

Self-Energies and the Interactions of Particles with Many-Body Systems

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Abstract

We present an alternative approach to the self-energy formalism for the interaction of a projectile with a many-body target. We illustrate the method with examples of charges or atoms interacting with a surface, and with charges or atoms interacting with order atoms. Further applications are briefly discussed.

1. Introduction

The inherent problem in the study of many-particle systems is the large number of degrees of freedom that must be considered. Consequently, one has to look for ways to reduce the complexity of the problem, usually by a reduction of the number of degrees of freedom. In this paper we wish to review our approach to one of these methods, the self-energy approach.

The typical many-particle system we wish to consider here can be thought of as a projectile interacting with a many-body target. In general, the projectile may be of the same or of different nature from those making up the target and all particles including the projectile may have internal degrees of freedom. In the absence of any interactions between target and projectile the wave function of the system is of the form

$$|i\rangle = \phi_i(\mathbf{r})|f_i\rangle| \{n_i\} \rangle \quad (1)$$

where $\phi_i(\mathbf{r})$ is a spatial wave function in the relative coordinate \mathbf{r} between projectile and target, $|f_i\rangle$ is the ket for the internal state of the projectile, and $| \{n_i\} \rangle$ is the ket for the many-body state of the target. The label $\{n_i\}$ indicates a set of occupation numbers. The simplest form of the interaction would be a pairwise sum of interactions between all components of the projectile and target,

$$V = \sum_{i,j} v_a(\mathbf{r}_i, \mathbf{r}_j) + \dots \quad (2)$$

and in general the potential will include the interactions with collective modes of the system. The examples discussed below will be strongly oriented towards the interaction of atoms and charges with surfaces, so the collective modes would be phonons, plasmons, optical phonon modes, etc.

One approach which has historically been particularly useful for projectiles which retain somewhat of an identity as single particles is to convert the many-body wave equation into an effective single particle problem in the relative coordinate. This is often expressed in terms of the nonlocal, complex, and energy dependent self-energy $\Sigma(\mathbf{r}, \mathbf{r}', E)$

as [1, 2]

$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 + v(\mathbf{r}) \right\} \phi_i(\mathbf{r}) + \int d\mathbf{r}' \Sigma(\mathbf{r}, \mathbf{r}', E_i) \phi_i(\mathbf{r}') = E_i \phi_i(\mathbf{r}) \quad (3)$$

Here $v(\mathbf{r})$ is the external potential plus any average potential due to the target. This equation can be further forced into the form of a single-body Schrödinger equation by defining the local self-energy projection $\Sigma_i(\mathbf{r})$ according to

$$\Sigma_i(\mathbf{r}) \phi_i(\mathbf{r}) = \int d\mathbf{r}' \Sigma(\mathbf{r}, \mathbf{r}', E_i) \phi_i(\mathbf{r}') \quad (4)$$

which leads to

$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 + v(\mathbf{r}) + \Sigma_i(\mathbf{r}) \right\} \phi_i(\mathbf{r}) = E_i \phi_i(\mathbf{r}) \quad (5)$$

This is basically a quasiparticle equation and $\Sigma_i(\mathbf{r})$ is often called the exchange and correlation potential. The usual prescription for determining the above self-energy involves many-body Green functions [1] and is often a lengthy process.

2. Formalism

We would like to present here an alternative approach for obtaining a self-energy [3]. This is a straightforward and simple approach which avoids all direct reference to many-body Green functions, although of course, they are implicitly always contained in the formalism.

One of the most important physical quantities that can be measured is the energy shift of the projectile as it interacts with the many-particle target. If the form of the potential of eq. (2) is known, this energy shift is given by the many-body Rayleigh-Schrödinger perturbation series using the non-interacting states of eq. (1).

