Z. Physik A 290, 13–17 (1979)

Zeitschrift
für Physik A

Variational Method for Inner-Shell Excitation in Heavy-Ion Collisions

D.H. Jakubassa*
Department of Physics, University of Bergen, Bergen, Norway

Received September 1; Revised Version November 2, 1978

In the framework of the monopole model we study a perturbation method for inner-shell excitation which covers the whole projectile velocity region. This is achieved by introducing a velocity-dependent variational parameter and minimizing the time-dependent perturbation. We apply the method to the K-excitation of nonrelativistic systems.

1. Introduction

In the theory of atomic processes such as inner-shell excitation and ionization during heavy-ion collisions [1] a basis set for the electronic states is chosen in a way that the remaining interaction is small, so that one may restrict oneself to the lowest orders of perturbation theory. In slow collisions the molecular basis is used [2] where the electron is allowed to adjust to the two-center potential at any given internuclear separation R. However, when the projectile velocity v is increased and becomes comparable with the orbiting velocity v_k of the electron to be excited this adiabatic picture is no longer true. For still higher velocities the electron tends to remain in the field of the nucleus to which it is initially bound and one can apply the atomic description [3].

In order to find an appropriate basis set which holds also for the region $v \approx v_k$ a variational principle is investigated.

A well-established method in the variational approach is to introduce parameters into the wave function and determine them by minimizing the expectation value of the Schrödinger operator. For static problems this gives in most cases a good approximation to the ground state. In the time-dependent case, however, the parameters have to be chosen complex if they depend on time [4]. Thus one does thereby not find the ground state at a fixed time, but has by means of the imaginary part of the parameters also an admixture of excited states and one has to project out on some final state in order to find the transition probability. This semiclassical method, though yielding good results for total cross sections [4] may fail if one is interested in differential cross sections.

In this paper we introduce a time-independent variational parameter λ into the Hamiltonian by splitting the perturbing potential V into λV, which we incorporate in H_0, and $(1-\lambda)V$, which will be the reduced perturbation. An additional perturbation is given by the operator $\partial/\partial t$, which arises since V and thus H_0 is time-dependent. λ is then obtained by minimizing the total perturbation and will be a function of the projectile velocity. Since λ determines both the initial and final state, the transition amplitude can be calculated in the usual quantum mechanical framework.

To illustrate the method which is described in Sect. 2, we apply in Sect. 3 the monopole model where the two-center potential is replaced by a time-dependent nuclear charge. Section 4 shows the extension to the two-center problem, and in Sect. 5 we give a discussion of the results.

2. Formulation of the Variational Principle

Let us consider the excitation of a K-shell electron in the target by the projectile moving with velocity v. Then we have in the single particle model

* This work was supported by the Deutsche Forschungsgemeinschaft

0340-2193/79/0290/0013/$01.00

$$H = H_0(t) + V(t) \tag{2.1}$$

where H_0 contains the interaction between the electron and the target nucleus, and V is due to the projectile perturbation. Expanding the electron wave function ψ in eigenstates of H_0 and inserting it into the Schrödinger equation one obtains for the transition amplitude into some final state f in first order perturbation theory

$$a_f = 1/i\hbar \int_{-\infty}^{\infty} dt \langle \psi_{f0} | V - i\hbar\, \partial/\partial t\, | \psi_{i0} \rangle \cdot \exp\left(i/\hbar \int_0^t dt' (\varepsilon_f - \varepsilon_i - V_{ii} + V_{ff}) \right) \tag{2.2}$$

where ε_i and ε_f are the eigenenergies to H_0. The introduction of the diagonal expectation values of the perturbation, V_{ii} and V_{ff}, into the energy exponent is the so-called distortion approximation [5] which reduces the contribution of higher-order terms in the perturbation series.

The low- and high-energy limit of (2.2) is well established. If $v \ll v_k$, one chooses $H_0 = H$ which means that the transition is only induced by $\partial/\partial t$. This is the molecular approach. On the other hand, if $v \gg v_k$, one takes $H_0 = H_T$, where H_T contains only the (time-independent) interaction with the target, so that there is just the projectile field V_P as perturbation.

