^2 + s^2, \quad s = r_0\sqrt{mu_0/\hbar^2} \tag{37}$$

As usual we consider low enough temperatures so that we can take the $k \to 0$ limit giving the typical asymptotic solution

$$R_{00}(r > \sigma + r_0) \sim \left(1 - \frac{a_s}{r}\right) \tag{38}$$

from where we can read of the s-wave scattering length as

$$a_s = \sigma - r_0 \left[\frac{\tan r_0 \sqrt{m u_0/\hbar^2}}{r_0 \sqrt{m u_0/\hbar^2}} - 1 \right] \tag{39}$$

Variations in the scattering length can be induced by changing either σ, r_0, or u_0. In order to avoid tauthologies, we simply define "diluteness" as systems whose energy can be quantitatively descrived by the scattering length only (at least in some limiting cases where r_0 and σ vanish in an appropriate way. Still, other properties may, and in general do depend on details of the potential.

We further note that for $m u_0 r_0^2/\hbar^2 = \pi^2/4$ we have a bound state at zero energy and the effective range of the potential is of order r_0. Therefore, we need $r_0 \ll a_s$ in order to keep effective range effects small, but still all values of the scattering length can be realised by modifying u_0. However, in order to keep away from two-particle bound states $m u_0 r_0^2 < \hbar^2 \pi^2/4$ is needed.

2. Many-body eigenstates: short range behavior of pair correlations

Let us consider an exact many-body eigenstate $\psi(\mathbf{R})$ of the Hamiltonian

$$H = -\sum_i \frac{\hbar^2 \nabla_i^2}{2m} + \sum_{i<j} v(r_{ij}) \tag{40}$$

where $\mathbf{R} = \mathbf{r}_1, \ldots, \mathbf{r}_N$ denotes all particle positions.

Let us consider a typical configuration $\mathbf{R}$ where the typical distance between particles is of order $n^{-1/3}$ and pick out two particles, i and j. Holding all other particles fix, we let these two particles approach each other, $r_{ij} \to 0$. In order to satisfy the Schrödinger equation, $H\Psi(\mathbf{R}) = E\Psi(\mathbf{R})$, we expect the wave function to asymptotically approach the solution of the two-body problem

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots \mathbf{r}_j) \sim R_{00}(r_{ij}) \widetilde{\Psi}(\mathbf{R}), \quad r_{ij} \ll n^{-1/3} \tag{41}$$

Up to know this is only a rewriting, but, as usual, one inserts this ansatz into the full Schrödinger equation and hopes that the reminder $\widetilde{\Psi}(\mathbf{R})$ will become more regular for $r_{ij} \to 0$, e.g. $\lim_{r_{ij}\to 0} \widetilde{\Psi}(\mathbf{R})$ remains finite for all particle's positions. This is of course, a much too strong condition, as we may simply put two or more particles on the same place and things will likely go nuts. However, our diluteness definition above implies some stronger conditions, in particular, since the energy should be expressible in terms of the scattering length only, we can require that

$$\frac{\int d\mathbf{R}^{(ij)} \Psi^*(\mathbf{r}_1, \ldots, \mathbf{r}'_i, \ldots \mathbf{r}'_j) \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots \mathbf{r}_j)}{\int d\mathbf{R} |\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots \mathbf{r}_j)|^2} \approx R_{00}(r_{ij}) R_{00}(r'_{ij}) \frac{C}{V^2}, \quad r_{ij} \ll n^{-1/3}, r'_{ij} \ll n^{-1/3} \tag{42}$$

where C is some constant smoothly depend on the details of the interaction potential such that it becomes a constant in the appropriate pseudo-potential limit ($d\mathbf{R}^{(ij)}$ denotes the integration over all particles but i and j). This somehow implies that intrinsic three-particle collisions are rare and can be neglecticted to leading order, as well as horrible scenarios as two/three etc. particle bound states are neglegible. (In a pragmatic way, as long as their effects are suppressed by density/temperature, the separation above will still hold approximately over some scale and the different relations can still be useful putten in a proper context.)

Note that C is not the usual definition of the "contact" [2] but we here it is more directly related to the pair correlation function $g(r)$.