$$\Delta E = \sum_l \frac{\langle i|V|l\rangle \langle l|V|i\rangle}{E_i - E_l + i\epsilon} + \sum_{l,l'} \frac{\langle i|V|l\rangle \langle l|V|l'\rangle \langle l'|V|i\rangle}{(E_i - E_l + i\epsilon)(E_i - E_{l'} + i\epsilon)} + \dots \quad (6)$$

where we have ignored the first order term since it usually vanishes, or else can be included in the average potential. Also not appearing in eq. (6) are some additional higher order terms [4]. Recall that the many-body matrix elements are of the form

$$\langle i|V|l\rangle = \int d\mathbf{r} \phi_i^*(\mathbf{r}) \langle f_i | \langle \{n_i\} | V | \{n_i\} \rangle | f_i \rangle \phi_i(\mathbf{r}) \quad (7)$$

with l the collective quantum index for the set $(\mathbf{k}_l, f_l, \{n_l\})$ and

the unperturbed energies will be

$$E_i = E_{k_i} + \mathcal{E}_{f_i} + E^c(\{n_i\}), \quad (8)$$

the sum of the translation energy of the projectile E_{k_i} , the internal excitation energy of the projectile \mathcal{E}_{f_i} , and the collective energy of the target system $E^c(\{n_i\})$.

We can rewrite the perturbation series in mixed representation

$$\begin{aligned} \Delta E &= \int d\mathbf{r} \\ &\times \sum_I \frac{\phi_i^*(\mathbf{r}) \langle f_i | \{n_i\} | V | \{n_i\} \rangle | f_i \rangle \phi_i(\mathbf{r}) \langle I | V | i \rangle}{(E_i - E_i + i\epsilon)} + \int d\mathbf{r} \sum_{I'} \\ &\times \frac{\phi_i^*(\mathbf{r}) \langle f_i | \{n_i\} | V | \{n_i\} \rangle | f_i \rangle \phi_i(\mathbf{r}) \langle I | V | I' \rangle \langle I' | V | i \rangle}{(E_i - E_i + i\epsilon)(E_i - E_{i'} + i\epsilon)} \\ &+ \dots \end{aligned} \quad (9)$$

where we have also inverted the usual sequence of summations and integrations.

We assert that this same energy shift ΔE may be written as the integral of the spatially dependent self-energy $\Sigma_i(\mathbf{r})$, weighted by the probability density of the projectile in its original state.

$$\Delta E_0 = \int d\mathbf{r} \phi_i^*(\mathbf{r}) \Sigma_i(\mathbf{r}) \phi_i(\mathbf{r}) \quad (10)$$

The self-energy is identified by equating integrands in the two expressions for ΔE .

$$\begin{aligned} \Sigma_i(\mathbf{r}) \phi_i(\mathbf{r}) &= \sum_I \frac{\phi_i(\mathbf{r}) \langle f_i | \{n_i\} | V | \{n_i\} \rangle | f_i \rangle \langle I | V | i \rangle}{(E_i - E_i + i\epsilon)} \\ &+ \sum_{I'} \frac{\phi_i(\mathbf{r}) \langle f_i | \{n_i\} | V | \{n_i\} \rangle | f_i \rangle \langle I | V | I' \rangle \langle I' | V | i \rangle}{(E_i - E_i + i\epsilon)(E_i - E_{i'} + i\epsilon)} + \dots \end{aligned} \quad (11)$$

This is certainly not a unique choice (a characteristic of any approach for obtaining a self-energy) but it is certainly a reasonable, and in a certain sense, a sufficient choice since it reproduces exactly the energy shift. Although we have exhibited only a few terms, the process can obviously be extended to all orders in perturbation theory. Hence as long as the perturbation series converges so will our choice of self-energy. In the cases which we have examined, this approach reproduces the self-energy obtained from the usual definitions of the correlation and exchange potential.

There is an alternative method of arriving at the same definition of eq. (11) if the initial single particle states $\phi_i(\mathbf{r})$ are plane waves, and this is through Fourier transformation of the transition matrix. The two terms exhibited in eq. (9) or (6) are also the first two terms in the diagonal elements of the transition matrix, or the transition matrix for forward scattering. If we make the extension of the transition matrix to non-diagonal contributions in the particle states, the two terms of eq. (11) are the Fourier transform with respect to the exchanged momentum. This same formal exercise can be carried out for all high order terms in the transition matrix, and for those terms in ΔE which do not appear in the transition matrix.

