SELF-ENERGIES AND THE INTERACTIONS OF PARTICLES WITH SURFACES

J. R. Manson

Department of Physics and Astronomy
Clemson University
Clemson, South Carolina 29634 USA

R. H. Ritchie

Health and Safety Research Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831 USA

P. M. Echenique

Departamento de Fisica, Facultad de Quimica
Apartado 1072
San Sebastian 20080 Spain

A. Gras-Marti

LCFCA, Department de Fisica
Facultat de Ciències
Universitat d'Alacant
Apt. 99 E-03080 Alacant Spain

SELF-ENERGIES AND THE INTERACTIONS OF PARTICLES WITH SURFACES

J. R. Manson

Department of Physics and Astronomy
Clemson University
Clemson, South Carolina 29634 USA

R. H. Ritchie

Health and Safety Research Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831 USA

P. M. Echenique

Departamento de Fisica, Facultad de Quimica
Apartado 1072
San Sebastian 20080 Spain

A. Gras-Marti

LCFCA, Department de Fisica
Facultat de Ciències
Universitat d'Alacant
Apt. 99 E-03080 Alacant Spain

Self-Energies and the Interactions of Particles with Surfaces

J. R. Manson[α], R. H. Ritchie[β], P. M. Echenique[γ]
and A. Gras-Marti[δ]

[α] Department of Physics and Astronomy,
Clemson University, Clemson, SC 29634.

[β] Health and Safety Research Division,
Oak Ridge National Laboratory, Oak
Ridge, Tennessee 37831, and Department
of Physics, University of Tennessee,
Knoxville, Tennessee 37996.

[γ] Euskal Herriko Unibertsitatea, Kimika
Fakultatea, Donostia, Euskadi, Spain.

[δ] Permanent address: L.C.F.C.A., Department
de Física, Facultat de Ciències, Universitat
d'Alacant, Apt. 99 E-03080 Alacant (Alicante),
Spain.

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 for the cases of a charge approaching a surface
and a charge bound near a surface. Other applications are briefly
discussed.

I. 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 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

$$|i> = \phi_i(\underline{r})|f_i>|\{n_i\}>$$ (1)

where $\phi_i(\underline{r})$ is a spatial wave function in the relative coordinate $\underline{r}$ between

projectile and target, $|f_i>$ is the internal state of the projectile, and $|\{n_i\}>$ is the many body state of the target. The simplest form of the interaction would be a pairwise sum of interactions between all components of the projectile and target,

$$V = \sum_{\substack{i,j \\ i \neq j}} v_a(\underline{r}_i, \underline{r}_j) + \cdots \tag{2}$$

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 $\Sigma(\underline{r}, r', E)$ as[1,2]

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

Here $v(\underline{r})$ 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 $\Sigma_i(r)$ according to

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

which leads to

$$\{-\frac{\hbar^2}{2m} \nabla^2 + v(\underline{r}) + \Sigma_i(\underline{r})\}\phi_i(\underline{r}) = E_i\phi_i(\underline{r}) \tag{5}$$

This is basically a quasiparticle equation and $\Sigma_i(\underline{r})$ 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.

II. 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 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).

$$\Delta E = \Sigma \; \frac{<i|V|\ell><\ell|V|i>}{E_i - E_\ell + i\epsilon}$$

$$+ \underset{\ell,\ell'}{\Sigma} \; \frac{<i|V|\ell><\ell|V|\ell'><\ell'|V|i>}{(E_i - E_\ell + i\epsilon)(E_i - E_{\ell'} + i\epsilon)} \qquad (6)$$

$$+ \underset{\ell,\ell',\ell''}{\Sigma} \; \frac{<i|V|\ell><\ell|V|\ell'><\ell'|V|\ell''><\ell''|V|i>}{(E_i - E_\ell + i\epsilon)(E_i - E_{\ell'} + i\epsilon)(E_i - E_{\ell''} + i\epsilon)} + \cdots$$

where we have ignored the first order term since it usually vanishes, or else can be included in the average potential. Recall that the many-body matrix elements are of the form