In the intermediate velocity region, $v \approx v_k$, neither this atomic description nor the adiabatic picture holds. Both operators, $\partial/\partial t$ as well as the projectile perturbation, will equally contribute to the transition. We therefore choose a basis which incorporates part of the projectile interaction by splitting the Hamiltonian in the following way

$$H = H_0(\lambda) + (1-\lambda)\, V_P \tag{2.3}$$

where $H_0(\lambda) = H_T + \lambda V_P$. The parameter λ we introduced here has to be velocity-dependent. Since H_0 depends on λ this holds also for the eigenstates ψ_{i0} and ψ_{f0}.

We determine λ by requiring that the absolute value of the transition matrix element is minimal. That means we choose the "ratio" between the two operators such that the higher-order terms in the transition amplitude will be reduced. As we are looking for a time-independent λ we must integrate the matrix element over time to get the whole contribution of the transition operators along the path. This leads to

$$d/d\lambda \left| \int_0^{\infty} dt \langle \psi_{f0} | (1-\lambda)\, V_P - i\hbar\, \partial/\partial t\, | \psi_{i0} \rangle \right|^2 = 0. \tag{2.4}$$

Since the only time-dependence of ψ_{i0} results from λV_P its time derivative is proportional to λ, and further also proportional to v. So we rediscover the limiting cases: For large v, λ must go to zero (atomic case) while for small v, $\lambda \to 1$ to reduce the potential perturbation as well (molecular case).

3. Study of λ in the Monopole Model

In order to find the behaviour of λ as a function of velocity or charge ratio one can apply an analytical model which makes the calculations very transparent and which yields results that are very similar to the two-center problem treated in the next section.

This model is based on the fact that for large momentum transfer in inner-shell excitation, the transition is dominated by the monopole expansion term of the two-center potential. It can be approximated by a one-center field with an effective charge Z that depends on the internuclear distance $R(b,t)$, where b is the impact parameter. Writing $Z = Z_2 + Z_1(t)$ where Z_2 is the target charge and $Z_1(t)$ the additional charge due to the projectile field, we have

$$H_0(\lambda) = -(\hbar^2/2m)\, \Delta - Z_2\, e^2/r - \lambda\, Z_1(t)\, e^2/r$$
$$V = -(1-\lambda)\, Z_1(t)\, e^2/r. \tag{3.1}$$

When the internuclear separation $R = 0$, $Z_1(t)$ is equal to the projectile charge Z_1 and goes to zero at infinite R. For our model calculations we choose

$$Z_1(t) = \frac{Z_1}{1 + \beta^2 (R/a_2)^2} \tag{3.2}$$

where $a_2 = a_0/Z_2$ is the K-shell radius of the target ($a_0 = \hbar^2/m\, e^2$) and β determines how fast $Z_1(t)$ decreases with R. (We shall take $\beta = 1$ if not indicated otherwise.)

The eigenfunctions of $H_0(\lambda)$ are simply hydrogenic functions belonging to the charge $Z = Z_2 + \lambda Z_1(t)$. λ is obtained by means of the variational equation (2.4). Since we are interested in a value of λ which could be used for excitations to any state f we take ψ_{f0} to be the lowest excited state ($2s$) where the matrix elements in (2.4) have their largest value. Actually one could also choose a different λ for each transition, by introducing into (2.4) the final state one is interested in. It turns out, however, that this leads only to small changes in the functional dependence of λ.

For similar reasons we evaluate (2.4) at zero impact parameter in the straight line approximation. A Coulomb path brings about changes which are smaller than 10% unless $v/v_k \leqq 0.1$ ($v_k/c = Z_2/137$) where λ is already very close to its limiting value 1. We obtain

