Electronic-recoil spectra of p waves in an electron gas

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The p-wave electronic recoil spectra and their spectral moments are evaluated for a free-electron gas subjected to various suddenly applied, local, spherically symmetric perturbations. The spectra depend on the form of the perturbation, except at threshold, where they exhibit shapes depending only on the Fermi-energy phase shifts.

I. INTRODUCTION

Any sudden perturbation of an electron gas sets up an electronic shock wave which dissipates energy by low-energy electron-hole-pair production. Photoemission of electrons from impurity or core states,[1] meson capture,[2] radioactive decay,[3] and electronic transitions within an atom all shock the surrounding electron gas. The spectrum of electronic recoil energies, that is, the probability that the electron gas recoils dissipating energy E, can be directly observed as an asymmetric line whenever the perturbing process would otherwise produce a discrete line in the case of zero recoil. Photoemission experiments[4,5] have produced such asymmetric lines, which have been studied extensively.

The theory of the electronic recoil profile is presently developing, with early work[1] having been confined to making general statements concerning the line shape very near threshold and with more recent studies having been devoted to solutions of specific models.[6–10]

In this paper, we present results of calculations of the p-wave recoil spectra of a free-electron gas, using the determinantal methods of Friedel,[11] Dow and Flynn,[7] and Swarts, Dow, and Flynn.[12,13] We demonstrate explicitly that Flynn's moment theorems[14] for the recoil line shapes are satisfied; we compare the p-wave profiles with corresponding s-wave profiles[7,13]; and we show how the line shapes change with different final-state interactions.

In Sec. II, we outline the theory, and in Sec. III, we present the results of the calculations. Section IV summarizes our conclusions, and the principal mathematical underpinnings of the work are contained in Appendix A.

II. THEORY

The recoil spectrum $I(E)$ is the probability that the electron gas will make a transition from the initial state $|i\rangle$ to the nth final state $|fn\rangle$, absorbing energy E.

$$I(E)=\sum_n \langle i|fn\rangle^2 \delta(E-E_{fn}+E_i) \quad . \tag{1}$$

This transition is induced by the sudden change of effective Hamiltonian from

$$H_{\text{init}}=\sum_{i=1}^{N}\frac{p_i^2}{2m}+U(\vec{r}_i) \tag{2}$$

to

$$H_{\text{final}}=\sum_{i=1}^{N}\frac{p_i^2}{2m}+U(\vec{r}_i)+V(\vec{r}_i) \quad . \tag{3}$$

In the present paper, we take U and V to be spherically symmetric and take either U or $U+V$ to be zero. Since the initial and final Hamiltonians are one-electron Hamiltonians, the eigenfunctions $|i\rangle$ and $|fn\rangle$ are Slater determinants of one-electron spin orbitals $\phi(\vec{r})\chi_\sigma$ and $\psi(\vec{r})\chi_\sigma$, respectively. The matrix element $\langle i|fn\rangle$ is itself a determinant, which factors into smaller determinants for each angular-momentum channel (l,m,σ). The resulting recoil profile can be written as a multiple convolution of the profiles for the individual channels[7]; so we consider here only one p-wave channel ($l=1$, $m=0$, $\sigma=\frac{1}{2}$) with N electrons

$$\langle i|fn\rangle=\begin{vmatrix}(\phi_1,\psi_1) & \cdots & (\phi_1,\psi_N)\\ \vdots & & \vdots\\ (\phi_N,\psi_1) & \cdots & (\phi_N,\psi_N)\end{vmatrix} \quad . \tag{4}$$

Expressions for the various matrix elements are given in Appendix A.

The procedure for computing a recoil spectrum is the same as that used for s waves[7,12]: the determinants $\langle i|fn\rangle$ are evaluated for a system of N p waves and N is steadily increased until a convergent spectrum is obtained for $N \sim 80$. A sphere with $N=80$ p waves per channel contains $N=2.28\times10^6$ electrons and has a diameter of 547 Å in sodium. The moments of the calculated spectra are evaluated

$$M^{(p)}(E) \equiv \int_{-\infty}^{E} I(E)(E-E_i)^p dE \tag{5a}$$

and compared with Flynn's moment theorems[14]

$$M^{(p)}(\infty) = \langle i|V^p|i\rangle \ . \tag{5b}$$

Finite moments do not exist for either the infinite barrier potential (for $p>0$) or the δ shell (for $p>1$); however, the high-energy asymptotic behavior of $I(E)$ can be deduced in these cases from the $N=1$ line shape.