3. Derivative of the energy and contact

Under all these assumptions, it is now straightforward to calculate the derivative of the energy with respect to the scattering length. We will take our explicit potential above to avoid technical complications resulting from the use of a contact pseudopotential, in particular we can use the theorem of Hellmann-Feynman to calculate energy derivatives

$$\frac{dE}{da_s} = \sum_{i<j} \frac{\int d\mathbf{R} |\Psi(\mathbf{R})|^2 dv(r_{ij})/da_s}{\int d\mathbf{R} |\Psi(\mathbf{R})|^2} \tag{43}$$

Changes in the scattering results can be obtained by changing r_0 holding σ and u_0 fix

$$\frac{\partial a_s}{\partial r_0} = -\tan^2 r_0\sqrt{mu_0/\hbar^2} \tag{44}$$

so that

$$\frac{dv(r)}{da_s} = \frac{\partial r_0}{\partial a_s}\frac{\partial v(r)}{\partial r_0} = \frac{u_0}{\tan^2 r_0\sqrt{mu_0/\hbar^2}}\delta(r-r_0-\sigma) \tag{45}$$

Note that $\delta(r)$ here is the one-dimensional radial delta function, e.g. $\int d^3r\delta(r-r_0) = 4\pi\int dr\, r^2\delta(r-r_0) = 4\pi r_0^2$ for $r_0 > 0$. Putting this expression into Hellmann-Feyman, we have

$$\frac{dE}{da_s} = \frac{N(N-1)}{2}\frac{4\pi\hbar^2 C}{mV}\frac{mu_0(r_0+\sigma)^2/\hbar^2}{\tan^2 r_0\sqrt{mu_0/\hbar^2}}\left(1-\frac{a_s}{r_0+\sigma}\right)^2 = \frac{N(N-1)}{2V}\frac{4\pi\hbar^2 C}{m}\frac{(\sigma+r_0-a_s)^2}{(\sigma+r_0-a_s)^2} \tag{46}$$

$$= \frac{N(N-1)}{2V}\frac{4\pi\hbar^2 C}{m} \tag{47}$$

and we see that the energy change with respect to the scattering length is entirely described by the behavior of the two-particle correlation function separating out the asymptotic two-body solution.

4. Momentum distribution: large k asymptotics

Let us consider the normalized many-body wavefunction $\Psi(\mathbf{R})$. Then the momentum distribution writes

$$n(k) = \frac{N}{V}\int d\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}}\int d\mathbf{R}\Psi(\mathbf{R}:\mathbf{r}_1)\Psi(\mathbf{R}:\mathbf{r}_1+\mathbf{r}) \tag{48}$$

Let us consider the situation where one of the particles $j \neq 1$ becomes very close to particle 1, much closer than any of the other particles. Then the most singular behavior of the wave functions is given by $\sim -a/|r_{1j}|$, and, similarly $\sim -a/|\mathbf{r}_{1j}+\mathbf{r}|$ for our deplaced one, entering the momentum distribution (assuming $\mathbf{r}\to 0$). Taking only account of this most singular terms we can write

$$n(k) \approx \frac{N(N-1)C}{V^3}\int d\mathbf{r}_1\int d\mathbf{r}_2\int d\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}}\left(1-\frac{a_s}{r_{12}}\right)\left(1-\frac{a_s}{|\mathbf{r}_{12}+\mathbf{r}|}\right) \tag{49}$$

If we now change integration variables from $\mathbf{r}$ to $\mathbf{x} = \mathbf{r}+\mathbf{r}_{12}$, we get

$$n(k) \approx \frac{N(N-1)C}{V^2}\int d\mathbf{r}_{12}e^{i\mathbf{k}\cdot\mathbf{r}_{12}}\left(1-\frac{a_s}{r_{12}}\right)\int d\mathbf{x}e^{-i\mathbf{k}\cdot\mathbf{x}}\left(1-\frac{a_s}{|\mathbf{x}|}\right) \tag{50}$$

$$= Cn^2\left(\frac{4\pi a_s}{k^2}\right)^2, \quad k\neq 0 \tag{51}$$

which gives a characteristic power law $\sim k^{-4}$ for large momenta [2]. Since corrections to the above considerations are more smoothly changing for small distances, the asymptotic k^{-4} is an exact property of the many-body momentum distribution, entirely determined by the contact parameter C.

Note: Here, we explicitly considered short-range interactions. The discussion can be extended also to long-range potentials, e.g. for Coulomb interactions where it involves the so-called Kato cusp conditions [3], and, of course, the asymptotic power laws are changed, but still given in terms of the asymptotic two-particle wave function behavior.

