Quantum reflection in the presence of dissipation

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(Received 30 November 1987)

We present a perturbation treatment of the scattering of low-energy long–de Broglie–wavelength electrons scattering from the surface of liquid helium in the presence of ripplonic effects. We analyze the problem in the so-called distorted-wave Born approximation and consider higher-order terms in perturbation theory. We show explicitly how quantum-mechanical effects enter in to modify the behavior of the reflection coefficient.

I. INTRODUCTION

The physics of a surface inelastic scattering experiment, when the incoming probe has very low energy, is rather unusual and intimately related to the quantum nature of the incoming particle. A correct quantum-mechanical treatment of scattering from a surface in the presence of strong inelastic scattering is at the core of a number of physically interesting situations including sticking, and the scattering of monoenergetic probes like helium from surfaces.

The essence of the problem is easily illustrated by a simple example. Imagine a potential well of depth V_0 and range l near some surface (Fig. 1). In addition, we wish to include some type of dissipative coupling of the particle when it is in the neighborhood of the surface. If, for a classical particle, we model the dissipative coupling by a frictional force then it will suffer a finite energy loss ΔE as it is accelerated in the potential well. For incident energies E small compared to ΔE the particle is trapped by the well so a classical particle has a sticking probability $\alpha(E)\rightarrow 1$ as $E\rightarrow 0$.[1] However, because of the low energy, an incoming particle of mass m has a de Broglie wavelength $\xi_E=\hbar/(2mE)^{1/2}$ which can be much larger than l. In this case quantum effects would seem to suppress the low-energy absorption probability since the bulk of the wave packet remains far from the surface. More specifically, in the so-called distorted-wave Born approximation[2] (DWBA) there is a wavelength mismatch between the wave function ψ inside and outside the well (Fig. 1). Matching ψ and ψ' at the step gives an amplitude reduction $T\approx 2\sqrt{E/V_0}$ in the well. The probability to be in the well is proportional to $|T|^2$, so that for a finite rate of emission, $\alpha(E)\approx\sqrt{E}$ for $E\ll V_0$ because the time spent near the surface only increases as $1/\sqrt{E}$. This means that for a quantum particle $\alpha(E)\rightarrow 0$ as $E\rightarrow 0$.

For low energies, based on such arguments, predictions of classical or semiclassical models are indeed in wild disagreement with quantum perturbation theory.[3] However, it is possible that higher-order inelastic effects could suppress phase coherence for the incoming particle, i.e., destroy our wave-function mismatch argument and validate the classical method. The question whether quantum reflection is or is not suppressed by inelastic scattering has an analog for waves traveling across an interface between two media of different refractive index whose transmission coefficients are also suppressed because of "impedance" mismatch. They may have an enhanced transmission coefficient because of inelastic scattering, as in the well-known case of Kapitza resistance.[4]

To gain some physical insight into the physical effects of quantum reflection on the differential cross section for low-energy inelastic scattering, we will discuss in detail a rather special case: inelastic scattering of electrons from bulk ^{4}He surfaces.[5] The great advantage of this case is that the surface potential is well understood and of the Coulomb form.[6] Thus *analytic* expressions for the probe wave function in the rigid potential are available, the interaction potential with surface phonons is known in detail, and ^{4}He surfaces are clean and uncontaminated. In addition the one-dimensional (1D) Coulomb potential or image potential which an incoming electron experiences is in a real sense the smoothest realistic potential. Unlike the simple square-well type of potential discussed it has no characteristic range l and quantum reflection effects from sudden changes in potential will be minimized. If quantum reflection is significant in the Coulomb case, it will certainly be so for other potentials.

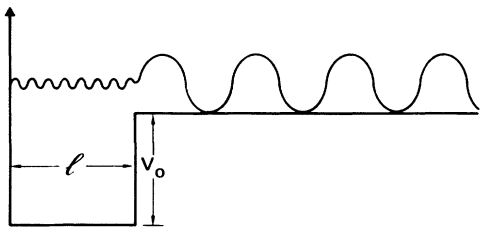

FIG. 1. Amplitude reduction of an incoming low-energy plane wave in a rectangular potential well of depth V_0 due to quantum reflection at the threshold of the well.

In this paper we will explicitly calculate the quantum reflection and sticking coefficients, for an electron incident on bulk ^{4}He, in the DWBA. We will also be able to estimate the range of validity of this perturbation expansion, by considering higher-order terms in perturbation theory.

II. ELECTRON-RIPPLON HAMILTONIAN

The Hamiltonian which characterizes our problem is given by

$$H = H_e + H_{\text{ripplon}} + H_{\text{int}} \ . \tag{1}$$

Here

$$H_e = \mathbf{p}^2/2m + V(z) \ . \tag{2}$$

$V(z)$ is the static image potential seen by an electron approaching a surface of bulk ^{4}He, i.e.,

$$V(z) = -\frac{\Lambda_0}{z}, \quad 0 < z < \infty \tag{3}$$

$$= V_0, \quad z < 0 \ . \tag{4}$$

The squared "effective charge" for the ^{4}He (dielectric constant ϵ_1) vacuum interface is

$$\Lambda_0 = \frac{e^2}{4}\frac{(\epsilon_1 - 1)}{(\epsilon_1 + 1)} \ . \tag{5}$$

The negative of the electron affinity $V_0 \cong 1$ eV is the energy required to put an electron into the helium assuming no bubble formation. The bound states of ^{4}He thus have a hydrogenlike spectrum $E_n = -E_R/n^2 (n = 1,2,\ldots)$. The corresponding Rydberg energy $E_R = m\Lambda_0^2/2\hbar^2$ is of order 10 K and the Bohr radius $a_B = \hbar^2/m\Lambda_0$ is of order 100 Å.

The quantity H_{ripplon} characterizes the long-wavelength normal mode vibrations (ripplons) of the free ^{4}He surface, i.e.,

$$H_{\text{ripplon}} = \sum_{\mathbf{q}} b_q^\dagger b_{\mathbf{q}} \omega_q \ , \tag{6}$$

where

$$\omega_q^2 = gq + (\sigma/\rho)q^3 \ . \tag{7}$$

Here g is the gravitational constant, σ the surface tension, and ρ the density of ^{4}He and q is the magnitude of the in-plane wave vector of the ripplon.

Equation (7) is the result of hydrodynamic arguments[7] and is accurate as long as the inverse wave vector q^{-1} is large compared to atomic (angstrom) distances. In our calculation we will be interested in electrons with energies in the 1 K range, i.e., with wavelengths $\xi_E \cong 10^2$ Å. The ripplons of importance will have comparable wave vectors. The energies of such ripplons ($\sigma/\rho \cong 1$ cm^3/sec^2) are approximately 10^{-2} K, i.e., very small. The gravitational term in Eq. (7) can be neglected for wave vectors in this range.