III. RESULTS

Calculated p-wave recoil profiles for cases in which $U=0$ and the final-state interaction V is either a spherical square well, impenetrable barrier, or δ shell are given in Figs. 1–3 for various Fermi-energy phase shifts δ_1 for an electron gas with $r_s=3.93$ (Na). Corresponding recoil spectra for turning the potential off ($U\neq0$, $U+V=0$) are also given in Figs. 4–6. Several features of the spectra merit comment.

The asymptotic approximation[1,7] to the line shape generally is valid only very near the threshold

$$\lim_{E\to E_T^+} I(E) = C_1(E-E_T)^{-1+\delta_1^2/\pi^2} \ . \tag{6}$$

Here C_1 is related to Anderson's constant.[7,15,16]

To illustrate this point, we display in Fig. 7 the asymptotic theory together with the exact results for $\Delta=\delta_1^2=0.20$, a typical exponent.[5] The dashed lines define the region around the asymptotic theory corresponding to the experimental uncertainty ±0.015 quoted in some fits of the asymptotic line shape to x-ray photoemission data.[5] Clearly the theoretical uncertainty, namely, the difference between asymptotic and exact theories, greatly exceeds the experimental uncertainty, namely, the difference between the asymptotic theory and data, for $E-E_T \gtrsim 0.5E_F$, a typical energy over which analyses occur.[5] A similar conclusion was obtained for the s-wave recoil profiles[12]; thus exponents Δ extracted by fitting data

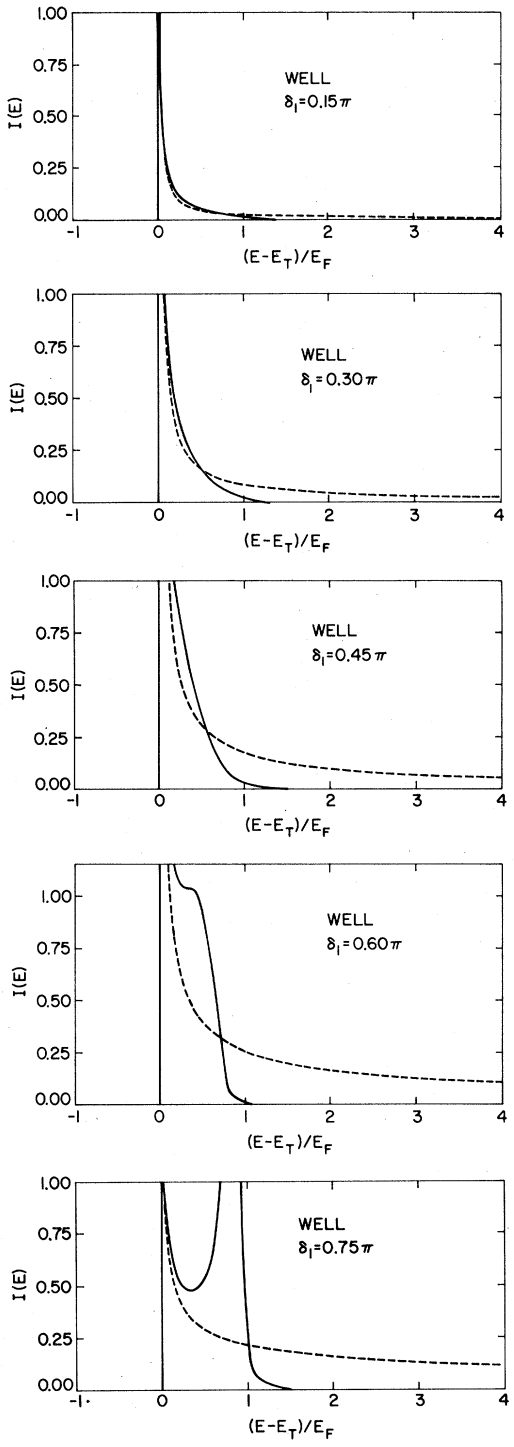

FIG. 1. Recoil profile for p waves subjected to a square-well final-state interaction V of increasing strength (specified by δ_1). The units of energy and length are the rydberg and Bohr radius. The well radius is $a=2$. Solid lines: present work; broken lines: asymptotic theory. Note the p-wave resonance for $\delta_1/\pi=0.6$, 0.75. (A p state is bound for $\delta_1=0.80\pi$.)