We note in passing that our definition of the self-energy can readily be extended to dynamical processes in which the projectile makes transitions to different states. Such dynamical processes are, in fact, implicit in eq. (11) in the form of certain imaginary parts as will be discussed below.

Although we have concentrated on the development of the local projection of the self-energy, it is immediately apparent that a nonlocal self-energy such as that appearing in eq. (3) can be obtained by an immediate extension of these methods. One simply rewrites the final matrix element in each of the terms of eq. (11) in a similar mixed form as in eq. (9). The nonlocal $\Sigma(\mathbf{r}, \mathbf{r}', E_i)$ is obtained by equating integrands between eq. (4) and eq. (11):

$$\begin{aligned} \Sigma(\mathbf{r}, \mathbf{r}', E_i) &= \sum_I \frac{\phi_i(\mathbf{r}) \langle f_i | \{n_i\} | V | \{n_i\} \rangle \langle f_i | \{n_i\} | V | \{n_i\} \rangle | f_i \rangle \phi_i^*(\mathbf{r}')}{E_i - E_i + i\epsilon} \\ &+ \dots \end{aligned} \quad (12)$$

Note that the nonlocal self-energy depends on the energy of the system, but not on the initial state $\phi_i(\mathbf{r})$.

We can, furthermore, relate the result of eq. (12) to previous work [1, 2] by noting that the local self-energy can be written in the well known G-W form

$$\Sigma(\mathbf{r}, \mathbf{r}', \omega) = \int d\omega' G(\mathbf{r}, \mathbf{r}'; \omega - \omega') W(\mathbf{r}, \mathbf{r}'; \omega') e^{-i\omega\omega'}$$

with single particle Green function taking the standard form

$$G(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{k_i} \frac{\phi_i(\mathbf{r}) \phi_i^*(\mathbf{r}')}{\omega - E_{k_i} + i\epsilon}$$

and the screened interaction term $W(\mathbf{r}, \mathbf{r}'; \omega)$ is given by

$$\begin{aligned} W(\mathbf{r}, \mathbf{r}'; \omega) &= \sum_{f_i} \sum_{\{n_i\}} \frac{\langle f_i | \{n_i\} | V | \{n_i\} \rangle | f_i \rangle \langle f_i | \{n_i\} | V | \{n_i\} \rangle | f_i \rangle}{\omega + \mathcal{E}_{f_i} + E^c(\{n_i\}) - \mathcal{E}_{f_i} - E^c(\{n_i\}) + i\epsilon} \end{aligned}$$

We have also tacitly assumed in this treatment that the initial state of the target $|\{n_i\}\rangle$ is unique, essentially implying a process carried out at a temperature $T = 0$. The case of nonzero target temperature is, in principle, handled by averaging the energy shift or self-energy over the appropriate ensemble of initial target states.

3. General form of the self-energy

The form of $\Sigma_i(\mathbf{r})$ as expressed in eq. (11) allows us immediately to make some statements about its nature. For example, looking at the first non-vanishing term (second order in the perturbation series) the self-energy is

$$\Sigma_i(\mathbf{r}) = \sum_{k_i, f_i, \{n_i\}} \frac{\phi_i(\mathbf{r}) \langle f_i | \{n_i\} | V | \{n_i\} \rangle | f_i \rangle \langle I | V | i \rangle}{\phi_i(\mathbf{r}) E_i - E_i + i\epsilon} \quad (13)$$

Since it is expressed in terms of summations over intermediate states much can be ascertained by considering the nature of the pole contributions. The important singularities are those in the energy denominator and those coming from the matrix elements of the potential. Clearly $\Sigma_i(\mathbf{r})$ will have both real and imaginary contributions. The real part is analogous to the ordinary potential in a Schrödinger equation. The imaginary part can be further subdivided into a conservative contribution and a non-conservative contribution. The non-conservative imaginary part describes a net real energy loss or gain of the projectile due to the exchange of real quanta of energy with the target. The conservative imaginary part is somewhat more subtle and arises because of the inherent many-particle nature of the problem. It describes virtual quantum exchanges with the target but does not give

rise to a net energy exchange [5]. To illustrate this discussion, consider the energy denominator. If initially the projectile and target are in their ground states and if the energy of relative motion is insufficient to create a real excitation of either target or projectile, only virtual excitations are possible. In the momentum space conjugate to the relative motion, the poles of the energy denominator lie on the imaginary axis, but $\Sigma_i(\mathbf{r})$ will in general have both real and imaginary parts, and the imaginary part will be conservative. On the other hand, if the energy of relative motion is sufficiently high, a real excitation can occur which corresponds to the pole of the energy denominator shifting down to lie on the real axis. This exchange of a real quantum will be described by the resulting non-conservative imaginary part, but there can also be at the same time imaginary parts which are conservative.