$$<i|V|\ell> = \int d\underline{r} \; \phi_i^*(\underline{r})<f_i|<\{n_i\}|V|\{n_\ell\}>|f_\ell>\phi_\ell(\underline{r}) \qquad (7)$$

with ℓ the collective quantum index for the set $(\underline{k}_\ell,\; f_\ell,\; \{n_\ell\})$ and the unperturbed energies will be

$$E_\ell = E_{\underline{k}_\ell} + E_{f_\ell} + E^c_{\{n_\ell\}} \quad , \qquad (8)$$

the sum of the translation energy of the projectile $E_{\underline{k}_\ell}$, the internal excitation energy of the projectile E_{f_ℓ}, and the collective energy of the target system $E^c_{\{n_\ell\}}$.

We can rewrite the perturbation series in mixed representation

$$\Delta E = \int d\underline{r} \; \underset{\ell}{\Sigma} \; \frac{\phi_i^*(\underline{r})<f_i|\{n_i\}|V|\{n_\ell\}>|f_\ell>\phi_\ell(\underline{r})<\ell|V|i>}{(E_i - E_\ell + i\epsilon)}$$

$$\qquad (9)$$

$$+ \int d\underline{r} \; \underset{\ell,\ell'}{\Sigma} \; \frac{\phi_i^*(\underline{r})<f_i|\{n_i\}|V|\{n_\ell\}>|f_\ell>\phi_\ell(\underline{r})<\ell|V|\ell'><\ell'|V|i>}{(E_i - E_\ell + i\epsilon)(E_i - E_{\ell'} + i\epsilon)} + \cdots$$

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 $\Sigma_i(\underline{r})$, weighted by the probability density of the projectile in its original state.

$$\Delta E_o = \int d\underline{r} \; \phi_i^*(\underline{r}) \; \Sigma_i(\underline{r}) \; \phi_i(\underline{r}) \qquad (10)$$

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

$$\Sigma_i(\underline{r}) \ \phi_i(\underline{r}) = \sum_{\ell} \frac{\phi_\ell(\underline{r}) <f_i|<\{n_i\}|V|\{n_\ell\}>|f_\ell><\ell|V|i>}{(E_i - E_\ell + i\epsilon)}$$

$$+ \sum_{\ell,\ell'} \frac{\phi_\ell(\underline{r}) <f_i|<\{n_i\}|V|\{n_\ell\}>|f_\ell><\ell|V|\ell'><\ell'|V|i>}{(E_i - E_\ell + i\epsilon)(E_i - E_{\ell'} + i\epsilon)} + \cdots \quad (11)$$

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 many cases which we have examined, this approach reproduces the self-energy obtained from the usual definitions of the correlation and exchange potential.

We note in passing that this 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 the nonlocal self-energy 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 $\Sigma(\underline{r},\underline{r}',E_i)$ is obtained by equating integrands between eq. (4) and eq. (11):

$$\Sigma(\underline{r},\underline{r}',E_i) = \sum_\ell \frac{\phi_\ell(\underline{r}) <f_i|<\{n_i\}|V|\{n_\ell\}>|f_\ell><f_\ell|\{n_\ell\}|V|\{n_i\}>|f_i>\phi_\ell^*(\underline{r}')}{E_i - E_\ell + i\epsilon} + \cdots \quad (12)$$

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

We have also tacitly assumed in this treatment that the initial state of the target $|\{n_i\}>$ 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.

III. General Form of the Self-Energy

The form of $\Sigma_i(\underline{r})$ 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

$$\Sigma_i(\underline{r}) = \sum_{k_\ell, f_\ell\{n_\ell\}} \frac{\phi_\ell(\underline{r})}{\phi_i(\underline{r})} \frac{\langle f_i|\langle\{n_i\}|V|\{n_\ell\}\rangle|f_\ell\rangle\langle\ell|V|i\rangle}{E_i - E_\ell + i\epsilon} \tag{13}$$

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 $\Sigma_i(\underline{r})$ 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.[4] 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 $\Sigma_i(\underline{r})$ 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.