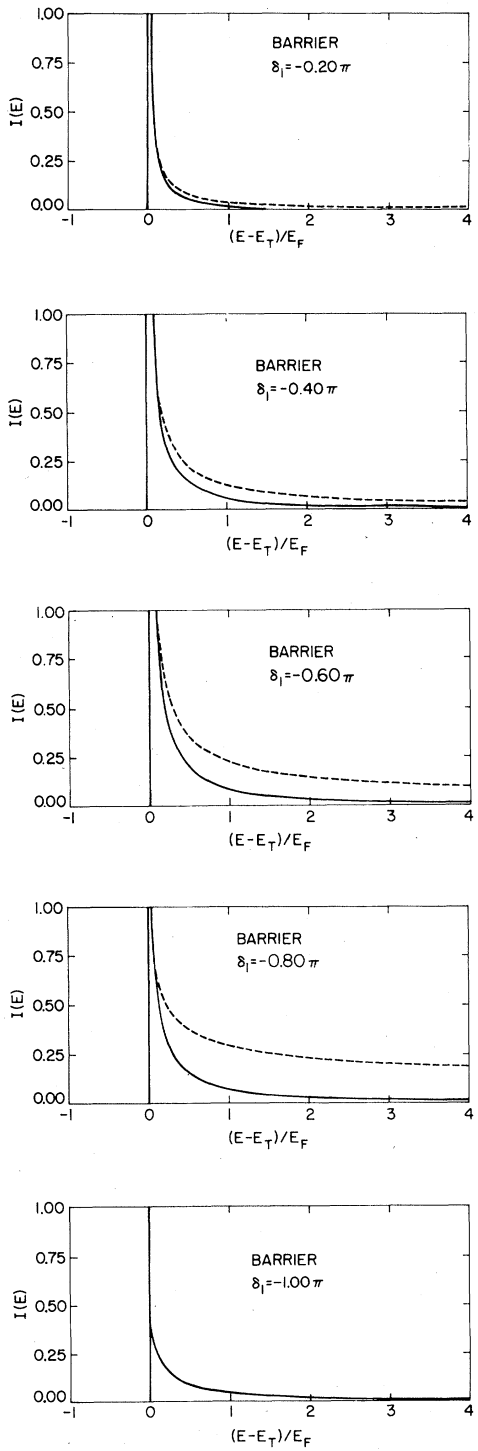

FIG. 2. Recoil profile for p waves subjected to an impenetrable barrier final-state interaction V of increasing radius (specified by δ_l). Solid line: present work; broken line: asymptotic theory.

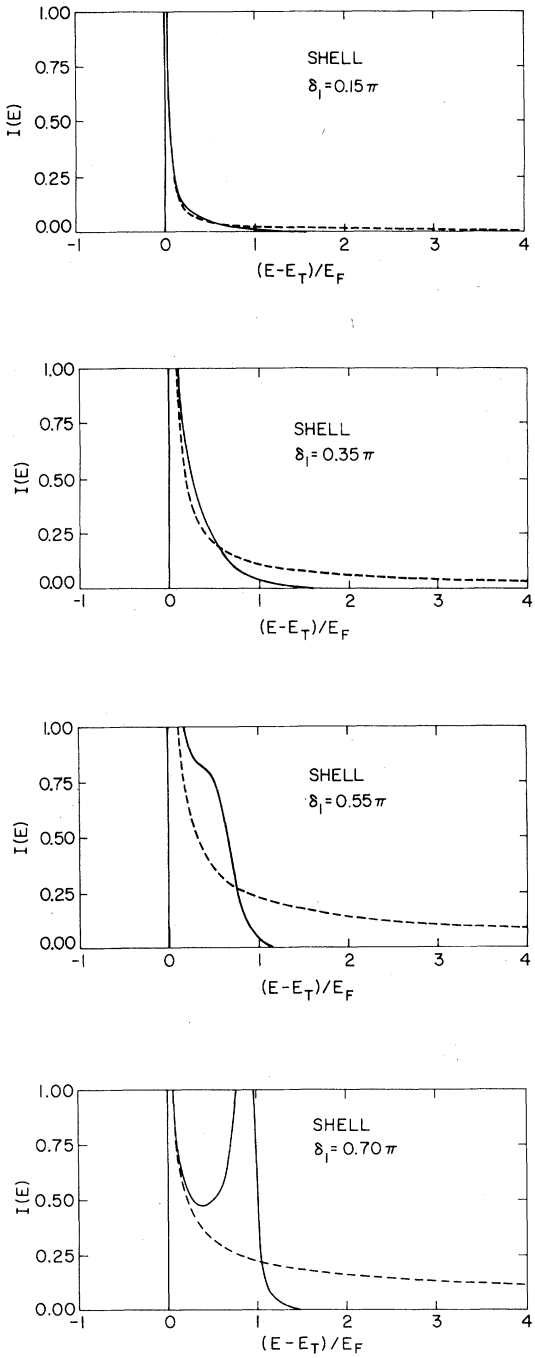

FIG. 3. p wave recoil profile for a δ shell final-state interaction V of increasing strength (specified by δ_l). Solid line: present work; broken line: asymptotic theory. Note p-wave resonance for $\delta_l/\pi = 0.55, 0.70$. (A p state is bound for $\delta_l = 0.75\pi$.)