4. Examples

4.1. Charge interacting with a surface

As an example of the application of the self-energy approach, we begin with the problem of a charge interacting with a surface. This problem is of interest because knowledge of the charge-surface interaction potential is important in all surface experiments using electrons as probes, i.e., LEED, electron energy loss spectroscopies, and electron tunneling microscopy. In addition there is renewed interest in experiments involving the interactions of positrons and surfaces.

Outside the surface the forces on a charge are due to collective surface electronic excitations, e.g., surface plasmons on metals and surface optical phonons on insulators, and we can ignore the fields due to bulk excitations except for very small separations. Far away from a metal surface the self-energy must approach the classical image potential $-e^2/4z$ while near the surface it will be strongly altered because of quantum effects. Among these near surface effects are the exchange of real quanta (energy loss or gain), finite velocity saturation, and recoil. The self-energy potential weakens and eventually saturates due to the velocity of the charge because the collective electronic excitations of the surface cannot follow faithfully the motion. Recoil is the kickback due to conservation of momentum each time the charge exchanges a real or virtual quantum, and this recoil motion also serves to weaken the attractive potential.

The interaction potential between a charge and surface can be written as

$$V = \Phi(\mathbf{r}) = \alpha \sum_{\mathbf{Q}} \Gamma_{\mathbf{Q}} e^{-Q|z|+i\mathbf{Q}\cdot\mathbf{R}} (a_{\mathbf{Q}}^{\dagger} + a_{-\mathbf{Q}}) \quad (14)$$

where \mathbf{R} and \mathbf{Q} are, respectively, the displacement and wavevector parallel to the surface, and $a_{\mathbf{Q}}^{\dagger}$ is the creation operator for the collective surface excitations. The coupling constant is $\Gamma_{\mathbf{Q}}^2 = e^2 \pi \hbar \omega / Q$ and for metals (surface plasmons) $\alpha = 1$, while for ionic solids where the excitations are surface optical phonons

$$\alpha = \frac{\epsilon_0 - 1}{\epsilon_0 + 1} - \frac{\epsilon_{\infty} - 1}{\epsilon_{\infty} + 1} \quad (15)$$

For the remainder of this section we will specialize to the case of metal surfaces with a dispersionless surface plasmon frequency given by $\omega_s = \omega_p / \sqrt{2}$, where ω_p is the bulk plasmon frequency. Using plane waves for the unperturbed states $\phi_i(\mathbf{r})$ the second order term for $\Sigma_i(\mathbf{r})$ of eq. (13) can be

readily evaluated. There are a number of special cases depending mainly on whether the initial translational energy is large (sufficiently great so that real surface plasmons are excited) or small (only virtual plasmon excitations are possible). We present here several of these interesting results.

In the higher energy case and for large distance z away from the surface the real and imaginary parts of the self-energy are

$$\text{Re } \Sigma_i(z) \xrightarrow{z \rightarrow \infty} -\frac{e^2}{4|z|} \left\{ 1 - \frac{v^2}{2\omega_s z^2} + \dots \right\} \quad (16)$$

$$\text{Im } \Sigma_i(z) \xrightarrow{z \rightarrow \infty} \frac{e^2 v}{8\omega_s z^2} \left\{ 1 - \frac{3v^2}{2\omega_s z^2} + \dots \right\} \quad (17)$$

where v is the speed of the charge. These asymptotic series can be expressed in closed form in terms of exponential integrals [4]. The correction terms to the classical image force are energy dependent and become important at electron energies of the order of ω_p .