IV. Examples

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. 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 its velocity because the collective electronic excitations of the surface cannot follow faithfully the motion of the charge. 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

$$V = \phi(\underline{r}) = \alpha \sum_{\underline{Q}} \Gamma_Q e^{-Q|z|+i\underline{Q}\cdot\underline{R}} (a_Q^+ - a_{-Q}) \tag{14}$$

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

$$\alpha = \frac{\varepsilon_o - 1}{\varepsilon_o - 1} - \frac{\varepsilon_\infty - 1}{\varepsilon_\infty - 1} \tag{15}$$

For the remainder of this paper 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 $\phi_\ell(\underline{r})$ the second order term for $\Sigma_i(\underline{r})$ 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

$$\text{Re } \Sigma_i(z) \underset{z \to \infty}{\to} - \frac{e^2}{4|z|} \left\{ 1 - \frac{v^2}{2\omega_s z^2} + \cdots \right\} \tag{16}$$

$$\text{Im } \Sigma_i(z) \underset{z \to \infty}{\to} \frac{e^2 v}{8\omega_s} \frac{1}{z^2} \left\{ 1 - \frac{3v^2}{2\omega_s z^2} + \cdots \right\} \tag{17}$$

where v is the speed of the charge. These asymptotic series can be expressed in closed form in terms of exponential integrals.[3] 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 $\Sigma_i(r)$ which varies inversely as v:

$$\Sigma_i(z) \underset{z \to \infty}{\to} - \frac{\pi e^2 \omega_s}{2v} \left\{ 1 - \frac{i}{\pi} \ln \left[1 - \frac{\sqrt{1 - 2\,\hbar\omega_s/mv^2}}{1 - \hbar\omega_s/mv^2} \right] \right\} \tag{18}$$

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[5-8] 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

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

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

$$v(z) = -\hbar^2 \lambda_o m \delta(z) \quad . \tag{20}$$

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

$$\phi_o(z) = \sqrt{\lambda_o} \, e^{-\lambda_o z} \quad . \tag{21}$$

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:

$$\Sigma_i(z) \underset{z \to \infty}{\to} -\frac{e^2}{4z} \left\{ 1 + \frac{\lambda_o}{z} + \cdots \right\} \tag{22}$$

The higher order correction terms depend on energy similarly to eq. (16). Eq. (22) is essentially the same result obtained by Jonson[12] 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.

V. Conclusions

We have in this paper reviewed the method of treating many-body problems by means of an effective interaction self-energy. We have developed an alternative approach to the self-energy which is simpler and more straight-forward than standard methods, and we have illustrated its use with two examples of a charge interacting with a metal surface. In each case the self-energy produces the classical image potential together with corrections due to quantum mechanical effects.

This method has also been successfully applied to the problem of an atom interacting with a surface. Corrections to the Van der Waals dispersion force are obtained, and via the non-conservative imaginary parts to $\Sigma_i(z)$ we discuss transition rates and energy exchange.[13]

However, the method is not limited to the interactions of charges or atoms with condensed matter. It has been successfully applied to the problem of a charge or atom (viewed as the projectile) interacting with another atom (the target). Here, the fully quantum mechanical nature of this self-energy approach facilitates the discussion of non-adiabatic and recoil effects which arise in situations where the Born-Oppenheimer approximation is not valid, for example when an electron, positron or positronium interacts with an atom.[14]