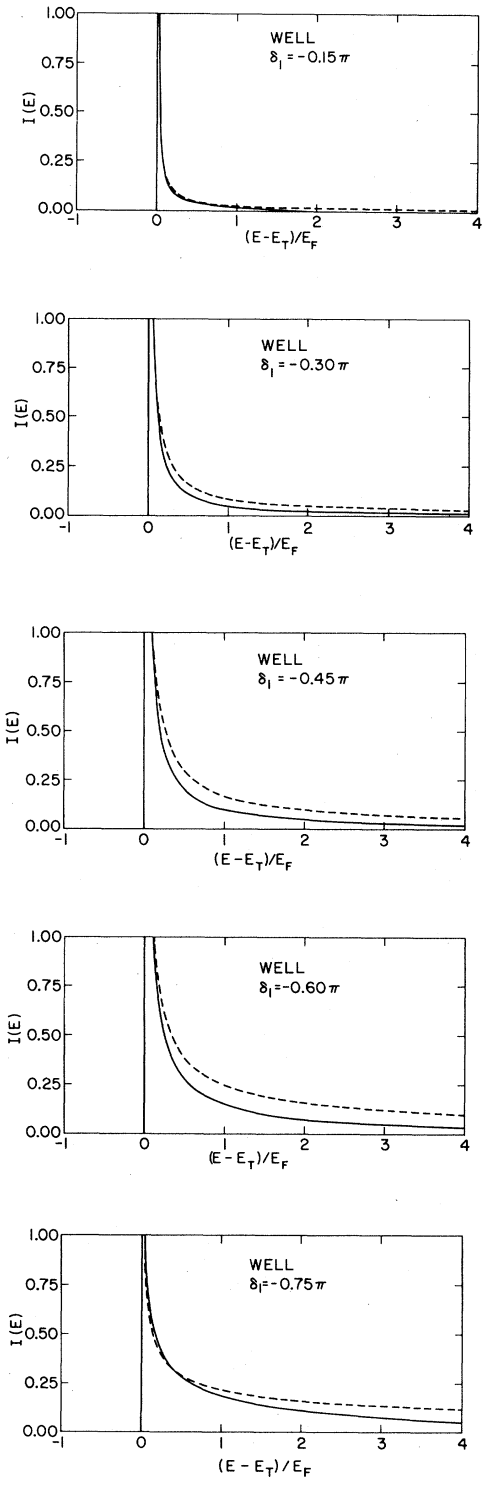

FIG. 4. Recoil profile for p waves with a square-well initial-state interaction U of increasing strength (specified by δ_1). Solid line: present work; broken line: asymptotic theory.