Near the surface, still at high energies, the finite velocity of the charge causes a saturation of $\Sigma_i(\mathbf{r})$ which varies inversely as v :

$$\Sigma_i(z) \xrightarrow{z \rightarrow 0} -\frac{\pi e^2 \omega_s}{2v} \left\{ 1 - \frac{i}{\pi} \ln \left[1 - \frac{\sqrt{1 - 2\hbar\omega_s/mv^2}}{1 - \hbar\omega_s/mv^2} \right] \right\} \quad (18)$$

Note that this is only the surface contribution, bulk contributions have been ignored. The saturation value in eq. (18) is bigger by a factor of two than that found by others [6-9] because we find an important contribution to recoil.

The question of recoil has very interesting consequences which are perhaps most easily illustrated at low energies where finite velocity effects disappear. In the limit $v = 0$ we can write the self-energy for all z in terms of tabulated functions

$$\Sigma_i(z) = -\frac{e^2}{4|z|} \{ 1 - e^{-Q_s|z|} + Q_s|z| E_2(Q_s|z|) \} \quad (19)$$

where $Q_s^2 = 2m\omega_s/\hbar$ and $E_2(x)$ is the associated exponential integral. Note that the recoil effects decay rapidly away from the surface with a characteristic length $1/Q_s$. The form of the recoil terms depends strongly on retaining its full three-dimensional nature, and in fact the saturation value of $-e^2 Q_s/2$ is substantially smaller than that obtained from a two-dimensional estimate [9, 10].

A typical example of the self-energy is shown in Fig. 1 which gives the real and imaginary parts of $\Sigma_i(z)$ for a case where the energy is greater than ω_s . We note that both the real and imaginary parts saturate at the surface. Oscillatory terms appear after the charge penetrates the surface and these are due to the excitation of real surface plasmons.

2. Charge in a bound state near the surface

As the second example of this self-energy formalism we consider a charge bound in a one-dimensional potential at the surface, a problem directly related to the question of a tunneling electron [11]. We choose one of the simplest forms for the potential, an attractive δ -function

$$v(z) = -\hbar^2 \lambda_0 m \delta(z). \quad (20)$$

The complete set of states for this potential consists of reflected and transmitted plane waves, together with a single

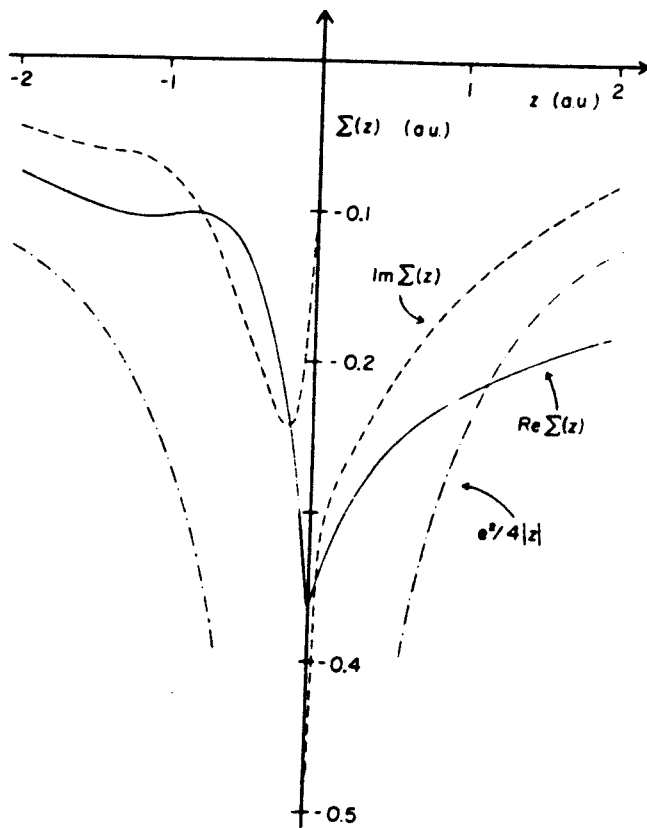


Fig. 1. The self-energy of an electron near a metal surface. The real and imaginary parts of $\Sigma_i(z)$ are compared to the classical image potential with $\omega_s = 0.5$ a.u. and $v = 2.0$ a.u.