References

1. L. Hedin and S. Lundqvist, Solid State Phys. **23**, 1 (1969).

2. John C. Inkson, Surf. Sci. **28**, 69 (1971).

3. J. R. Manson and R. H. Ritchie, Phys. Rev. B **24**, 4867 (1981).

4. F. Flores and F. Garcia-Moliner, J. Phys. C **12**, 907 (1979).

5. M. Sunjic, G. Toulouse and A. A. Lucas, Solid State Commun. **11**, 1629 (1972).

6. R. Ray and G. D. Mahan, Phys. Lett. **42A**, 301 (1972).

7. D. Chan and P. Richmond, Surf. Sci. **39**, 437 (1973).

8. J. Heinrichs, Phys. Rev. B **8**, 1346 (1973).

9. E. Evans and D. L. Mills, Phys. Rev. B **8**, 4004 (1973).

10. R. M. Nieminen and C. H. Hodges, Phys. Rev. B **18**, 2568 (1978).

11. P. M. Echenique, A. Gras-Marti, J. R. Manson and R. H. Ritchie, to be published.

12. M. Jonson, Solid State Comm. **33**, 743 (1980).

13. J. R. Manson and R. H. Ritchie, Phys. Rev. B **29**, 1084 (1984); J. R. Manson, R. H. Ritchie and T. L. Ferrell, Phys. Rev. B **29**, 1080 (1984).

14. J. R. Manson and R. H. Ritchie, Phys. Rev. Lett. **54**, 785 (1985); Phys. Rev. A **32**, 3782 (1985).
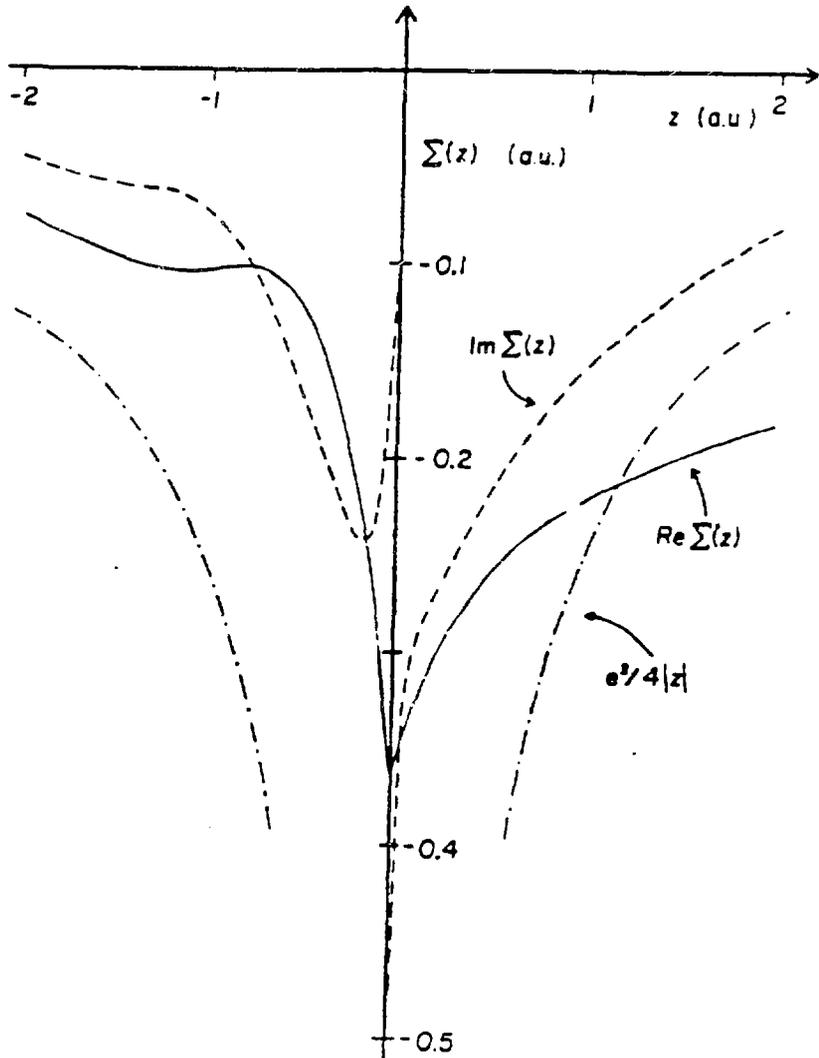
Figure 1. The self-energy of an electron near a metal surface. The real and
imaginary parts of $\Sigma_i(z)$ are compared to the classical image
potential with $\omega_s = 0.5$ au and $v = 2.0$ au.