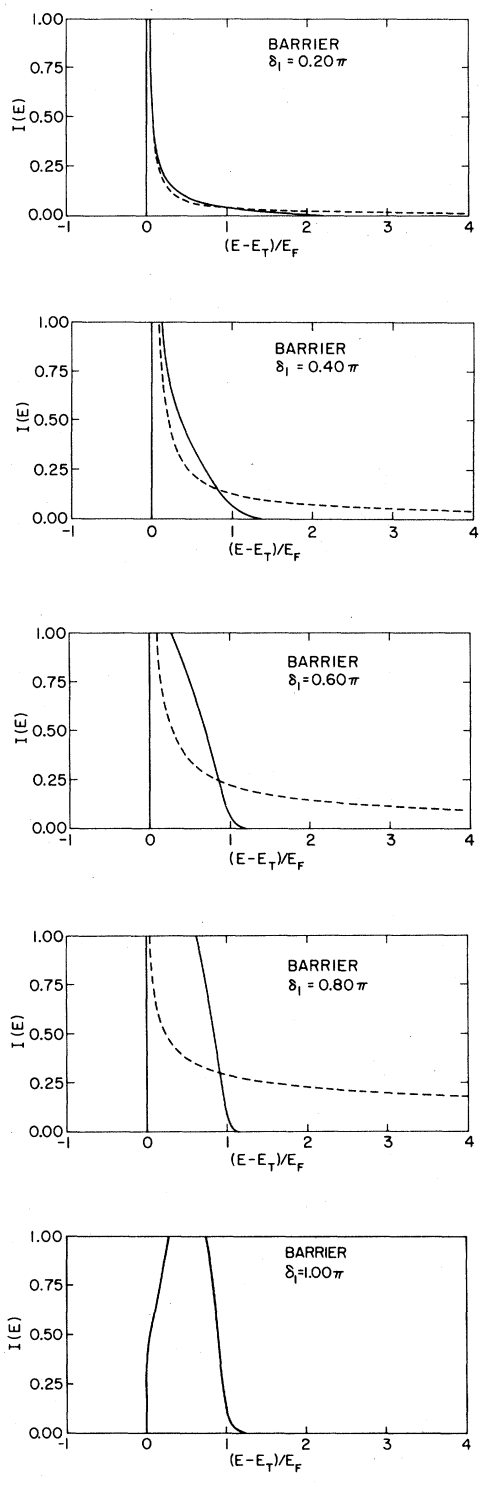

FIG. 5. Recoil profile for p waves with an impenetrable barrier initial-state interaction U of increasing radius (specified by δ_1). Solid line: present work; broken lines: asymptotic theory.

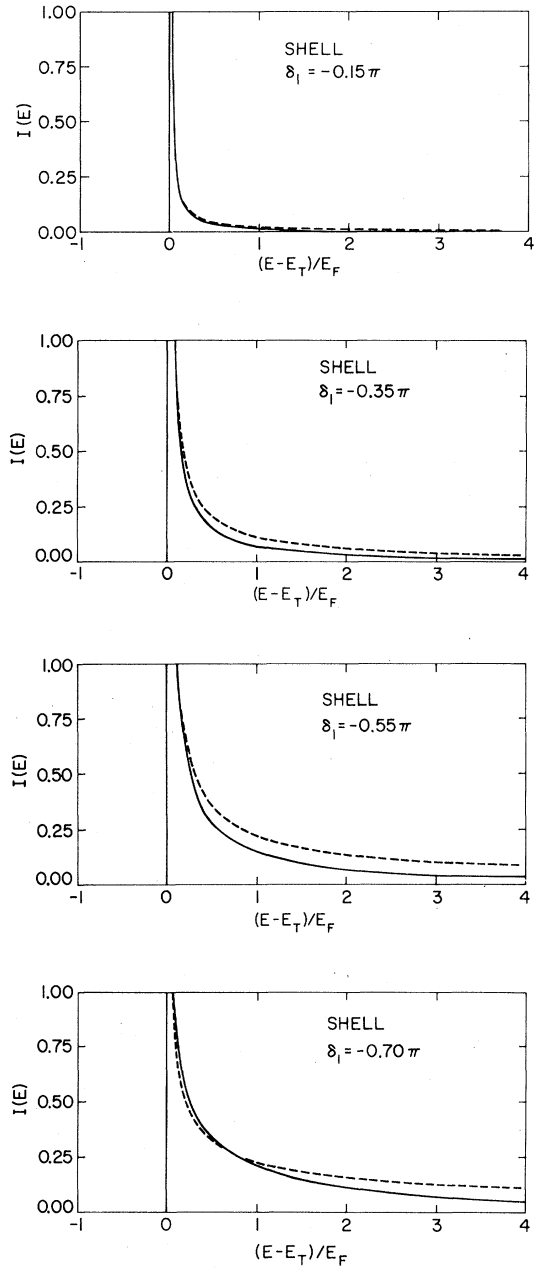

FIG. 6. Recoil profile for p waves subjected to a δ shell initial-state interaction U of increasing strength (specified by δ_1). Solid line: present work; broken line: asymptotic theory.

with the asymptotic theory should be regarded with great caution and may be unrelated to the true exponent $\Delta = \sum_{l=0}^{\infty} 2(2l+1)\delta_l^2/\pi^2$.

The recoil spectra depend strongly on the form of the electron-hole interaction V, as demonstrated in Fig. 8. Although the shapes at threshold depend only

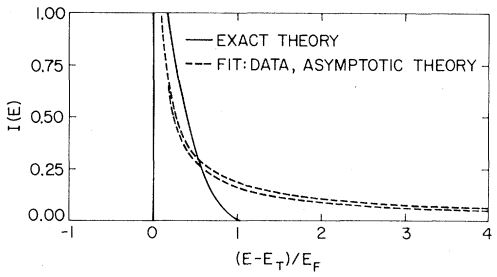

FIG. 7. p-wave recoil profile for a square-well final-state interaction $V = V_0\Theta(2-r)$ and a Fermi-energy phase shift of $\delta_1 = 0.45\ \pi$, giving $\Delta = 0.20$. The asymptotic theory for $\Delta = 0.20 \pm 0.015$ is dashed; this corresponds to exponents extracted from Na data by fitting the asymptotic theory to the x-ray photoemission line shape throughout $0 \lesssim E - E_T \lesssim 0.5E_F$. Clearly the uncertainty in the fit of the asymptotic theory to data (the difference between dashed lines) is small compared with the difference between exact and asymptotic theories.

on the phase shift δ_1, the absolute values of the spectra and their energy dependences away from threshold are quite sensitive to the form of the final-state interaction.