If $V(z)$ is the interaction potential between electrons and a flat ^{4}He surface, then a deformation $u(\mathbf{r}_\parallel)$ in the height of the surface will lead to a correction term. If $V(z)$ is only due to interaction between the electron and the surface immediately below it, hence independent of the shape of the surface away from the point of impact, then the corrected potential is just $V[z + u(\mathbf{r}_\parallel)]$ where $\mathbf{r}_\parallel$ is the impact point. For $z \gg u$, we expand

$$V[z + u(\mathbf{r}_\parallel)] \cong V(z) + u(\mathbf{r}_\parallel) V'(z) \ . \tag{8}$$

After quantization of $u(\mathbf{r}_\parallel)$, the interaction Hamiltonian becomes

$$H_{\text{int}} = \frac{1}{\sqrt{S}} \sum_{\mathbf{q}} Q_q V_q'(z)(a_{\mathbf{q}} + a_{-\mathbf{q}}^\dagger)\exp(i\mathbf{q}\cdot\mathbf{r}_\parallel) \ , \tag{9}$$

with $V_q'(z) = \Lambda_0/z^2$ and $Q_q = (\hbar q/2\rho\omega_q)^{1/2}$. This cannot be quite right because it allows $\mathbf{q}=0$ electron-ripplon coupling. A uniform shift of the ^{4}He surface (a $\mathbf{q}=0$ ripplon) should not affect the scattering probability.

Because of the long-range nature of the Coulomb potential the image potential of the electron does, however, depend on the shape of the surface away from the impact point. Shikin and Monarkha[6] showed that this leads to large corrections to $V_q(z)$ for $qz \ll 1$:

$$V_q'(z) = \frac{\Lambda_0}{z^2} - \frac{\Lambda_0}{z} q K_1(qz) \ , \tag{10}$$

with K_1 the modified Bessel function.

For $x \ll 1$,

$$K_1(x) \simeq \frac{1}{x} + \tfrac{1}{2} x \ln(x/2) \ , \tag{11}$$

so the interaction potential $V_q(z)$ depends on q as $q^2 z \ln(qz)$ for long-wavelength ripplons ($qz \ll 1$). The electron-ripplon scattering cross section is thus suppressed in the specular scattering direction ($q \to 0$), i.e., the interaction is short ranged and there is no coupling to $q=0$ ripplons. This is somewhat similar to scattering of electrons from acoustic phonons in bulk metals by a deformation potential which leads to a $q^{1/2}$ dependence in the electron-phonon matrix element.

For $x \gg 1$,

$$K_1(x) \simeq \sqrt{\pi/2x}\, e^{-x} \ , \tag{12}$$

so for short-wavelength ripplons ($qz \gg 1$), the interaction potential is independent of q and falls off as $1/z^2$ as expected from our naive argument [Eq. (8)].

III. LOWEST-ORDER INELASTIC SCATTERING

The rate of an incoming electron, with energy E_i, to scatter from the helium surface (assumed to be at $T=0$) and emerge with an energy E_f leaving the helium surface with a single-phonon excitation is given by the golden rule

$$W = \frac{2\pi}{\hbar} \sum_f |\langle f | H_{\text{int}} | i \rangle|^2 \delta(\epsilon_f - \epsilon_i) \ . \tag{13}$$

The state $|i\rangle$ is a product of an incoming electron wave function $e^{-i\mathbf{k}_\parallel^i \cdot \mathbf{r}} \psi_i(z)$ in the rigid Coulomb potential with all ripplons in their ground state, i.e., $\epsilon_i = E_i$ the electron energy. The state $|f\rangle$ is the product of an outgoing

electron wave function $e^{-i\mathbf{k}_\parallel^f\cdot\mathbf{r}}\psi_f(z)$ and a single excited ripplon consistent with energy and momentum conservation. Here $\mathbf{k}_\parallel$ is the component of $\mathbf{k}$ in the scattering surface. The scattering geometry is shown in Fig. 2. The final-state energy is thus,

$$\epsilon_f = E_f + \hbar\omega_q \ . \tag{14}$$

The matrix element in Eq. (13) reduces to

$$\langle f \mid H_{\text{int.}} \mid i \rangle = M\delta(\mathbf{k}_\parallel^i - \mathbf{k}_\parallel' - \mathbf{q}) \ , \tag{15}$$

where M is the electronic part of the matrix element which for fixed $\mathbf{q}$ is

$$M = \frac{(2\pi)^2}{\sqrt{S}} Q_q \langle \psi_f(z) \mid V_q'(z) \mid \psi_i(z) \rangle \ . \tag{16}$$

In an actual experiment at 1 K we are, relative to typical ripplon energies, at high temperatures. Thus we should, in principle, consider a thermal distribution of initial states, i.e., the possibility of emission and absorption of ripplons. The essential quantum-mechanical aspects of the problem are, however, illustrated by considering the $T=0$ situation which only involves ripplon emission.

The momentum δ function in Eq. (15) puts very few restrictions on the scattering process since $\mathbf{q}$ is a two-dimensional phonon wave vector. There is no conservation of momentum in the z direction, i.e., the surface provides arbitrary momentum in that direction and as we shall see, it is almost always possible to satisfy the energy momentum delta functions. Surface sound excitation is thus somewhat similar to Bremsstrahlung. In the following we consider separately the two cases of scattering of the particle into the continuous spectrum of outgoing states (A) and into the discrete spectrum of bound states (B).

A. Continuum scattering

In this case the differential rate to scatter into some solid angle is given by

$$\frac{dW}{d\Omega} = \frac{1}{\hbar}\frac{VS}{(2\pi)^2}\int \mid \langle \psi_f(z) \mid V_q'(z) \mid \psi_i(z) \rangle \mid^2 Q_q^2 k^{f\,2} dk^f \delta(E_f - E_i - \hbar\omega_q) \ , \tag{17}$$

where $\mathbf{q} = \mathbf{k}_\parallel^i - \mathbf{k}_\parallel^f$ and V is the scattering volume. Since $k^f \simeq k^i$, the usual triangle construction (Fig. 2) gives, for q and ϕ_f in the angle the ripplon wave vector makes with the plane of incidence.

$$q \simeq k^i(\sin^2\theta^i + \sin^2\theta^f + 2\sin\theta^i\sin\theta^f\cos\phi^f)^{1/2} \ , \tag{18a}$$

$$\phi_q \simeq \pi + \frac{\phi^f}{2} \ . \tag{18b}$$

The angles θ^i, θ^f, and ϕ^f are defined in Fig. 2. Since $\hbar\omega_q$ is small compared to E_f [a good approximation, see the discussion after Eq. (7)] then the integral over k^f is trivial, i.e.,

$$\frac{dW}{d\Omega} = \frac{m^{3/2} \mid \langle \psi_f \mid V_q' \mid \psi_i \rangle \mid^2 Q_q^2 \sqrt{2E_f}\, VS}{(2\pi)^2\hbar^4} \ . \tag{19}$$

To compute the matrix element in Eq. (19) we need the appropriate solutions of the Schrödinger equation

$$H_e\psi(z) = E\psi(z) \ , \tag{20}$$

with H_e given in Eq. (2). In Eq. (20) E is not the total incident energy (E_i) but only the contribution to E_i of the motion in the normal direction, i.e., $E = \hbar^2 k_z^{i\,2}/2m$ with k_z^i the projection of the incoming wave vector along the normal.