C. Pseudo-potentials (analytical calculations)

The idea of pseudo-potentials is to replace the true scattering potentials by a model. The model is chosen to simplify the calculations still maintaining the scattering properties. In particular, it can be convienient to use general operators instead of the more realistic physical interaction in terms of strictly local potentials in real space.

A particular simple potential for analytical calculations would be a delta-function potential $g\delta(\mathbf{r})$. However, inserting it together with Eq. (14) (continued to $\mathbf{r}=0$) in Eq. (15), we get $f=-2m_r g/4\pi \lim_{r\to 0}[1+f/r]$. As long as we would restrict to first order in $f\sim g$, we get a simple result, but the second order is diverging. Note that the small corrections in r'^2/r^2 neglected in Eq. (14) to describe the full behavior outside the scattering potential do not change this result.

Since the simple delta-function potential cannot be used in general, let us try a regularized delta-function potential

$$\tilde{V}_\delta(\mathbf{r}) = g\delta(\mathbf{r})\left[\frac{d}{dr}r\cdot\right] \tag{52}$$

which eliminates the above problems, as we will see. The scattering amplitude, Eq. (15), is now given by

$$f(\mathbf{k}',\mathbf{k};E=k^2/2m_r+i\epsilon) \;=\; -\frac{2m_r}{4\pi}\int d\mathbf{r}' e^{-i\mathbf{k}'\cdot\mathbf{r}'}V_\delta(r')\phi^+_{\mathbf{k}}(\mathbf{r}') = -\frac{2m_r g}{4\pi}\lim_{r\to 0}\frac{d}{dr}\left(r\phi^+_{\mathbf{k}}(r)\right) \tag{53}$$

which gives a close relation using Eq. (14) for $\phi^+_{\mathbf{k}}(r\to 0)$:

$$f(\mathbf{k}',\mathbf{k};E=k^2/2m_r+i\epsilon) = -\frac{2m_r g}{4\pi}\left[(1+i\mathbf{k}\cdot\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}+ikf(\mathbf{k}',\mathbf{k};E=k^2/2m_r+i\epsilon)e^{ikr}\right]\Big|_{r=0} \tag{54}$$

or

$$f(\mathbf{k}',\mathbf{k};E=k^2/2m_r+i\epsilon) = -\frac{2m_r g}{4\pi}\frac{1}{1+ik2m_r g/4\pi} \tag{55}$$

In order to recover the scattering length for vanishing momenta, we set $g=4\pi a/2m_r$ and get

$$f(\mathbf{k}',\mathbf{k};E=k^2/2m_r+i\epsilon) = -\frac{a}{1+ika} \tag{56}$$

Note that acting with the regularized pseudopotentials, Eq. (52) on functions which are regular at the origin, reduces to the action of a simple delta-function potential.

The exact solution of the two-body wave function for the regularized pseudo-potential is

$$\phi^+_{\mathbf{k}}(\mathbf{r}) \;=\; e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{a}{1+ika}\frac{e^{\pm ikr}}{r} \tag{57}$$

Let us explicitly verify that Eq. (57) is indeed a solution of the Schrödinger equation. Using that

$$\Delta\frac{f(r)}{r} = \Delta\frac{1}{r}+\Delta\frac{f(r)-1}{r} = 4\pi\delta(\mathbf{r})+\frac{f''(r)}{r} \tag{58}$$

for any radial function $f(r)$ with $f(0)=1$ and the laplacian operator in $d=3$. Note that $\Delta f(r)=f''(r)+(D-1)f'(r)/r$ and $[\nabla f(r)]\nabla 1/r = f'(r)/r$ such that we obtain the above result. We can further write

$$\Delta\phi^+_{\mathbf{k}}(\mathbf{r}) = \Delta e^{i\mathbf{k}\cdot\mathbf{r}}+f\Delta\frac{ikr}{r} = \Delta e^{i\mathbf{k}\cdot\mathbf{r}}+f\Delta\frac{1}{r}+f\Delta\frac{e^{ikr}-1}{r} \tag{59}$$

so that we have

$$-\Delta\phi^+_{\mathbf{k}}(\mathbf{r}) = k^2\phi^+_{\mathbf{k}}(\mathbf{r})-\frac{4\pi a}{1+ika}\delta(\mathbf{r}) \tag{60}$$

We then get

$$\left[-\Delta+2m_r\hbar^{-2}V_\delta(\mathbf{r})\right]\phi^+_{\mathbf{k}}(\mathbf{r}) = k^2\phi^+_{\mathbf{k}}(\mathbf{r})-\frac{4\pi a}{1+ika}\delta(\mathbf{r})+2m_r\hbar^{-2}g\delta(\mathbf{r})\left[1-\frac{iak}{1+ika}\right] = k^2\phi^+_{\mathbf{k}}(\mathbf{r}) \tag{61}$$

so that $\phi^+_{\mathbf{k}}(\mathbf{r})$ is an energy-eigenfunction with energy $k^2/2m_r$.