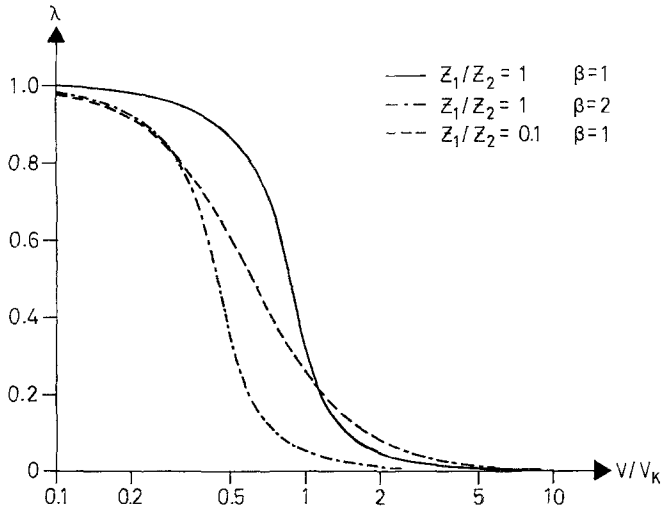

Fig. 1. Variational parameter λ for K-shell excitation as a function of the projectile velocity v in terms of the velocity v_k of the target K electron shown for different values of the interaction strength β and charge ratio Z_1/Z_2 in the monopole model

$$\int_0^\infty dt \langle \psi_{2s} | (1-\lambda)\, V_P - i\hbar\, \partial/\partial t \,| \psi_{1s} \rangle$$
$$= 4\sqrt{2}\hbar/27 \left[-(1-\lambda) \frac{\pi}{2\beta(v/v_k)} Z_1/Z_2 (1+\lambda Z_1/2Z_2) \right.$$
$$\left. + i\, 8/3 \ln(1+\lambda Z_1/Z_2) \right] \tag{3.3}$$

and by means of (2.4)

$$\beta\, v/v_k = 3\pi/16\, Z_1/Z_2 \cdot \sqrt{\frac{(1-\lambda)(1+\lambda Z_1/2Z_2)(1+(2\lambda-1) Z_1/2Z_2)(1+\lambda Z_1/Z_2)}{Z_1/Z_2 \ln(1+\lambda Z_1/Z_2)}}. \tag{3.4}$$

Due to the scaling properties of the Hamiltonian (3.1) λ is only a function of Z_1/Z_2. The dependence on v is shown in Fig. 1. The change from the molecular behaviour to the atomic region occurs at $v/v_k \sim 1$.

The details of the functional dependence of λ on v are due to the change of ψ_i with time. We have $d\psi_i/dt = (dZ/dt)\, d\psi_i/dZ$ and thus two contributions, the first expressing the slope of the interaction potential, which we represented by the parameter β. Increasing β results in a shift of the function to smaller values of v since at a given v the electron can the less adjust to the actual field the faster the potential changes. This becomes important in the relativistic case where there is an additional dependence on Z_2, so that v and β enter independently into the derivative of the potential. The second contribution to $d\psi_i/dt$ originates from the shape of the wave function, i.e. depends on the charge ratio Z_1/Z_2, and leads to a slower fall-off of $\lambda(v)$ for more asymmetric systems, as is shown in Fig. 1.

The nonadiabaticity of the electronic motion is taken into account by using basis functions which differ from the molecular functions, although one has to keep in mind that they are determined by a static calculation since λ is time-independent. The degree of nonadiabaticity can be displayed by means of the ground state energy of the electron as a function of time for fixed velocity v:

$$\varepsilon_{1s}(t) = -e^2/2a_0 (Z_2 + \lambda Z_1(t))^2. \tag{3.5}$$

The adiabatic value (for $v=0$) is the less reached the more v increases (Fig. 2) until one arrives at the constant atomic energy.

The variational model introduced above reduces the excitation process to a first order process in the region $v \approx v_k$ since it includes changes in the wave function and energy in the first order term. This holds, however, only as long as higher order terms would be restricted to these effects. In case of strong coupling and resonance effects the higher order terms are still needed.