In Appendix A we show that

$$\psi_i(z) = N\left[\frac{z}{\xi_E}\right]\left[\frac{\pi R}{e^{\pi R}-1}\right]^{1/2} \times \exp(-iz/\xi_E)\,{}_1F_1\left[1 - i\frac{R}{2}, 2, \frac{2iz}{\xi_E}\right] \ . \tag{21}$$

Here $R = -\Lambda_0/\xi_E E$, ${}_1F_1$ is the confluent hypergeometric function, and N is a normalization factor. We can express the low-energy limit $E \ll E_R$ (the Rydberg) in a simpler form if we use the result[8] that, for $ka_B \to 0$ ($k \equiv \sqrt{2mE}/\hbar$):

$${}_1F_1\left[1 + \frac{i}{k}, 2, 2ikx\right] = \frac{1}{\sqrt{2x}} J_1(\sqrt{8x}) \ , \tag{22}$$

where $J_1(x)$ is the first-order Bessel function. If we apply

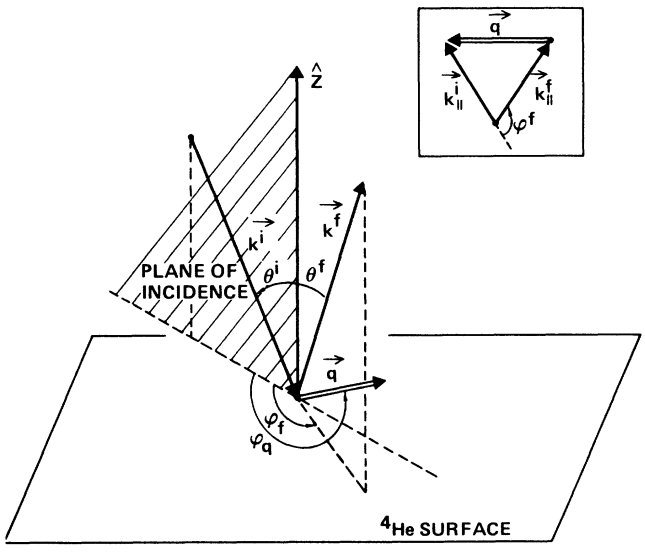

FIG. 2. Scattering geometry. The incoming electron has a wave vector $\mathbf{k}^i$, the scattered electron a wave vector $\mathbf{k}^f$. θ^i and θ^f are the angle of $\mathbf{k}^i$ and $\mathbf{k}^f$ with the surface normal $\hat{z}$. The in-plane components $\mathbf{k}_\parallel^i$ and $\mathbf{k}_\parallel^f$ are related to the ripplon wave vector $\mathbf{q}$ by $\mathbf{k}_\parallel^i = \mathbf{k}_\parallel^f + \mathbf{q}$ (see inset). The angles of $\mathbf{k}_\parallel^f$ and $\mathbf{q}$ with the plane of incidence are ϕ_f and ϕ_q.

this to Eq. (21), we find that

$$\psi_i(z)\cong N\sqrt{\pi}\left[\frac{E}{E_R}\right]^{1/4}\sqrt{z/a_B}J_1(\sqrt{8z/a_B}) \tag{23}$$

for $E\to 0$. The factor $(E/E_R)^{1/4}$ is the reduction in amplitude of the wave function near the surface due to quantum reflection. Remember that in the Introduction we argued that this factor was of order $\sqrt{E/V_0}$ for a rectangular well. The characteristic energy below which quantum reflection becomes important is thus E_R, the Rydberg, and the reduction for this smooth potential is weaker than for a square well. Alternatively, we can write Eq. (23) as

$$\psi_i(z)\simeq N(\pi k_z^i z)^{1/2}J_1(\sqrt{8z/a_B}) , \tag{24}$$

Eq. (24) is valid for $z\ll\xi_E$. Note the peculiar feature that for $z\ll\xi_E$, the wavelength of $\psi_i(z)$ is determined by a_B not the de Broglie wavelength. For $z\gg\xi_E$, Eq. (21) reduces to

$$\psi_i(z)\cong N\sin\left[k_z^i z-\frac{R}{2}\ln(2k_z^i z)+\delta\right] \tag{25}$$

which is the appropriate sum of ingoing and outcoming waves. The phase shift δ is a constant.

To fix the normalization N we simply note that the incident probability current density is [see Eq. (25)]

$$J_z=\left[\frac{\hbar}{2m}\right]|N|^2k_z^i . \tag{26}$$

The integral of J_z over a surface S parallel to the ^{4}He surface gives us the total flux of incoming particles. If we require the initial flux to be one particle per cm^2 per sec then

$$N=\left[\frac{2m}{\hbar k_z^i S}\right]^{1/2} . \tag{27}$$

In Appendix A we also show that the correct final-state wave function is

$$\psi_f(z)=\frac{1}{\sqrt{V}}e^{\pi(R/2)}\left[\frac{\pi R}{1-e^{-\pi R}}\right]^{1/2}y^1(z/\xi_E) , \tag{28}$$

where y^1 is not an elementary function and is defined in Eq. (A11). Now R and ξ_E should be evaluated using the final energy $E=\hbar^2 k_z^{f\,2}/2m$ where k_z^f is the projection of the final wave vector along the normal. In the limit $E\ll E_R$, Eq. (28) implies that

$$\psi_f(z)\simeq\frac{1}{\sqrt{V}}\sqrt{\pi k_z^f z}\,H_1^{(1)}(\sqrt{8z/a_B}) \tag{29}$$

for $z\ll\xi_E$. Note the similarity with Eq. (24). We merely replaced the J_1 Bessel function by the $H_1^{(1)}$ Hankel function.

For $z\gg\xi_E$

$$\psi_f(z)\simeq\frac{1}{\sqrt{V}}\exp\{i[k_z^f z-R/2\ln(2k_z^f z)+\bar{\delta}]\} . \tag{30}$$

Comparing Eqs. (29) and (30) we note that the amplitude ratio $|\psi_f(0)|^2/|\psi_f(\infty)|^2$ is of order $\sqrt{E/E_R}$ so near the surface ψ_f is significantly reduced, again due to impedance mismatch.

The matrix element is found by using Eqs. (9), (21), and (28) in Eq. (16), i.e.,

$$\langle\psi_f|V_q'|\psi_i\rangle=\int_0^\infty dz\frac{1}{\sqrt{V}}e^{\pi R_f/2}\left[\frac{\pi R_f}{1-e^{-\pi R_f}}\right]^{1/2}y^1(z/\xi_{E_f})\left[\frac{\Lambda_0}{z^2}-\frac{\Lambda_0}{z}qK_1(qz)\right]$$
$$\times N(z/\xi_{E_1})\left[\frac{\pi R_i}{e^{\pi R_i}-1}\right]^{1/2}\exp(-iz/\xi_{E_i})\,{}_1F_1\left[1-i\frac{R_i}{2},2,\frac{2iz}{\xi_{E_i}}\right] , \tag{31}$$

with ξ_{E_i}, R_i, ξ_{E_f}, and R_f the values of ξ_E and R evaluated for the incoming and outgoing particle.