END

DATE FILMED

07 / 06 / 88

CONF-870155--9

DE88 010451

DISCLAIMER

SELF-ENERGIES AND THE INTERACTIONS OF PARTICLES WITH SURFACES

J. R. Manson

Department of Physics and Astronomy
Clemson University
Clemson, South Carolina 29634 USA

R. H. Ritchie

Health and Safety Research Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831 USA

P. M. Echenique

Departamento de Fisica, Facultad de Quimica
Apartado 1072
San Sebastian 20080 Spain

A. Gras-Marti

LCFCA. Department de Fisica
Facultat de Ciències
Universitat d'Alacant
Apt. 99 E-03080 Alacant Spain

SELF-ENERGIES AND THE INTERACTIONS OF PARTICLES WITH SURFACES

J. R. Manson

Department of Physics and Astronomy
Clemson University
Clemson, South Carolina 29634 USA

R. H. Ritchie

Health and Safety Research Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831 USA

P M. Echenique

Departamento de Fisica, Facultad de Quimica
Apartado 1072
San Sebastian 20080 Spain

A. Gras-Marti

LCFCA, Department de Fisica
Facultat de Ciències
Universitat d'Alacant
Apt. 99 E-03080 Alacant Spain

Self-Energies and the Interactions of Particles with Surfaces

J. R. Manson[a], R. H. Ritchie[b], P. M. Echenique[c]
and A. Gras-Marti[d]

[a] Department of Physics and Astronomy,
Clemson University, Clemson, SC 29634.

[b] Health and Safety Research Division,
Oak Ridge National Laboratory, Oak
Ridge, Tennessee 37831, and Department
of Physics, University of Tennessee,
Knoxville, Tennessee 37996.

[c] Euskal Herriko Unibertsitatea, Kimika
Fakultatea, Donostia, Euskadi, Spain.

[d] Permanent address: L.C.F.C.A., Department
de Física, Facultat de Ciències, Universitat
d'Alacant, Apt. 99 E-03080 Alacant (Alicante),
Spain.

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 for the cases of a charge approaching a surface
and a charge bound near a surface. Other applications are briefly
discussed.

I. 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 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

$$|i> = \phi_i(\underline{r}) |f_i>|\{n_i\}> \qquad (1)$$

where $\phi_i(\underline{r})$ is a spatial wave function in the relative coordinate $\underline{r}$ between

projectile and target, $|f_i\rangle$ is the internal state of the projectile, and $|\{n_i\}\rangle$ is the many body state of the target. The simplest form of the interaction would be a pairwise sum of interactions between all components of the projectile and target,

$$V = \sum_{\substack{i,j \\ i \neq j}} v_a(\underline{r}_i, \underline{r}_j) + \cdots \tag{2}$$

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 $\Sigma(\underline{r},r',E)$ as[1,2]

$$\{-\frac{\hbar^2}{2m}\nabla^2 + v(\underline{r})\}\phi_i(\underline{r}) + \int d\underline{r}' \; \Sigma(\underline{r},\underline{r}',E_i)\phi_i(\underline{r}') = E_i\phi_i(\underline{r}) \tag{3}$$

Here $v(\underline{r})$ 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 $\Sigma_i(r)$ according to

$$\Sigma_i(\underline{r})\phi_i(\underline{r}) = \int d\underline{r}' \; \Sigma(\underline{r},\underline{r}',E_i)\phi_i(\underline{r}') \tag{4}$$

which leads to

$$\{-\frac{\hbar^2}{2m}\nabla^2 + v(\underline{r}) + \Sigma_i(\underline{r})\}\phi_i(\underline{r}) = E_i\phi_i(\underline{r}) \tag{5}$$

This is basically a quasiparticle equation and $\Sigma_i(\underline{r})$ 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.