Qualitatively, the spectra exhibit many of the features characteristic of s-wave recoil, although s- and p-wave profiles differ significantly, as shown in Fig. 9.

One interesting feature of the p-wave recoil spectra is the appearance of a p-wave resonance (Figs. 1 and 3).[17] At one time there was speculation that such resonances might influence the optical spectra of alkali metals,[18] but it is now generally believed that the required large phase shifts do not occur in the simple metals. However, such resonances should be observed in semiconductors sufficiently heavily

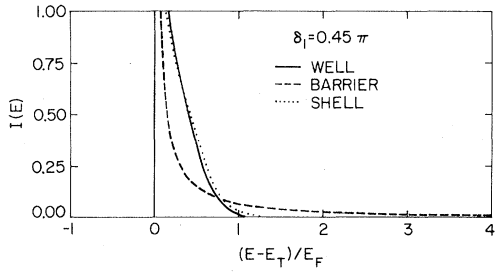

FIG. 8. p-wave recoil profile for Fermi-energy phase shift of 0.45 π for a final-state interaction V of different forms. Solid line: square well; broken line: impenetrable barrier (for the case $\delta_1 = -0.45\ \pi$, not $+0.45\ \pi$); dotted line: δ shell.

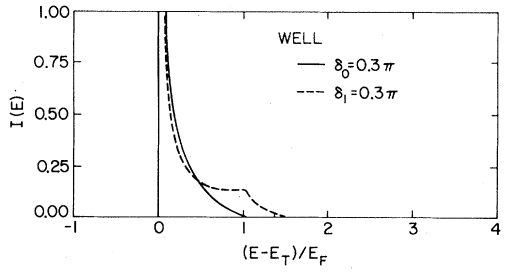

FIG. 9. Recoil profiles for square-well final-state interactions V. Solid line: s-wave recoil for $\delta_1=0.3\pi$; broken line: p-wave recoil for $\delta_0=0.3\pi$.

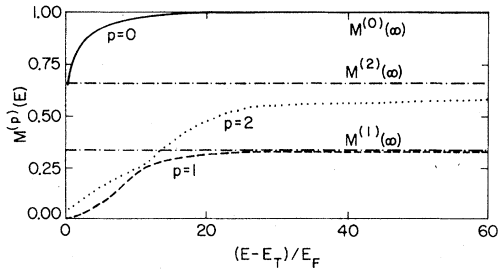

FIG. 11. Spectral moments $M^{(p)}(E)$ of the p-wave recoil profile for a square-well initial-state interaction U of radius 2, giving a Fermi-level phase shift of $\delta_1=0.45\pi$. (Units of energy are rydbergs.) Solid line: zeroth moment; broken line: first moment; dotted line: second moment; dash-dot lines: $E=\infty$ values of moments, $\langle i|V^p|i\rangle$.

doped that the interelectron radius is comparable with the $2p$ exciton radius.

For a sufficiently strong final-state interaction, a $2p$ exciton is bound, and a second threshold appears in the recoil spectrum. Hopfield[19] and Combescot and Nozieres [20] have discussed how the exponent for this threshold is related to the square of the excess charge localized in its channel, giving an exponent in the asymptotic approximation of $(\delta_1-\pi)^2/\pi^2$ rather than δ_1^2/π^2 as for the first threshold. The spectra in Figs. 1–9 are plotted as functions of $E-E_T$. For reference, the threshold energies E_T are given in Fig. 10. As expected, the spectral moments of the recoil profile satisfy Flynn's moment theorems.[14] Indeed, the first few moments are saturated at relatively low energies, as demonstrated in Fig. 11.

IV. SUMMARY

The present work shows that the p-wave recoil profiles of independent electron metals can be computed in a straightforward way, using the determinantal method. For physically interesting recoil energies, the resulting recoil line shapes can differ significantly from the asymptotic theory[1] profiles; hence, attempts to accurately describe data should rely on exact line-shape calculations rather than on the asymptotic approximation. The sensitivity of the line shapes to the form of the final-state interaction indicates that this interaction must be well understood before reliable comparisons with data can be made.