We did not succeed in evaluating this expression analytically, but the limits $E_i\ll E_R$ and $E_i\gg E_R$ can be found. First take the limit $E_i\ll E_R$ where we can use Eqs. (24) and (29). Then

$$\langle\psi_f|V_q'|\psi_i\rangle\cong\pi N\Lambda_0\frac{(k_z^i k_z^f)^{1/2}}{\sqrt{V}}\int_0^\infty dz\,z\,H_1^{(1)}(\sqrt{8z/a_B})\left[\frac{1}{z^2}-\frac{q}{z}K_1(qz)\right]J_1(\sqrt{8z/a_B}) \tag{32}$$

or

$$\langle\psi_f|V_q'|\psi_i\rangle=N\Lambda_0\frac{(k_z^i k_z^f)^{1/2}}{\sqrt{V}}g(qa_B) , \tag{33}$$

where

$$g(x)=\pi\int_0^\infty dz\,H_1^{(1)}(\sqrt{z})J_1(\sqrt{z})\left[\frac{1}{z}-\frac{x}{8}K_1\left[\frac{xz}{8}\right]\right] . \tag{34}$$

In Appendix B it is shown that $g(x)$ is proportional to $x^{1/2}$ for $x\ll 1$. The differential scattering probability $dW/d\Omega$ is [see Eq. (19)]

$$\frac{dW}{d\Omega}=\frac{\sqrt{2}}{4\pi^2}\left[\frac{q}{\rho\omega_q}\right]\frac{m^{5/2}k_z^f}{\hbar^4}\Lambda_0^2 g^2(qa_B)(E_f)^{1/2} . \tag{35}$$

In the limit $E\gg E_R$, we can directly use the Born approximation, i.e., use the asymptotic expression Eqs. (25) and (30) for ψ_i and ψ_f. In this limit

$$\langle \psi_f \mid V_q' \mid \psi_i \rangle \cong N\Lambda_0 \frac{(k_z^i k_z^f)^{1/2}}{\sqrt{V}} f\left[\frac{q}{(k_z^i k_z^f)^{1/2}}, (k_z^i/k_z^f)^{1/2}\right], \quad (36)$$

with

$$f(x,y)=\int_0^\infty dz \sin(yz)\left[\frac{1}{z^2}-\frac{x}{z}K_1(xz)\right]e^{iz/y}. \quad (37)$$

The differential scattering rate for $E \gg E_R$ is thus

$$\frac{dW}{d\Omega} \cong \frac{\sqrt{2}}{4\pi^2}\left[\frac{q}{\rho\omega_q}\right]\frac{m^{5/2}k_z^f\Lambda_0^2}{\hbar^4} \times \left| f\left[\frac{q}{(k_z^i k_z^f)^{1/2}}, (k_z^i/k_z^f)^{1/2}\right]\right|^2 (E_f)^{1/2}. \quad (38)$$

The function $f(x,y)$ is also discussed in Appendix B. The angular distribution of scattering probabilities for $E \ll E_R$ and $E \gg E_R$ are quite different. For $E \gg E_R$ [Eq. (38)] scattering is predominantly into the cone $|k_z^f| \cong |k_z^i|$ if $q \ll k_z$, as shown in Appendix B [Eq. (B13)]. We thus recover momentum conservation along the z direction as is expected for high energy. For $E \ll E_R$, [Eq. (35)] the angular distribution is broad as a function of θ_f with no trace of momentum conservation along the z direction.

In the limit we have analyzed the problem, i.e., where the ripplon frequencies may be neglected, it is possible to simply include finite temperature effects into the scattering rate Eq. (38). Specifically one needs only to multiply Eq. (38) by $k_B T/\hbar\omega_q$.

B. Absorption

The absorption probability α is computed in much the same way as the scattering probability except that the sum over final states in Eq. (13) is only over the bound-state spectrum. This partial rate is conventionally denoted by α. The nth bound-state wave function is, for large n,

$$\psi_n^f(\mathbf{r}) \simeq -\frac{1}{n^{3/2}}\left[\frac{2z}{Sa_B^2}\right]^{1/2} J_1(\sqrt{8z/a_B}) \times \exp(-i\mathbf{k}_\parallel^f\cdot\mathbf{r}-z/na_B). \quad (39)$$

Note that the final state is now normalized over the area S, not over the scattering volume. Of course, now there is no amplitude reduction factor, as in Eq. (29), because there is no impedance mismatch. Dropping the $\exp-(z/na_B)$ factor in Eq. (39), since the dominant effects come from large n, we can write the matrix element of ψ_n^f with a low-energy incoming state [Eq. (23)] as

$$\langle f \mid H_{\rm int} \mid i \rangle = \frac{(2\pi)^2 N}{Sn^{3/2}}\left[\frac{2\pi k_z^i}{a_B^2}\right]^{1/2}\Lambda_0 \times \sum_{\mathbf{q}} Q_q e(qa_B)\delta(\mathbf{q}+\mathbf{k}_\parallel^f-\mathbf{k}_\parallel^i), \quad (40)$$

where

$$e(x)=\int_0^\infty dz\, J_1^2(\sqrt{z})\left[\frac{1}{z}-\frac{x}{8}K_1\left[\frac{xz}{8}\right]\right], \quad (41)$$

$$\alpha=\sum_{\mathbf{q},k_\parallel^f,n}\frac{(2\pi)^4 \mid N \mid^2 k_z^i}{\hbar n^3/Sa_B^2}\Lambda_0^2 Q_q^2 e^2(qa_B) \times\delta(\mathbf{q}+\mathbf{k}_\parallel^f-\mathbf{k}_\parallel^i)\delta(E_f+\hbar\omega_q-E_i), \quad (42)$$

where we have replaced one δ function by $S/(2\pi)^2$. The final result is

$$\alpha \cong \frac{\mid N \mid^2 k_z^i \Lambda_0^2 Sm}{\hbar^3 a_B^2}\int_0^{2\pi} d\phi\, Q_{q(\phi)}^2 e^2(q(\phi)a_B)\sum_{n=1}^\infty \frac{1}{n^3}, \quad (43)$$

where

$$q(\phi)=k^i(\sin^2\theta^i+1-2\sin\theta^i\cos\phi)^{1/2}.$$

is the wave vector of the emitted ripplon. For small x, $e(x)=(1/\pi)\sqrt{x/2}$ [Eq. (B14)] so for $k^i a_B \ll 1$, Eq. (43) reduces to

$$\alpha \simeq \frac{Z(3)}{2\pi^2}\frac{m^2\Lambda_0^2}{a_B\hbar^3\sqrt{\sigma\rho}}k^{i\,1/2} \times\int_0^{2\pi} d\phi(1+\sin^2\theta^i-2\sin\theta^i\cos\phi)^{1/4}, \quad (44)$$

where $Z(3)\approx 1.202$ is the Riemann ζ function. We have used Eqs. (7) and (27) for ω_q and N. For the case of absorption, even though the ripplon frequency may be neglected in all situations of physical interest, it is not possible to simply multiply Eq. (44) by $k_B T/\hbar\omega_q$ as we have done for Eq. (35) to include finite-temperature effects. The problem of how to include finite temperature for the absorption probability is much more complicated and interesting, and will be discussed in a future publication.

Equation (35) and (44) are our principal results. The physical implications will be discussed in Sec. V but first we will consider the validity of perturbation theory.

IV. HIGHER-ORDER PERTURBATION THEORY

The expression we used [Eq. (13)] for the single ripplon emission rate W is, of course, only the first term of a perturbation series in $H_{\rm int}$. Higher-order corrections will contain electron self-energy corrections and electron-ripplon vertex corrections. For instance, when $k_z \to 0$ we should expect in higher order some type of polaronic mass enhancement for the electron. In this section we will determine the expansion parameter of the perturbation theory and the validity of neglecting higher-order corrections.