II. 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 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).

$$\Delta E = \Sigma \frac{<i|V|\ell><\ell|V|i>}{E_i - E_\ell + i\epsilon}$$

$$+ \sum_{\ell,\ell'} \frac{<i|V|\ell><\ell|V|\ell'><\ell'|V|i>}{(E_i - E_\ell + i\epsilon)(E_i - E_{\ell'} + i\epsilon)} \tag{6}$$

$$+ \sum_{\ell,\ell',\ell''} \frac{<i|V|\ell><\ell|V|\ell'><\ell'|V|\ell''><\ell''|V|i>}{(E_i - E_\ell + i\epsilon)(E_i - E_{\ell'} + i\epsilon)(E_i - E_{\ell''} + i\epsilon)} + \cdots$$

where we have ignored the first order term since it usually vanishes, or else can be included in the average potential. Recall that the many-body matrix elements are of the form

$$<i|V|\ell> = \int d\underline{r}\ \phi_i^*(\underline{r})<f_i|<\{n_i\}|V|\{n_\ell\}>|f_\ell>\phi_\ell(\underline{r}) \tag{7}$$

with ℓ the collective quantum index for the set $(\underline{k}_\ell,\ f_\ell,\ \{n_\ell\})$ and the unperturbed energies will be

$$E_\ell = E_{\underline{k}_\ell} + E_{f_\ell} + E^c_{\{n_\ell\}} \quad, \tag{8}$$

the sum of the translation energy of the projectile $E_{\underline{k}_\ell}$, the internal excitation energy of the projectile E_{f_ℓ}, and the collective energy of the target system $E^c_{\{n_\ell\}}$.

We can rewrite the perturbation series in mixed representation

$$\Delta E = \int d\underline{r}\ \sum_\ell \frac{\phi_i^*(\underline{r})<f_i|\{n_i\}|V|\{n_\ell\}>|f_\ell>\phi_\ell(\underline{r})<\ell|V|i>}{(E_i - E_\ell + i\epsilon)}$$

$$+ \int d\underline{r}\ \sum_{\ell,\ell'} \frac{\phi_i^*(\underline{r})<f_i|\{n_i\}|V|\{n_\ell\}>|f_\ell>\phi_\ell(\underline{r})<\ell|V|\ell'><\ell'|V|i>}{(E_i - E_\ell + i\epsilon)(E_i - E_{\ell'} + i\epsilon)} + \cdots \tag{9}$$

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 $\Sigma_i(\underline{r})$, weighted by the probability density of the projectile in its original state.

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

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

$$\Sigma_i(\underline{r}) \ \phi_i(\underline{r}) = \sum_{\ell} \frac{\phi_\ell(\underline{r}) <f_i|<\{n_i\}|V|\{n_\ell\}>|f_\ell><\ell|V|i>}{(E_i - E_\ell + i\epsilon)}$$

$$+ \sum_{\ell,\ell'} \frac{\phi_\ell(\underline{r}) <f_i|<\{n_i\}|V|\{n_\ell\}>|f_\ell><\ell|V|\ell'><\ell'|V|i>}{(E_i - E_\ell + i\epsilon)(E_i - E_{\ell'} + i\epsilon)} + \cdots \tag{11}$$

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 many cases which we have examined, this approach reproduces the self-energy obtained from the usual definitions of the correlation and exchange potential.

We note in passing that this 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 the nonlocal self-energy 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 $\Sigma(\underline{r},\underline{r}',E_i)$ is obtained by equating integrands between eq. (4) and eq. (11):

$$\Sigma(\underline{r},\underline{r}',E_i) = \sum_{\ell} \frac{\phi_\ell(\underline{r}) <f_i|<\{n_i\}|V|\{n_\ell\}>|f_\ell><f_\ell|\{n_\ell\}|V|\{n_i\}>|f_i>\phi_\ell^*(\underline{r}')}{E_i - E_\ell + i\epsilon} + \cdots \tag{12}$$

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

We have also tacitly assumed in this treatment that the initial state of the target $|\{n_i\}>$ 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.