As an example we study the cross section for the $2s$ excitation in symmetric systems by means of

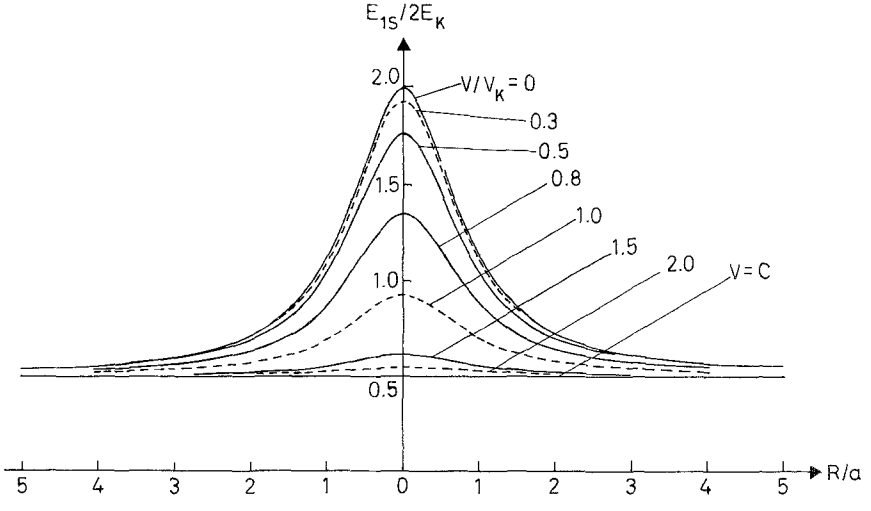

Fig. 2. Ground state energy in terms of the target $1s$ energy E_k as a function of the internuclear separation R in terms of the target K-shell radius a_k for symmetric systems colliding with different velocities v

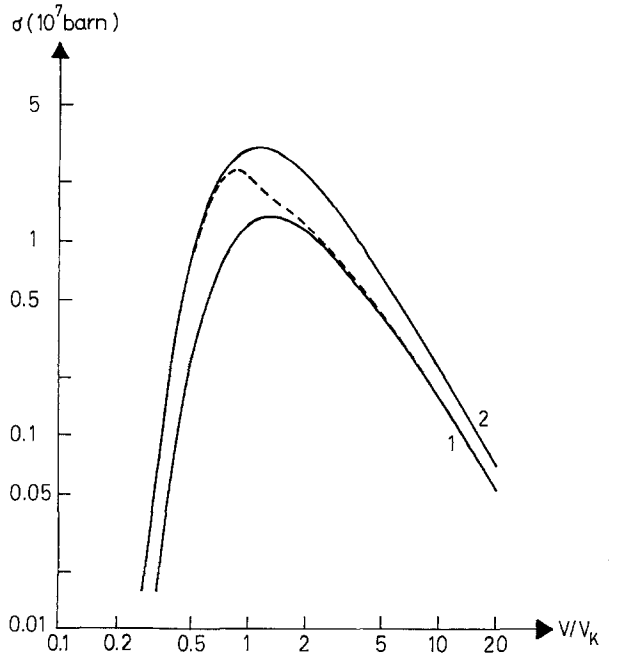

Fig. 3. Cross section for the $1s-2s$ excitation of symmetric systems ($Z_1=Z_2=1$) in the monopole model as a function of the projectile velocity v. Curve *1* = atomic basis ($\lambda=0$), Curve *2* = molecular basis ($\lambda=1$) and the dashed line corresponds to $\lambda(v)$

$$\sigma(v)=2\pi\int b\,db\,|a_f|^2 \tag{3.6}$$

together with (2.2), (3.1) and (3.4). Figure 3 gives a comparison of (3.6) with the molecular and atomic limit. The transition between the two limits occurs in the region of $0.5\lesssim v/v_k\lesssim 2$. The fact that our result differs from experiment [6] by at most a factor of 3 shows that our monopole model is quite reasonable in spite of its drastic simplifications.

4. Extension to the Two-Center Case

Instead of (3.1) we now have

$$H_0(\lambda)=-(\hbar^2/2m)\Delta-Z_2\,e^2/|\mathbf{r}-\mathbf{x}|-\lambda\,Z_1\,e^2/|\mathbf{r}-\mathbf{R}-\mathbf{x}|$$
$$V=-(1-\lambda)\,Z_1\,e^2/|\mathbf{r}-\mathbf{R}-\mathbf{x}| \tag{4.1}$$

where we have chosen the origin of the electron at a distance x from the target ($\mathbf{x}=-x_0\,\mathbf{R}$). We approximate the eigenfunctions of H_0 by one-center functions to a charge Z which is determined together with x by minimizing the expectation value of H_0 with respect to the trial function $\psi_{i0}=\pi^{-1/2}(Z/a_0)^{3/2}\exp(-Z\,r/a_0)$ at fixed internuclear separation [7].