bound state

$$\phi_0(z) = \sqrt{\lambda_0} \exp(-\lambda_0 |z|). \quad (21)$$

With this set of states the relevant matrix elements can be readily calculated for an evaluation of $\Sigma_i(z)$ from the second order term of eq. (13). We quote here only one result, the asymptotic correction to the classical image potential:

$$\Sigma_i(z) \xrightarrow{z \rightarrow \infty} -\frac{e^2}{4z} \left\{ 1 + \frac{\lambda_0}{z} + \dots \right\} \quad (22)$$

The higher order correction terms depend on energy similarly to eq. (16). Equation (22) is essentially the same result obtained by Jonson [13] for the case of a charge tunneling through a rectangular potential, except that with his more approximate method he obtains an imaginary contribution which is not present here. Many other results have been calculated, including the energy shifts of the δ -function potential states due to the presence of the surface [12].

3. Atom-surface interaction

A logical extension of this work is to consider the interaction of an atom with a surface. This problem is important in the study of chemical reactions, in the interactions of atoms passing near submicron structures, and in the field of surface analysis by thermal energy atom scattering. As opposed to the charge-surface problem, the atom is a neutral particle and interacts with the surface through an induced polarization as it is excited into virtual states. The only major change in the formalism is that we must consider the internal states of the atom. The lowest non-vanishing order expression of eq. (11)

becomes [14]

$$\Sigma_i(\mathbf{r}) = \sum_{\{n\}} \sum_I \sum_k \frac{\phi_k(\mathbf{r})}{\phi_k(\mathbf{r})} \frac{\langle f_i | \langle \{n_i\} | V | \{n\} \rangle | f_i \rangle \int d\mathbf{r}' \phi_k(\mathbf{r}') \langle f_i | \langle \{n\} | V | \{n_i\} \rangle | f_i \rangle \phi_k(\mathbf{r}')}{E_k - E_k - \omega_n - \varepsilon_i + i\eta} \quad (23)$$

where, as above ω_n is the surface plasmon (or optical phonon) frequency and ε_i is the atomic excitation energy measured from the ground state. The potential is the interaction energy between the atomic charge distribution and the induced surface field

$$V = \int d\mathbf{r}' \rho(\mathbf{r}') \Phi(\mathbf{r} + \mathbf{r}') \quad (24)$$

where $\rho(\mathbf{r})$ is the atomic charge density and Φ is the induced surface field for an isolated charge of eq. (14).

All the necessary sums in eq. (23) can be carried out in a variety of cases. We present here the asymptotic expansion of $\Sigma_i(\mathbf{r})$ for motion perpendicular to the surface [13, 14]

$$\text{Re } \Sigma_i(z) \rightarrow \frac{Ze^2 Q_s^2}{12} \sum_I \frac{\langle f_i | \hat{p} | f_i \rangle^2}{(Q_s^2 + q_i^2)} \frac{1}{z^3} \times \left\{ 1 - \frac{12k_i^2}{(Q_s^2 + q_i^2)^2} \frac{1}{z^2} + \dots \right\} \quad (25)$$

$$\text{Im } \Sigma_i(z) \rightarrow \frac{Ze^2 Q_s^2 k_0}{4} \sum_I \frac{\langle f_i | \hat{p} | f_i \rangle^2}{(Q_s^2 + q_i^2)^2} \frac{1}{z^4} \times \left\{ 1 - \frac{20k_i^2}{(Q_s^2 + q_i^2)^2} \frac{1}{z^2} + \dots \right\} \quad (26)$$

where Z is the atomic charge number, $q_i^2 = 2m\varepsilon_i/\hbar^2$ and \hat{p} is the atomic polarization operator. The leading term in $\text{Re } \Sigma_i(z)$ is the well known Lifshitz form of the Van der Waals potential. The correction terms are energy dependent and the entire imaginary contribution is multiplied by the velocity.