III. General Form of the Self-Energy

The form of $\Sigma_i(\underline{r})$ 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

$$\Sigma_i(\underline{r}) = \sum_{\underline{k}_\ell, f_\ell\{n_\ell\}} \frac{\phi_\ell(\underline{r})}{\phi_i(\underline{r})} \frac{<f_i|<\{n_i\}|V|\{n_\ell\}>|f_\ell><\ell|V|i>}{E_i - E_\ell + i\varepsilon} \tag{13}$$

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 $\Sigma_i(\underline{r})$ 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.[4] 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 $\Sigma_i(\underline{r})$ 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.

IV. Examples

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. 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 its velocity because the collective electronic excitations of the surface cannot follow faithfully the motion of the charge. 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

$$V = \phi(\underline{r}) = \alpha \sum_{\underline{Q}} \Gamma_Q e^{-Q|z|+i\underline{Q}\cdot\underline{R}} (a_Q^+ - a_{-Q}) \tag{14}$$

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

$$\alpha = \frac{\epsilon_o - 1}{\epsilon_o - 1} - \frac{\epsilon_\infty - 1}{\epsilon_\infty - 1} \tag{15}$$

For the remainder of this paper 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 $\phi_\ell(\underline{r})$ the second order term for $\Sigma_i(\underline{r})$ 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

$$\text{Re } \Sigma_i(z) \underset{z \to \infty}{\to} - \frac{e^2}{4|z|} \left\{ 1 - \frac{v^2}{2\omega_s z^2} + \cdots \right\} \tag{16}$$

$$\text{Im } \Sigma_i(z) \underset{z \to \infty}{\to} \frac{e^2 v}{8\omega_s} \frac{1}{z^2} \left\{ 1 - \frac{3v^2}{2\omega_s z^2} + \cdots \right\} \tag{17}$$

where v is the speed of the charge. These asymptotic series can be expressed in closed form in terms of exponential integrals.[3] 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 $\Sigma_i(r)$ which varies inversely as v:

$$\Sigma_i(z) \underset{z \to \infty}{\to} - \frac{\pi e^2 \omega_s}{2v} \left\{ 1 - \frac{1}{\pi} \ln \left[1 - \frac{\sqrt{1 - 2\hbar\omega_s/mv^2}}{1 - \hbar\omega_s/mv^2} \right] \right\} \tag{18}$$

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[5-8] 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

$$\Sigma_i(z) = - \frac{e^2}{4|z|} \left\{ 1 - e^{-Q_s|z|} + Q_s|z| \, E_z(Q_s|z|) \right\} \tag{19}$$

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

$$v(z) = -\hbar^2 \lambda_o m \delta(z) \quad . \tag{20}$$

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

$$\phi_o(z) = \sqrt{\lambda_o} \; e^{-\lambda_o z} \quad . \tag{21}$$

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:

$$\Sigma_i(z) \underset{z \to \infty}{\to} -\frac{e^2}{4z} \left\{ 1 + \frac{\lambda_o}{z} + \cdots \right\} \tag{22}$$

The higher order correction terms depend on energy similarly to eq. (16). Eq. (22) is essentially the same result obtained by Jonson[12] 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.

V. Conclusions

We have in this paper reviewed the method of treating many-body problems by means of an effective interaction self-energy. We have developed an alternative approach to the self-energy which is simpler and more straight-forward than standard methods, and we have illustrated its use with two examples of a charge interacting with a metal surface. In each case the self-energy produces the classical image potential together with corrections due to quantum mechanical effects.

This method has also been successfully applied to the problem of an atom interacting with a surface. Corrections to the Van der Waals dispersion force are obtained, and via the non-conservative imaginary parts to $\Sigma_i(z)$ we discuss transition rates and energy exchange.[13]

However, the method is not limited to the interactions of charges or atoms with condensed matter. It has been successfully applied to the problem of a charge or atom (viewed as the projectile) interacting with another atom (the target). Here, the fully quantum mechanical nature of this self-energy approach facilitates the discussion of non-adiabatic and recoil effects which arise in situations where the Born-Oppenheimer approximation is not valid, for example when an electron, positron or positronium interacts with an atom.[14]