Since we expect that also the N-body wave function of a gas must be an eigenfunction of the two-body Hamiltonian for two particles coming arbitrary close to each other, the wave function must be proportional to Eq. (57) when all the other $N-2$ particles are kept fixed. At low temperatures, we can use the limit $k\to 0$ and we get

$$\Psi_N(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\to(1-a/|\mathbf{r}_i-\mathbf{r}_j|)\tilde{\Psi}_{ij}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N),\quad \text{for any } \mathbf{r}_i\to\mathbf{r}_j \tag{62}$$

where $\tilde{\Psi}_{ij}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$ is regular when $\mathbf{r}_i\to\mathbf{r}_j$. Notice that the wave function is well defined for all $|\mathbf{r}_i-\mathbf{r}_j|$, including distances smaller than a, so that the a/r in the wave function will dominate the momentum distribution at large k, leading to an universal behavior.

Relations as shown above involving the contact C, can be similarly derived within the pseudo-potential approach [4].

1. Delta-Potential truncated in momentum space

Perturbation expansions of the many-body problem are often done in Fourier-space, and the application of the real-space pseudopotential is not always simple there. In this case, we can define a smooth potential by

$$V_\eta(\mathbf{k}) = \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} V(r) = g_0 \eta(k) \tag{63}$$

with $\eta(k) = 1$ for $k \ll k_c$ and $\eta(k) = 0$ for $k \gg k_c$. The true delta function would be described by $k_c \to \infty$, but this will introduce divergent expressions, circumvented by the use of a large, but finite k_c.

Let us look directly at the T-matrix given by

$$T_{\mathbf{k},\mathbf{k}'} = \langle \mathbf{k}|V|\Psi^+_{\mathbf{k}'}\rangle \tag{64}$$

which can be generalized inserting the Lippmann-Schwinger equation, Eq. (8), to obtain the operator equation (for general E)

$$T(E) = V + V\frac{1}{E - H_0 + i\epsilon}T(E) \tag{65}$$

Note the connection to the scattering amplitude, Eq. (15),

$$\langle \mathbf{k}|T(E = k^2/2m + i\epsilon)|\mathbf{k}'\rangle = -\frac{4\pi}{2m_r} f(\mathbf{k},\mathbf{k}'; k^2/2m_r + i\epsilon) \tag{66}$$

We then have for our model potential

$$T_{\mathbf{k}\mathbf{k}'}(E) = g_0\eta(\mathbf{k}-\mathbf{k}') + \int \frac{d\mathbf{q}}{(2\pi)^3}\frac{g_0\eta(\mathbf{k}-\mathbf{q})}{E - q^2/2m_r + i\epsilon} T_{\mathbf{q}\mathbf{k}'}(E) \tag{67}$$

For E around $k^2/2m_r$ we can approximate $T_{\mathbf{q}\mathbf{k}'}(E) \approx T_{\mathbf{k}\mathbf{k}'}(E)$ since the nominator is peaked around $q \approx k$. We then get

$$T_{\mathbf{k}\mathbf{k}'}(E) = g_0\eta(\mathbf{k}-\mathbf{k}') + T_{\mathbf{k}\mathbf{k}'}(E)\int \frac{d\mathbf{q}}{(2\pi)^3}\frac{g_0\eta(\mathbf{k}-\mathbf{q})}{E - q^2/2m_r + i\epsilon} \tag{68}$$

or

$$T_{\mathbf{k}\mathbf{k}'}(E) = \frac{g_0\eta(\mathbf{k}-\mathbf{k}')}{1 + g_0\int \frac{d\mathbf{q}}{(2\pi)^3}\frac{\eta(\mathbf{k}-\mathbf{q})}{E - q^2/2m_r + i\epsilon}} \tag{69}$$