A result of particular interest is what happens to the potential at very small separation distance, because this is where recoil should play a role. However, since all atoms are at least three orders of magnitude more massive than an electron, recoil will play no measurable role whatsoever. On the other hand, a very light atomic system exists, namely positronium. Furthermore positronium is becoming increasingly popular as a surface probe due to a series of recent experiments in which metal surfaces are used as a source of thermal energy positronium after the crystal is bombarded by positrons [16].

We find that for positronium recoil effects have an exponential decay away from the surface governed by the range parameter

$$\alpha = \sqrt{Q_s^2 + q_i^2} = \sqrt{2m(\hbar\omega_s + \varepsilon_i)/\hbar} \approx 2\text{\AA}^{-1}, \quad (27)$$

thus they can extend outward a reasonable distance. Very close to the surface the recoil causes a saturation of the Van der Waals potential. This is most easily shown by considering the atom as a point polarizable dipole in which case the $1/z^3$ attraction weakens to a $1/z$ form

$$\Sigma_i(z) \xrightarrow{z \rightarrow 0} \frac{Ze^2 Q_s^2}{8} \frac{\langle f_i | p^2 | f_i \rangle}{z}. \quad (28)$$

In the general case the surface contribution to the dispersion potential saturates to a constant [17].

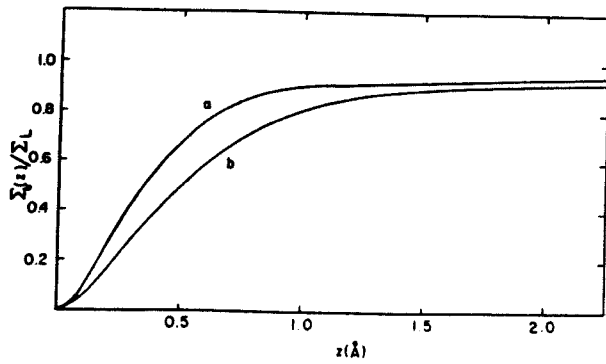


Fig. 2. Ratio of the real part of the atom-surface self-energy $\Sigma_r(z)$ to the semiclassical Lifshitz term as a function of distance z from the surface. Shown are two cases of slow positronium moving perpendicularly to a metal surface. Curve a, 4 eV Ps and Al with $\hbar\omega_s = 11.2$ eV, and curve b, 2 eV Ps and Cs with $\hbar\omega_s = 2.5$ eV.

Figure 2 illustrates the velocity and recoil effects on the positronium-metal self-energy potential. Shown is the ratio of $\text{Re } \Sigma_r(z)$ to the Lifshitz term for slow positronium near an Al and a Cs surface. The saturation due to recoil is evident near the surface, while the reduction of the potential due to finite velocity extends outward to rather large distances.

4. Charge-atom interaction

As an example of the versatility of the self-energy approach we consider the interaction potential between a charge (the projectile) and a hydrogen-like atom (the target). It is well known that the virtual excitation of an atom by a nearby charge gives rise to a polarization force, represented by the dispersion potential

$$\Sigma(R) \xrightarrow{R \rightarrow \infty} -\frac{1}{R^4} \sum_I \frac{|\langle f_I | \hat{z} | f_I \rangle|^2}{\epsilon_I} \quad (29)$$

where R is the separation distance, ϵ_I is again the atomic excitation energy and \hat{z} is the z -component of the atomic polarization operator, and we use atomic units.

The first nonvanishing contribution to the self-energy is again the second order term of eq. (11). If we choose τ_1 and τ_2 as the vectors to the atomic nucleus and to the scattering charge, respectively, and if ϱ is the vector to the atomic electron, the perturbing potential is then

$$V = -\frac{1}{|\tau_1 - \tau_2|} + \frac{1}{|\varrho - \tau_2|}, \quad (30)$$

the sum of the potentials between the incident charge and the atomic nucleus and atomic electron. Since the matrix elements only involve $\phi_k(\mathbf{r})$ and atomic states, the mathematics is straightforward and we quote some of the results. In the asymptotic region the self-energy is expanded as [17]

$$\Sigma_r(R) = -\frac{1}{R^4} \sum_I \frac{|\langle f_I | \hat{z} | f_I \rangle|^2}{\epsilon_I} \left\{ 1 + \frac{i2k_I}{\epsilon_I R} - \frac{6k_I^2}{\epsilon_I^2 R^2} + \dots \right\} \quad (31)$$

The finite velocity weakens the dispersion term with an energy dependent $1/R^2$ correction. In addition there is a conservative imaginary part which is proportional to the velocity. These velocity dependent terms are non-adiabatic corrections. They are a result of the breakdown of the Born-Oppenheimer approximation or the inability of the electronic cloud to faithfully follow the external charge.