Acknowledgements

References

1. L. Hedin and S. Lundqvist, Solid State Phys. **23**, 1 (1969).

2. John C. Inkson, Surf. Sci. **28**, 69 (1971).

3. J. R. Manson and R. H. Ritchie, Phys. Rev. B **24**, 4867 (1981).

4. F. Flores and F. Garcia-Moliner, J. Phys. C **12**, 907 (1979).

5. M. Sunjic, G. Toulouse and A. A. Lucas, Solid State Commun. **11**, 1629 (1972).

6. R. Ray and G. D. Mahan, Phys. Lett. **42A**, 301 (1972).

7. D. Chan and P. Richmond, Surf. Sci. **39**, 437 (1973).

8. J. Heinrichs, Phys. Rev. B **8**, 1346 (1973).

9. E. Evans and D. L. Mills, Phys. Rev. B **8**, 4004 (1973).

10. R. M. Nieminen and C. H. Hodges, Phys. Rev. B **18**, 2568 (1978).

11. P. M. Echenique, A. Gras-Marti, J. R. Manson and R. H. Ritchie, to be published.

12. M. Jonson, Solid State Comm. **33**, 743 (1980).

13. J. R. Manson and R. H. Ritchie, Phys. Rev. B **29**, 1084 (1984); J. R. Manson, R. H. Ritchie and T. L. Ferrell, Phys. Rev. B **29**, 1080 (1984).

14. J. R. Manson and R. H. Ritchie, Phys. Rev. Lett. **54**, 785 (1985); Phys. Rev. A **32**, 3782 (1985).
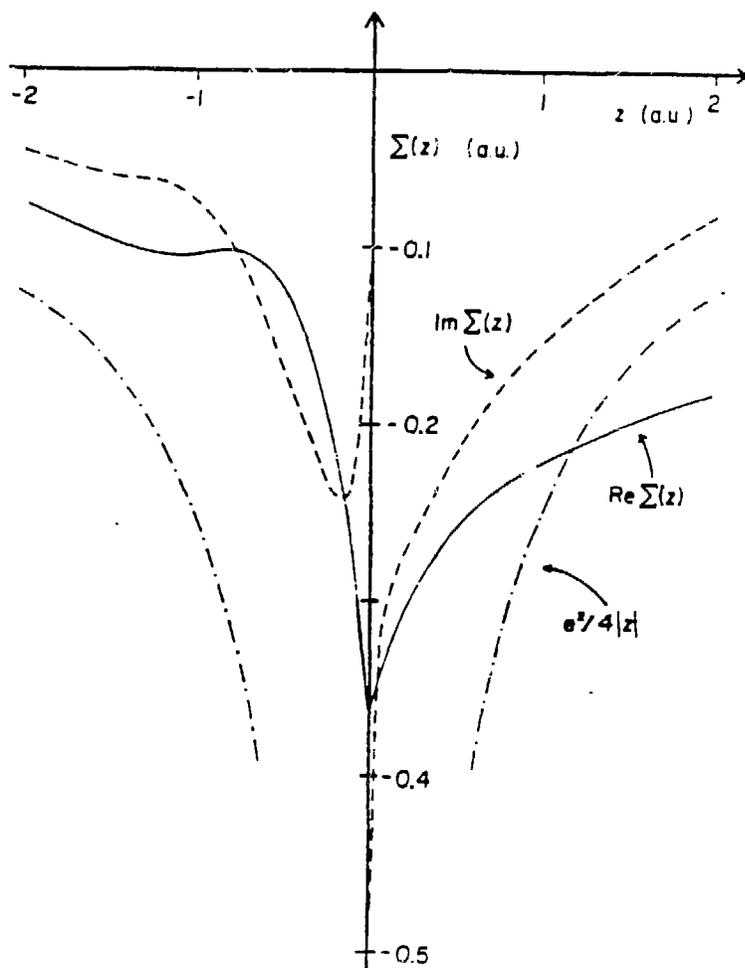
Figure 1. The self-energy of an electron near a metal surface. The real and
imaginary parts of $\Sigma_i(z)$ are compared to the classical image
potential with $\omega_s = 0.5$ au and $v = 2.0$ au.