Let us now look at low energy properties, $E \sim k^2/2m_r \approx 0$, and relate the on-shell T-matrix with the scattering amplitude, Eq. (66), and using the pseudo-potential expression for s-wave scattering, we have

$$T_{\mathbf{k}\mathbf{k}'}(E = k^2/2m_r) = \frac{4\pi a}{2m_r}\frac{1}{1 + ika} \tag{70}$$

so that we can eliminate g_0 in favour of a, e.g. from Eq. (68) for $E \sim k^2/2m \to 0$, which we write as

$$\frac{1}{g_0} = \frac{1 + ika}{4\pi a/2m_r} - \int \frac{d\mathbf{q}}{(2\pi)^3}\frac{\eta(\mathbf{q})}{(q^2 - k^2)/2m_r - i\epsilon} \tag{71}$$

We can further simplify by evaluating the integral on the rhs

$$\begin{aligned}
2m_r\int \frac{d\mathbf{q}}{(2\pi)^3}\frac{\eta(\mathbf{q})}{q^2 - k^2 - i\epsilon} &= \frac{m_r}{\pi^2}\int_0^\infty dq \frac{\left[q^2 - k^2 + k^2\right]\eta(\mathbf{q})}{q^2 - k^2 - i\epsilon} && (72)\\
&= \frac{m_r}{\pi^2}\left[\int_0^\infty dq\eta(\mathbf{q}) + \frac{k^2}{2}\int_{-\infty}^\infty dq \frac{\eta(q)}{(q - k - i\epsilon)(q + k + i\epsilon)}\right] && (73)\\
&= \frac{m_r}{\pi^2}\left[\pi C k_c/2 + i\frac{\pi}{2}k\right] && (74)
\end{aligned}$$

where $\pi C/2 = \int_0^\infty d(q/kc)\eta(q/k_c)$ is a constant of order one. Inserting on the rhs of Eq. (71), we get

$$\frac{1}{g_0} = \frac{1}{4\pi a/2m_r} - \frac{2m_r C k_c}{4\pi} = \frac{1}{g} - \frac{Cak_c}{g} \tag{75}$$

where $g = 4\pi a/2m_r$. We then have

$$g_0 = \frac{g}{1 - Cak_c} \tag{76}$$

or

$$g = \frac{g_0}{1 + 2m_r C g_0 k_c/4\pi} \tag{77}$$

Notice that second order effects in g_0 are not proprotional to second order effects in a.

Appendix: Some results for the phase shifts

We have chosen the normalization for the radial wavefunction such that for $u_l(kr) = R_l(kr)/r$, we have

$$\int_0^\infty dr u_l(kr) u_l(k'r) = 2\pi\delta(k - k') \tag{78}$$

in the continuum limit.

Let us denote $u_{nl}^{(0)}(r)$ the free solution of Eq. (24) for vanishing potential

$$-\frac{\hbar^2}{2\mu}\frac{d^2 u_{nl}^{(0)}(r)}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} u_{nl}^{(0)}(r) = E_{nl} u_{nl}^{(0)}(r) \tag{79}$$

$$\frac{u_l^{(0)}(kr)}{kr} = 2j_l(kr) \tag{80}$$

We multiply Eq. (24) with $u_{nl}^{(0)}(r)$ from the left and subtract Eq. (79) multiplied by $u_{nl}(r)$. Integrating over r from 0 to R we obtain

$$\frac{2\mu}{\hbar^2}\int_0^R dr\, u_l^{(0)}(kr) V(r) u_l(kr) = -u_l(kR)\frac{du_l^{(0)}(kr)}{dr}\Big|_{r=R} + u_l^{(0)}(kR)\frac{du_l(kr)}{dr}\Big|_{r=R} \tag{81}$$

where we have integrated by parts and used that u_l and $u_l^{(0)}$ vanish at $r = 0$. For large R we can use the asymptotic expressions and obtain

$$\begin{aligned} u_l(kR)\frac{du_l^{(0)}(kr)}{dr}\Big|_{r=R} - u_l^{(0)}(kR)\frac{du_l(kr)}{dr}\Big|_{r=R} &= -4k\sin\left(kr - l\frac{\pi}{2} + \delta_l\right)\cos\left(kr - l\frac{\pi}{2}\right) + 4k\sin\left(kr - l\frac{\pi}{2}\right)\cos\left(kr - l\frac{\pi}{2} + \delta_l\right) \\ &= -4k\sin\delta_l \end{aligned} \tag{82}$$

We obtain a quite useful result

$$\int d\mathbf{r}\frac{u_l^{(0)}(rk)}{2kr} V(r)\frac{u_l(rk)}{2kr} = -\frac{4\pi\hbar^2}{m}\frac{\sin\delta_l}{k} \tag{83}$$

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