The lowest-order corrections to the one-ripplon emission rate involve intermediate states with one virtual ripplon. From continuum perturbation theory:[9]

$$W=\frac{2\pi}{\hbar}\sum_f\left|H_{i,f}^{\rm int}+\sum_{r,r'}\frac{H_{f,r}^{\rm int}H_{r,r'}^{\rm int}H_{r',i}^{\rm int}}{(\epsilon_i-\epsilon_r)(\epsilon_i-\epsilon_r')}\right|^2\delta(\epsilon_i-\epsilon_f), \quad (45)$$

with ϵ_i and ϵ_f the initial- and final-state energy, respectively, and with r and r' intermediate states. As shown in Fig. 3, there are three types of intermediate states included in Eq. (45).

(a) Emission of a virtual ripplon $\mathbf{q}'$, followed by reabsorption and emission of a real ripplon $\mathbf{q}$ (this is an electron self-energy correction).

(b) Emission of a virtual ripplon $\mathbf{q}'$ followed by emission of a real ripplon $\mathbf{q}$ and reabsorption $\mathbf{q}'$ (a vertex correction).

(c) Emission of a real ripplon $\mathbf{q}$ followed by emission and reabsorption of a virtual ripplon $\mathbf{q}'$ (a self-energy correction once more).

The intermediate electron states are taken to be of low energy ($E_i \ll E_R$). First because we are interested in low-energy initial states and the main contribution in Eq. (45) will come from intermediate states with $\epsilon_r \cong \epsilon_i$. Furthermore, for $E \approx 0$ both the bound states and scattering states have, as we saw before, a wavelength which is energy independent so there are no interference terms in the matrix elements. For intermediate states with energies $|E_r| \gg E_R$ interference terms appear and the matrix elements are reduced. We thus use E_R as an energy "cutoff" for intermediate states. We first consider intermediate scattering states. We need to evaluate matrix elements such as

$$ {}_{\pm}\langle \mathbf{k} \mid H_{\rm int} \mid \mathbf{k} \rangle_{\pm} , \tag{46} $$

where $|\mathbf{k}\rangle_{\pm}$ is an outgoing or incoming solution of the Schrödinger equation and $H_{\rm int}$ is given by Eq. (9). Matrix elements between an incoming and an outgoing wave contain (for $E \to 0$) an oscillating phase e^{2iz/a_B} and are neglected. Remaining matrix elements are of the form

$$ {}_{+}\langle \mathbf{k} \mid H_{\rm int} \mid \mathbf{k}' \rangle_{+} = \frac{\sqrt{S}}{V} \int d^2\mathbf{q}\, Q_q \delta(\mathbf{q}+\mathbf{k}'_{\parallel}-\mathbf{k}_{\parallel}) \sqrt{k_z k'_z}\, h(qa_B) , \tag{47} $$

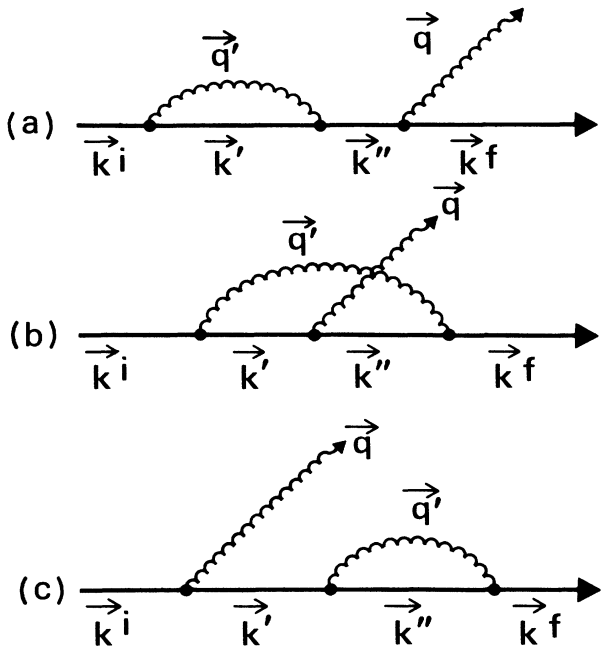

FIG. 3. (a), (b), and (c): Higher-order corrections to the single ripplon emission rate. The wave vectors of intermediate states of the electron are $\mathbf{k}'$ and $\mathbf{k}''$, of the ripplon $\mathbf{q}'$. The emitted ripplon has a wave vector $\mathbf{q}$ while $\mathbf{k}^i$ and $\mathbf{k}^f$ are the wave vectors of the incoming and outgoing electron.

where

$$ h(x) = \pi \int_0^{\infty} dz\, |H_1^{(1)}(\sqrt{z})|^2 \left[\frac{1}{z} - \tfrac{1}{8} x K_1(xz) \right] . \tag{48} $$

The first diagram in Fig. 3 contributes a factor

$$ \sum_{\mathbf{k}',\mathbf{k}',\mathbf{q}} \frac{\langle i \mid H_i \mid \mathbf{k}',\mathbf{q}' \rangle_{++} \langle \mathbf{q}',\mathbf{k}' \mid H_{\rm int} \mid \mathbf{k}'' \rangle_{++} \langle \mathbf{k}'' \mid H_{\rm int} \mid f \rangle}{\{E_i - [\hbar^2(\mathbf{k}')^2/2m] - \hbar\omega'_q\}\{E_i - [\hbar^2(\mathbf{k}'')^2/2m]\}} , \tag{49} $$

where $\langle i \mid$ is still the standing-wave superposition of an incoming and an outgoing solution of wave vector $\mathbf{k}^i$. The energy $E_i = \hbar^2 \mathbf{k}^{i\,2}/2m$. $|f\rangle$ is an outgoing state of momentum $\mathbf{k}^f$ and a real ripplon of momentum $\mathbf{q}$. Using Eq. (47) gives, after some elementary algebra,

$$ \left[\frac{1}{(2\pi)^4} \int dk'_z \int dk''_z \int d^2q' \frac{k'_z k''_z \Lambda_0^2 Q_q^2 h^2(q'a_B)}{\left[E_i - \frac{\hbar^2}{2m}[(\mathbf{k}^i_{\parallel}-\mathbf{q}')^2 + k'^2_z] - \hbar\omega'_q \right] \frac{\hbar^2}{2m}(k_z^{i\,2} - k''^2_z)} \right] \langle i \mid H_{\rm int} \mid f \rangle . \tag{50} $$

The factor in large parentheses is thus a dimensionless correction term to the first-order matrix element $\langle i \mid H^{\rm int} \mid f \rangle$ for ripplon emission. For perturbation theory to hold, it should be small compared to one. To compute the integrals we must specify the integration path around the singularities. This is done by allowing an infinitesimal damping term $-i\epsilon$ in the energy ϵ_r of an intermediate state. The resulting integrals over k'_z and k''_z are elementary:

$$ \int_0^{1/a_B} dk''_z \frac{k''_z}{\frac{\hbar^2}{2m}(k_z^{i2} - k''^2_z) + i\epsilon} = -\frac{m}{\hbar^2} \left[\ln \left[\frac{E_R}{\frac{\hbar^2}{2m} k_z^{i\,2}} \right] + i\pi \right] , \tag{51} $$

$$\int_0^{1/a_B} dk_z' \frac{k_z'}{E_i - \frac{\hbar^2}{2m}(\mathbf{k}_\parallel^i - \mathbf{q}')^2 - \hbar\omega_{\mathbf{q}}' - \frac{\hbar^2}{2m}k_z'^2 + i\epsilon}$$

$$= -\frac{m}{\hbar^2}\left[\ln\left[\frac{E_R}{\left|E_i - \frac{\hbar^2}{2m}(\mathbf{k}_\parallel^i - \mathbf{q}')^2 - \hbar\omega_q'\right|}\right] + i\pi\Theta\left[\frac{\hbar^2}{2m}(\mathbf{k}_\parallel^i - \mathbf{q}')^2 + \hbar\omega_{\mathbf{q}}' - E_i\right]\right], \quad (52)$$

with $\Theta(x)$ the step function. In Eq. (52) we assumed that the energy of the intermediate ripplon $|\hbar\omega_q| \ll E_R$.