The present work will probably find more applications to the theory of heavily doped semiconductors than to the theory of metals. Friedel's sum rule governs the phase shifts of degenerate metals

$$\sum_{l,m,\sigma}\delta_{lm\sigma}/\pi=\sum_{l=0}^{\infty}2(2l+1)\delta_l/\pi=1 \tag{7}$$

and effectively limits the p-wave phase shift to small values $0<\delta_1<\frac{1}{8}\pi$. As a result, the p-wave contribution to the total recoil profile in simple metals is often small, having a contribution to observed line asymmetries comparable with experimental uncertainties. However, in less degenerate metals or in doped semiconductors, the p-wave phase shift can be large, and phenomena such as p-wave resonances and bound states can become important. The Hamiltonians [Eqs. (2) and (3)] describe effective-mass electrons in the conduction band of a semiconducor with m being replaced by the effective mass m^*. However, the energy scale on which the recoil phenomena exist in semiconductors is reduced by a factor $m^*/m\epsilon_0^2$ where ϵ_0 is the dielectric constant.

One way to observe the strong-scattering recoil profile in semiconductors is to study the effects of increased doping (electron-gas density) on the shapes of photoemission spectra associated with transitions from impurity levels. To our knowledge, such high-resolution impurity photoemission measurements have not yet been reported for heavily doped semiconductors.

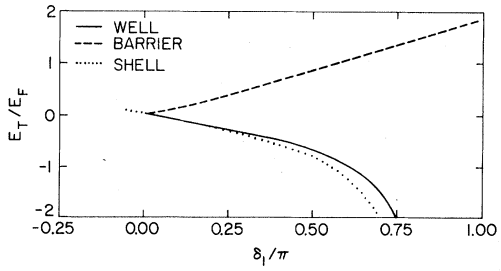

FIG. 10. Recoil threshold energies for final-state interactions V of different types as a function of the Fermi-level phase shift. Solid line: square well; broken line: impenetrable barrier (for this case, $-\delta_1$ is plotted instead of δ_1); dotted line: δ shell.

ACKNOWLEDGMENT

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APPENDIX A: MATHEMATICAL DETAILS

The radial wave functions are

$$R_l(r;k)\,Y_{lm}(\Theta,\phi)\chi_\sigma \ .$$

with $l=1$ and $\sigma=\frac{1}{2}$. Here χ_σ is a two-component spinor and Y_{lm} are spherical harmonics. In the unperturbed state ϕ_k, we have

$$R_1(r;k)=\tilde{C}j_1(kr) \ ,$$

where j_1 is the ordinary spherical Bessel function of order unity and the normalization constant is

$$\tilde{C}=k\sqrt{2}\left[S-\frac{\sin(2kS)}{2k}\right]^{-1/2} \ .$$

The wave-vector magnitudes k are determined by the condition the R_1 vanish on the surface of a sphere of radius S

$$j_1(kS)=0$$

and the sphere radius is fixed by the Fermi wave vector and the condition

$$S=Z^{(N)}/k_F \ ,$$

where $Z^{(N)}$ is the Nth zero of j_1.

In the perturbed state $\psi_{k'}$, for r outside the range a of the perturbation, the radial wave function is

$$R_1^{>}(r,k')=B_{k'}[\cos\delta_1(k')j_1(k'r)-\sin\delta_1(k')y_1(k'r)] \ ,$$

where y_1 is the spherical Neumann function, $\delta_1(k')$ is the phase shift, and k' is fixed by the condition $R_1^{>}(S,k')=0$.

For $r<a$, we have (i) for an infinite barrier, $R_1^{<}(r,k')=0$; (ii) for a δ shell, $R_1^{<}(r,k')=A_{k'}j_1(k'r)$; and (iii) for a square well, $R_1^{<}(r,k')=D_{k'}j_1(\chi r)$ with $\chi=(k'^2+V_0)^{1/2}$, V_0 being the well depth. The constants are $A_{k'}=R_1^{>}(a,k')/j_1(k'a)$ and $D_{k'}=R_1^{>}(a,k')/j_1(\chi a)$. The normalization constant $B_{k'}$ can be evaluated by the condition

$$\int_0^a R_1^{<}(r,k')^2r^2\,dr+\int_a^S R_1^{>}(r,k')^2r^2\,dr=1$$

using the integrals

$$\int r^2f_1(kr)g_1(qr)\,dr=\frac{r^2[qf_1(kr)g_0(qr)-kg_1(qr)f_0(kr)]}{k^2-q^2} \ ,$$

$$\int r^2f_1(qr)g_1(qr)\,dr=r^2[rq\,(f_0(qr)g_0(qr)+f_1(qr)g_1(qr)\ -2g_0(qr)f_1(qr)-g_1(qr)f_0(qr)]/2q \ ,$$

where f_1,g_1 denote either j_1 or y_1, and f_0, g_0 denotes the corresponding j_0 or y_0.