Recoil is another non-adiabatic manifestation and it can be readily shown that such effects decay with separation distance as $\exp(-aR)$ with

$$a^2 = \frac{2(m+1)}{m+2} \epsilon_I \approx 2\epsilon_I \quad (32)$$

with m the nuclear mass. At close distances the recoil alone can cause a saturation of the self-energy. The recoil motion effectively spreads out the nuclear and scattering charge into clouds and the interaction energy of these clouds is finite [19].

5. Atom-atom interaction

An extension of the above example is the attractive interaction between two atoms. The dispersion force is the attractive Van der Waals interaction arising from mutual polarization. The calculation follows very closely that for the charge-atom system so we simply state the most important results. The simplest case is for two identical hydrogen-like atoms where the asymptotic expansion is [19]

$$\Sigma_i(R) = \frac{1}{R^6} \sum_{ij} \frac{|Q_{ij}|^2}{\epsilon_i + \epsilon_j} \times \left\{ 1 + \frac{i6k_i}{(m+1)(\epsilon_i + \epsilon_j)R} - \frac{48k_i^2}{(m+1)(\epsilon_i + \epsilon_j)R^2} + \dots \right\} \quad (33)$$

with

$$Q_{ij} = 2\langle f_i | z_1 | f_i \rangle \langle g_j | z_2 | g_j \rangle - \langle f_i | x_1 | f_i \rangle \langle g_j | x_2 | g_j \rangle - \langle f_i | g_j | f_i \rangle \langle g_j | y_2 | g_j \rangle \quad (34)$$

where $|f_i\rangle$ or $|g_j\rangle$ are respectively internal states of the two atoms with corresponding energies ϵ_i and ϵ_j , and m is the nuclear mass. The leading term is the well known London expression for the Van der Waals potential, and the corrections are the velocity dependent non-adiabatic terms [21].

As discussed above, this self-energy formalism is particularly useful for a study of non-adiabatic and recoil effects because the Born-Oppenheimer approximation is not made. The effects of recoil motion are manifest only at small separation distances, decaying exponentially as $\exp(-bR)$ with

$$b^2 = 2\mu(\epsilon_i + \epsilon_j) \quad (35)$$

where μ is the reduced mass of the two atom system, $\mu = (m_1 + 1)(m_2 + 1)/(m_1 + m_2 + 2)$. Again it is clear that one of the atoms must be very light (e.g., positronium) for recoil to be important. At very close distances of approach, the recoil motion causes the nuclear charges to spread into charge clouds and the interaction self-energy saturates to a finite value [19].

V. conclusions

We have in this paper reviewed the method of treating many-particle problems by means of a self-energy. We have reviewed our development of an alternative approach for obtaining the self-energy and applied it to a number of examples involving particle surface interactions and atomic physics. These examples illustrate that the self-energy approach is suitable for a broad range of problems, and is in fact not at all limited to condensed matter applications. For the atomic physics

applications we have shown that the present approach is particularly useful for doing fully quantum mechanical calculations which do not depend on the Born–Oppenheimer approximation. This is of importance for the interactions of atoms with particles of small mass such as electrons, positrons or positronium. In these cases nonadiabatic corrections and recoil at close distances can affect the interaction potential.

Left undiscussed here is a broad range of problems in inelastic scattering and energy loss. Transition rates and energy exchanges are contained in the nonconservative imaginary part of the self energy [22]. Other problems to which this method has recently been applied are a detailed treatment of the interaction of a charge with a surface or metal-insulator interface including the coupling with both bulk and surface modes [23, 24]; and treatments of precursor states to chemical reactions such as the hydrated electron [25].

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