This reduces the self-energy correction to

$$\frac{1}{(2\pi)^3}\left[\frac{m\Lambda_0}{\hbar}\right]^2 \left[\ln\left[\frac{E_R}{\hbar^2 k_z^{i2}/2m}\right] + i\pi\right]_{q<q_{\max}} \int d^2q\, Q_q^2 h^2(qa_B)$$

$$\times \left[\ln\left[\frac{E_R}{\left|E_i - \frac{\hbar^2}{2m}(\mathbf{k}_\parallel^i - \mathbf{q})^2 - \hbar\omega_q\right|}\right] + i\pi\Theta\left[\frac{\hbar^2}{2m}(\mathbf{k}_\parallel^i - \mathbf{q})^2 + \hbar\omega_q - E_i\right]\right] \langle i \mid H_{\text{int}} \mid f\rangle , \quad (53)$$

where $q_{\max}$ is the maximum ripplon wave vector. To estimate this (complex) integral, we note that the dependence on $\mathbf{q}$ in the logarithm is weak. In the limit $\hbar^2 k_z^{i2}/2m \ll E_R$, the integral is of order

$$= \left[\frac{m\Lambda_0}{\hbar^2}\right]^2 \ln\left[\frac{E_R}{\hbar^2 k_z^{i2}/2m}\right] \left[\int_0^{q_{\max}} dq\, qQ_q^2\hbar^2(qa_B)\right] \langle i \mid H_{\text{int}} \mid f\rangle . \quad (54)$$

Since both h and Q are slowly varying for order-of-magnitude estimates we replace the integral over q by $q_{\max}^2 Q_{q_{\max}}^2 h^2(q_{\max}a_B)$. The final result is then

$$\approx \left[\frac{m\Lambda_0}{\hbar^2}\right]^2 \ln\left[\frac{E_R}{\hbar^2 k_z^{i2}/2m}\right] q_{\max}^2 Q_{q_{\max}}^2 h^2(q_{\max}a_B) \langle i \mid H_{\text{int}} \mid f\rangle . \quad (55)$$

We must add to Eq. (55) the contribution from highly excited virtual bound states. A completely analogous calculation shows that they give a contribution similar to Eq. (53), but exactly canceling the logarithmic divergence for $k_z^i \to 0$. The other two diagrams of Fig. 3 are similar to Eq. (55). We conclude that the dimensionless expansion parameter of the perturbation series is

$$\lambda = (q_{\max}^2 Q_{\max}^2) h^2(q_{\max}a_B)/a_B^2 . \quad (56)$$

A physically more transparent form for the expansion parameter is found by noting that the expression

$$\langle u^2\rangle \equiv \int_0^{q_{\max}} qQ_q^2 dq \approx q_{\max}^2 Q_{q_{\max}}^2 \quad (57)$$

is the mean square of fluctuations in the surface height $u(\mathbf{r}_\parallel)$ due to zero-point motion. Thus the expansion parameter is

$$\lambda \cong (\langle u^2\rangle/a_B^2) h^2(q_{\max}a_B) . \quad (58)$$

Once the quantum fluctuations in $u(\mathbf{r}_\parallel)$ become comparable to the Bohr radius a_B of the incident particle, perturbation theory may break down. However, for electrons $a_B = 100$ Å so with $\langle u^2\rangle^{1/2} \simeq 1$ Å, $q_{\max} \approx 10A_0^{-1}$, $\lambda \approx 10^{-3}$ and perturbation theory is amply justified. The criterion $\langle u^2\rangle \ll a_B^2$ basically means that zero-point fluctuations of the surface do not disturb the bound-state spectrum. The result $\lambda \sim \langle u^2\rangle/a_B^2$ could already have been inferred from Eq. (8).

V. DISCUSSION AND CONCLUSION

In the Introduction we posed the question whether quantum reflection leads to zero adsorption probability in the limit $E \to 0$. Within DWBA we found [Eq. (44)]

$$\alpha \approx k^{i\,1/2} m^2 \Lambda_0^2/(a_B\hbar^3\sqrt{\sigma\rho}) \quad (59)$$

so $\alpha(E)$ is proportional to $E^{1/4}$ for Coulomb scattering. For potentials which are less smooth (e.g., $1/z^2$) quantum reflection is expected to be further enhanced. For a square well $\alpha(E) \sim E^{1/2}$ so, in general, we would expect that $\alpha(E) \sim E^\gamma$ with $\frac{1}{2} \le \gamma \le \frac{1}{4}$, but the exponent depends also on the q dependence of Q_q and V_q'. Comparing adsorption with inelastic scattering we see that the inelastic scattering rate [Eq. (35)]

$$W(E) \approx (k^f a_B) k_z^f \,|\, \mathbf{k}_\parallel^f \,|^{1/2} \frac{m^2\Lambda_0^2}{\hbar^3} (\sigma\rho)^{-1/2} \quad (60)$$

is reduced compared to $\alpha(E)$ by a factor of order E/E_R, due to the amplitude reduction of the outgoing wave near $z=0$ as discussed in Sec. III. Low-energy scattering and adsorption are thus completely dominated by quantum effects if the incident energy is small compared with the

characteristic energy of the adsorption potential and if perturbation theory holds. Including higher-order terms did not change the conclusion that $\alpha(0)=0$. We believe that $\alpha(0)=0$ to all orders in perturbation theory.

The expansion parameter of the perturbation theory is $\lambda\sim\langle u^2\rangle/a_B^2$ in the case of Coulomb potential. The Coulomb potential, as is true for any power-law potential, has no length scale. The coupling to the ripplons does not add a new length scale to the problem while for $E\ll E_R$ the wave function is basically independent of ξ_E. The only remaining length scales are $\langle u^2\rangle^{1/2}$ and a_B so $\lambda=\langle u^2\rangle/a_B^2$ is a "natural" expansion parameter. For electron scattering from ^{4}He surfaces $\lambda\ll 1$ so Eq. (44) should be valid and quantum reflection effects should be huge for incident energies less that 10 K.

For adsorption of charged ions on ^{4}He, $\lambda\sim 1$ and perturbation theory breaks down. Now $\alpha(0)$ could be finite and the bound-state spectrum will be severely affected. In a separate publication we will discuss the strong coupling regime where we indeed find $\alpha(0)\neq 0$ and crossover to quasiclassical behavior. Since $\alpha(0)$ appears to be zero in perturbation theory this indicates that either there is a "phase transition" in $\alpha(0)$ or that it has an essential singularity at $\lambda=0$ such as $\exp(-1/\lambda)$.