The phase shifts are obtained as follows: (i) for an impenetrable barrier, we have $\delta_1(k')=\arctan[j_1(k'a)/y_1(k'a)]$; (ii) for a δ-shell potential $V=V_0a\,\delta(r-a)$, we have

$$\delta_1(k')=\arctan\frac{V_0a^3k'j_1^2(k'a)}{V_0a^3k'j_1(k'a)y_1(k'a)-1} \ ,$$

and (iii) for a square well $V=-V_0\Theta(a-r)$, we have

$$\delta_1(k')=\arctan\frac{\chi j_0(\chi a)j_1(k'a)-k'j_0(k'a)j_1(\chi a)}{\chi j_0(\chi a)y_1(k'a)-k'y_0(k'a)j_1(\chi a)} \ .$$

The overlap matrix elements $(\phi_k,\psi_{k'})$ are (i) for an impenetrable barrier

$$(\phi_k,\psi_{k'})=\tilde{C}B_{k'}\left[\cos\delta\int_a^S r^2j_1(kr)j_1(k'r)\,dr-\sin\delta\int_a^S r^2j_1(kr)y_1(k'r)\,dr\right] \ ,$$

where δ stands for $\delta_1(k')$; (ii) for a δ shell

$$(\phi_k,\psi_{k'})=\tilde{C}\left[A_{k'}\int_0^a r^2j_1(kr)j_1(k'r)\,dr+B_{k'}\cos\delta\int_a^S r^2j_1(kr)j_1(k'r)\,dr-B_{k'}\sin\delta\int_a^S r^2j_1(kr)y_1(k'r)\,dr\right] \ ,$$

and (iii) for a square well

$$(\phi_{k'},\psi_{k'})=\tilde{C}\left[D_{k'}\int_0^a r^2j_1(kr)j_1(\chi r)\,dr+B_{k'}\cos\delta\int_a^S r^2j_1(kr)j_1(k'r)\,dr-B_{k'}\sin\delta\int_a^S r^2j_1(kr)y_1(k'r)\,dr\right] \ .$$

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[1]S. Doniach and M. Sunjic, J. Phys. C 3, 285 (1970).
[2]J. D. Dow, C. A. Swarts, and R. Naumann (unpublished).
[3]C. P. Flynn (private communication).
[4]L. Ley, F. R. McFeely, S. P. Kowalczyk, J. G. Jenkin, and D. A. Shirley, Phys. Rev. B 11, 600 (1975).
[5]P. H. Citrin, G. K. Wertheim, and Y. Baer, Phys. Rev. B 16, 4256 (1977).
[6]A. Kotani and Y. Toyozawa, J. Phys. Soc. Jpn. 41, 1699 (1976).
[7]J. D. Dow and C. P. Flynn, J. Phys. C 13, 1341 (1980); summarized in J. D. Dow, Nuovo Cimento 39, 465 (1977).
[8]V. I. Grebennikov, Yu. A. Babanov, and O. B. Sokolov, Phys. Status Solidi 80, 73 (1977).
[9]P. Minnhagen, Phys. Lett. A 56, 327 (1976).
[10]L. C. Davis and L. A. Feldkamp, J. Appl. Phys. 50, 1944 (1979).
[11]J. Friedel, Comments Solid State Phys. 2, 21 (1952); Philos. Mag. 43, 153, 1115 (1952).
[12]C. A. Swarts, J. D. Dow, and C. P. Flynn, Phys. Rev. Lett. 43, 158 (1979); C. A. Swarts and J. D. Dow (unpublished).
[13]C. A. Swarts, Ph.D. thesis (University of Illinois, 1979) (unpublished).
[14]C. P. Flynn, Phys. Rev. B 14, 5294 (1976).
[15]P. W. Anderson, Phys. Rev. Lett. 18, 1049 (1967).
[16]We have used $C_1=(C\delta_1^2/2\pi^2E_F)(2E_F)^{1-\delta_1^2/\pi^2}$, where C is Anderson's constant. This result has been derived in Ref. 7, for cases when the lowest-energy states of the electron gas are sufficiently independent of system size N. Corrections to this result have been discussed by L. C. Davis and L. A. Feldkamp (unpublished). In comparing the exact and asymptotic theories one should take care to compare line shapes rather than absolute magnitudes.
[17]M. A. Bowen and J. D. Dow, Semiconductors and Insulators (in press).
[18]F. K. Allotey, Solid State Commun. 9, 91 (1971).
[19]J. J. Hopfield, Comments Solid State Phys. 2, 40 (1969).
[20]M. Combescot and P. Nozières, J. Phys. (Paris) 32, 913 (1971).