An interesting remaining question is how sensitive our conclusions are, to the analytic structure of the Coulomb potential. Coulomb potentials have an accumulation point of bound states at the ionization threshold. Typical terms in our perturbation expansion in Sec. IV are of the form

$$\int dE\,(D(E)/E-E_0+i\epsilon)\ ,$$

where $D(E)$ is the density of intermediate states. For potentials *without* an accumulation point, $D(E)$ drops to zero at the ionization threshold and for E_0 equal to the ionization threshold there could be a logarithmic divergence, as in the Kondo problem, in which case we would not have a converging perturbation theory in the limit $E\to 0$. van der Waals potentials $(1/z^3)$ may or may not have accumulation points depending on the strength, and certainly need to be considered separately.

ACKNOWLEDGMENTS

We would like to thank Dr. J. Goodkind and Dr. G. Williams for useful conversations. This work was supported by National Science Foundation Grant No. DMR-8603217.

APPENDIX A

To find the scattering states of the 1D Coulomb potential we first write the Schrödinger equation in dimensionless units. Expressing length in units of $x=z/\xi_E$ and energy in units of $R=\Lambda_0/\xi_E E$ the Schrödinger equation reduces to

$$\frac{d^2y}{dx^2}+\left[1-\frac{R}{x}\right]y=0\ . \tag{A1}$$

The general solution of Eq. (A1) is then found by Laplace transformation[10]

$$y(x)=\int_C e^{xz}w(z)dz\ , \tag{A2}$$

with C some contour in the complex plane. Substitution into Eq. (A2) leads to a first-order equation for $w(z)$ with solution

$$y(x)=\frac{1}{\pi}\int_C e^{xz}(z-i)^{(Ri/2)-1}(z+i)^{(Ri/2)-1}dz\ . \tag{A3}$$

The integrand has branch points at $z=\pm i$ and $z=\infty$. The branch cuts are chosen to lie along the imaginary axis from $\pm i$ to $\pm\epsilon i$, with ϵ small, and then from $\pm\epsilon i$ to $-\infty$ parallel to the real axis [see Fig. 4(a)]. Different choices for C lead to different asymptotic properties. First, we take a contour C_1+C_2 surrounding both

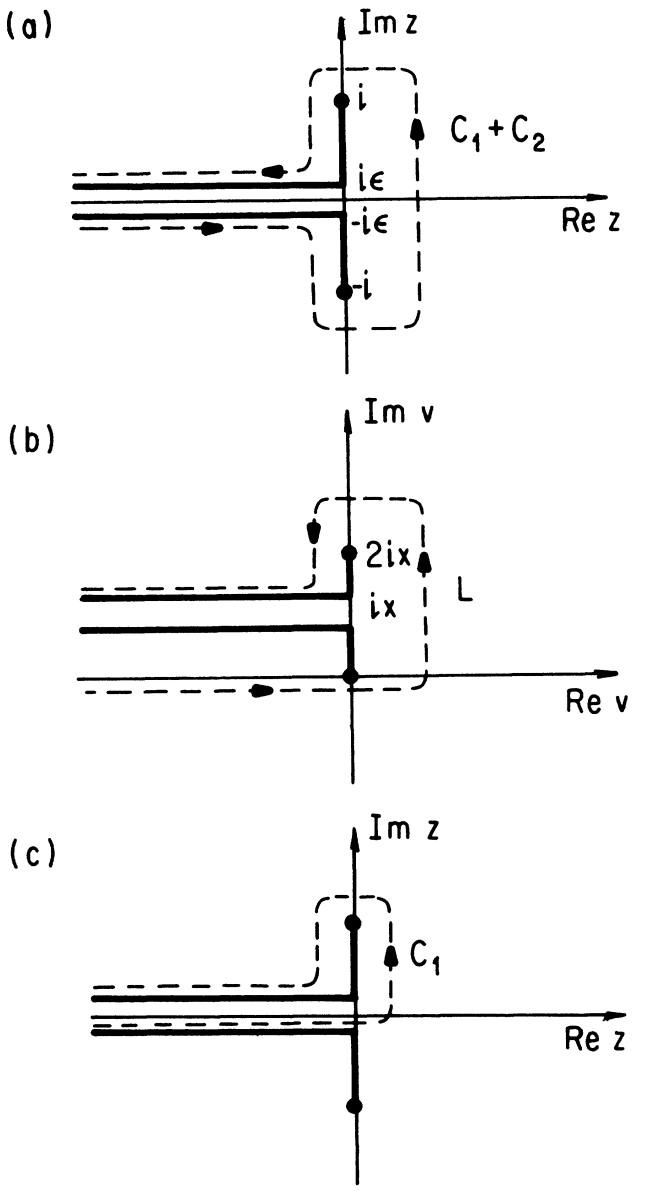

FIG. 4. (a) Branch cuts in the complex plane. (b) Contour L used in the definition of the elastically scattered solution [Eq. (A4)]. (c) Contour C_1 used in the definition of the outgoing solution [Eq. (A11)].

branch cuts and define the new variable $x=(z+i)x$. The result, $y^{+-}(x)$, is

$$y^{+-}(x)=\frac{1}{\pi}xe^{-ix}\int_L e^{v}v^{-2}\left[1-\frac{2ix}{v}\right]^{(Ri/2)-1}dv\ , \quad \text{(A4)}$$

where the contour L in the complex v plane is shown in Fig. 4(b). This contour integral is one of the representations[11] of the confluent hypergeometric function ${}_1F_1(\alpha,\gamma,z)$, so

$$y^{+-}(x)=2ixe^{-ix}{}_1F_1\left[1-\frac{iR}{2},2,2ix\right]\ . \quad \text{(A5)}$$

The asymptotic properties of ${}_1F_1$ can now be used. In the limit $z\to 0$, ${}_1F_1$ can be expressed as a power series:

$${}_1F_1(\alpha,\gamma,z)\simeq 1+\frac{\alpha z}{\gamma}+\cdots\ , \quad \text{(A6)}$$

so, for $x\to 0$,

$$y^{+-}(x)=2ix\ . \quad \text{(A7)}$$

On the other hand, for large z,

$${}_1F_1(\alpha,\gamma,z)=\frac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)}(-z)^{-\alpha}+\frac{\Gamma(\gamma)}{\Gamma(\alpha)}e^{z}z^{\alpha-\gamma}\ , \quad \text{(A8)}$$

which, for $x\to\infty$, leads to

$$y^{+-}(x)\simeq 2i\left[\frac{e^{\pi R}-1}{\pi R}\right]^{1/2}\sin\left[x-\frac{R}{2}\ln 2x+\delta\right]\ , \quad \text{(A9)}$$

with δ an irrelevant phase factor. This is the correct asymptotic form for $\psi_i(z)$, so we conclude that

$$\psi_i(z)=N\left[\frac{z}{\xi_E}\right]\left[\frac{\pi R}{e^{\pi R}-1}\right]^{1/2}\times\exp(-iz/\xi_E){}_1F_1\left[1-i\frac{R}{2},2,\frac{2iz}{\xi_E}\right]\ , \quad \text{(A10)}$$

with N the normalization factor.

To represent the outgoing wave we use a different contour. If the contour C_1 only surrounds one branch cut [Fig. 4(c)], the upper case, then the resulting function

$$y^{1}(x)=\frac{1}{\pi}\int_{C_1}e^{xz}(z-1)^{(Ri/2)-1}(z+1)^{(Ri/2)+1}dz\ , \quad \text{(A11)}$$

is not an elementary function. Its asymptotic properties were determined by Sexl.[10] For $x\to 0$

$$y^{1}(x)\simeq\frac{(1-e^{-\pi R})}{\pi R}+O(x)\ , \quad \text{(A12)}$$

while for $x\to\infty$,

$$y^{1}(x)=e^{-\pi r/2}\left[\frac{1-e^{-\pi R}}{\pi R}\right]^{1/2}\times\exp[i(x-R/2\ln 2x+\bar{\delta})]\ , \quad \text{(A13)}$$

with $\bar{\delta}$ again an irrelevant phase factor.

For large x, $y^{1}(x)$ is thus an outgoing plane wave. Note that, as expected, $y^{1}(0)\neq 0$. We conclude that

$$\psi_f(z)=\frac{1}{\sqrt{V}}e^{\pi(R/2)}\left[\frac{\pi R}{1-e^{-\pi R}}\right]^{1/2}y^{2}(z/\xi_E)\ , \quad \text{(A14)}$$

where now R and ξ_E should be evaluated using the final energy $E=k_z^{f\,2}/2m$.

APPENDIX B

In this Appendix we will discuss the various functions appearing in the evaluation of matrix elements. To evaluate the asymptotic behavior of

$$g(x)=\pi\int_0^\infty dz\,H_1^{(1)}(\sqrt{z})J_1(\sqrt{z})\left[\frac{1}{2}-\frac{x}{8}K_1(xz/8)\right] \quad \text{(B1)}$$

[see Eq. (3.4)] we separate the integral over z into two parts,

$$g(x)=\pi\left[\int_0^{8/x}dz\,H_1^{(1)}(\sqrt{z})J_1(\sqrt{z})\left[\frac{1}{x}-\frac{x}{8}K_1(xz/8)\right]+\int_{8/x}^\infty dz\,H_1^{(1)}(\sqrt{z})J_1(\sqrt{z})\left[\frac{1}{z}-\frac{x}{8}K_1(xz/8)\right]\right]\ . \quad \text{(B2)}$$

For $z<8/x$, the argument of the K_1 Bessel function is less than one, so we expand

$$K_1(z)\simeq\frac{1}{z}+\frac{z}{2}\ln(z/2)+\cdots\ . \quad \text{(B3)}$$

For $z>8/x$, $K(z)$ goes to zero exponentially fast. Using this in (B2) gives

$$g(x)\approx\pi\left[-\int_0^{8/x}dz\,H_1^{(1)}(\sqrt{z})J_1(\sqrt{z})\frac{x^2}{128}\ln(xz/16)+\int_{8/x}^\infty dz\,H_1^{(1)}(\sqrt{z})J_1(\sqrt{z})\frac{1}{z}\right]\ . \quad \text{(B4)}$$

We will consider separately the $x\to 0$ and $x\to\infty$ limits.

1. $\lim x\to 0$

The upper bound diverges in the first integral so the integral will be dominated by the large-z region. We can use the large-z expansions for the $H_1^{(1)}$ and J_1 Bessel functions, with the result

$$g(x)\approx-\frac{x^2}{32}\int_0^{\sqrt{8/x}}dz\,z^2\cos^2(z-3\pi/4)\times\ln(xz^2/16)+\sqrt{x/2}\ , \quad \text{(B5)}$$

where we have neglected a sine-cosine product in the first integral. The remaining integral can be expressed by the Ci or cosine integral function

$$g(x)\approx\sqrt{x/2}+\frac{x^2}{64}\left[\frac{2}{9}\left[\frac{8}{x}\right]^{3/4}-\tfrac{1}{2}\ln(4\sqrt{2/x})-\frac{\gamma}{4}+\mathrm{Ci}(4\sqrt{2/x})\right], \tag{B6}$$

where γ is Euler's constant. So to lowest order for $x\to 0$,

$$g(x)\simeq\sqrt{x/2}+O(x^{5/4}) . \tag{B7}$$

2. lim $x\to\infty$

For small z, $H_1^{(1)}(\sqrt{z})J_1(\sqrt{z})\approx -i/\pi$, and for $x\to\infty$ the integral is dominated by the small z region. Using this gives to lowest order (for $x\to\infty$)

$$g(x)\approx i\frac{x}{16}\ln(x/16) . \tag{B8}$$

To find the asymptotic properties of

$$f(x,y)=\int_0^\infty dz\,\sin(yz)\left[\frac{1}{z^2}-\frac{x}{z}K_1(xz)\right]e^{iz/y} \tag{B9}$$

for small x ($k^z\gg q$), we expand the K_1 Bessel function, with the result that

$$f(x,y)\approx\int_0^{2/x}dz\,\sin yz\,e^{iz/y}\left[\frac{x^2}{2}\ln\frac{xz}{2}\right] . \tag{B10}$$

Note that the quantity in large parentheses is a slow function of z so the integral will be strongly peaked near $y=\pm 1$. We are only interested in the region near $y=1$ where

$$f(x,y)\approx\frac{ix^2}{4}\int_0^{2/x}\exp\left[iz\left[\frac{1}{y}-y\right]\right]\ln(xz/2)$$

$$\approx\frac{ix}{2}\int_0^1 dw\,\exp\left[iw\frac{2}{x}\left[\frac{1}{y}-y\right]\right]\ln w . \tag{B11}$$

Expanding $y=1+\Delta y$ with $\Delta y\ll 1$,

$$f\simeq\frac{ix}{2}\int_0^1 dw\,e^{iw(\Delta y^2/x)}\ln w$$

$$\simeq\frac{ix}{2}\left[-\frac{x}{\Delta y^2}\left[\sin(x/\Delta y^2)+\frac{\pi}{2}\right]+\frac{ix}{\Delta y^2}[\gamma-\mathrm{Ci}(x/\Delta y^2)+\ln(x/\Delta y^2)]\right] , \tag{B12}$$

with γ Euler's constant. The limiting behavior of $f(x,y)$, for small x, is

$$f(x,y)\simeq\begin{cases}-\dfrac{ix}{2}, & (y-1)^2\ll x\\ -\dfrac{ix^3}{2(y-1)^4}, & (y-1)^2\gg x\end{cases} \tag{B13}$$

using the asymptotic expansions of the Ci function. This represents a peak at $y=1$ of width $\Delta y=\sqrt{x}$.

The functions $e(x)$ and $h(x)$ are evaluated in the same fashion as $g(x)$. We are mostly interested in the range $x<1$ where we can approximate

$$e(x)\approx\int_{8/x}^\infty dz\frac{1}{z}J_1^2(\sqrt{z}) , \tag{B14a}$$

$$h(x)\approx\pi\int_{8/x}^\infty dz\frac{1}{z}\,|H_1^{(1)}(\sqrt{z})|^2 , \tag{B14b}$$

with the result that both $e(x)$ and $h(x)$ are proportional to $\sqrt{x}$ for small x [$e(x)\approx(1/\pi\sqrt{2})\sqrt{x}$ and $h(x)\approx\sqrt{2x}$] just as $g(x)$.

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