Following the lines of the preceding section and inserting

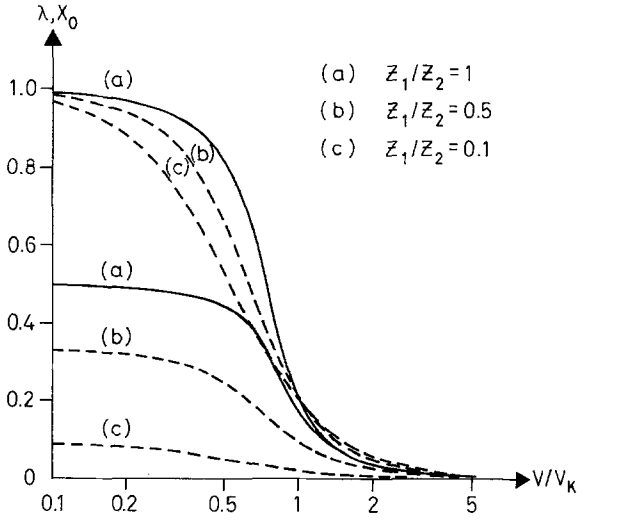

Fig. 4. Variational parameter λ as a function of v for the two-center potential at different charge ratios Z_1/Z_2 (upper curves). Also shown is the electron location x_0 at zero internuclear distance (lower curves)

$$\langle\psi_{2s}|\,V\,|\psi_{1s}\rangle=(\lambda-1)\,Z_1\,Z\,e^2/a_0(4\sqrt{2}/27)$$
$$\cdot\exp(-3/2\,Z(1-x_0)\,R/a_0)\,(1+3/2\,Z(1-x_0)\,R/a_0)$$
$$\langle\psi_{2s}|\,\partial/\partial t\,|\psi_{1s}\rangle=(32\sqrt{2}/81)\,\dot{Z}/Z \tag{4.2}$$

into (2.4) we obtain λ as shown in Fig. 4. Simultaneously we find $Z(t,\lambda)$ and $x(t,\lambda)$ for each velocity. Actually, introducing λ into H_0 results only in replacing the projectile charge Z_1 by λZ_1 which means that Z and x are scaled in the same way. A finite velocity (i.e. $\lambda<1$) corresponds thus to a smaller effective projectile charge.

In Fig. 4 we also plotted $\lambda(v)$ for different ratios Z_1/Z_2, and the results are very similar to the monopole case studied above. That for $Z_1=Z_2$ the slope of $\lambda(v)$ coincides nearly completely with the monopole calculations means that the interaction strength in the region of interest is well represented by (3.2) (with $\beta=1$).

The nonadiabaticity of slow collisions is also indicated by the location x of the electron when $R\to 0$. In the adiabatic case $x_0(R=0)$ is given by the center of charge. For finite v we have $x_0(R=0)=\lambda Z_1/(\lambda Z_1+Z_2)$ which is closer to the target. The velocity dependence of this quantity is shown in Fig. 4.

5. Discussion and Concluding Remarks

Having found $H_0(\lambda)$ for each v one can now calculate the transition probabilities according to (2.2). Thus we obtained a description of how to combine the adiabatic and the high-energy limit. For symmetric systems the atomic description is valid for velocities

$v/v_k \gtrsim 3$ [5]. The range of validity of the molecular representation has been examined only for asymmetric systems [8] and extends approximately up to $v/v_k \sim 0.3$. This is roughly in agreement with our calculations (Fig. 3) if one takes into account that for asymmetric systems the transition region is much larger (Fig. 4).

The degree of nonadiabaticity in slow collisions can be seen by the charge Z and the electron location x at small internuclear separation. The fact that x does not coincide with the center of charge leads to dipole transitions in symmetric systems which are not present in the adiabatic description. They can for example be measured by the asymmetry in the angular distribution of secondary electrons emitted during slow collisions of symmetric systems.

For the excitation of electrons in higher shells with main quantum number n the transition between the molecular and atomic region occurs at $v/v_k \approx 1/n$, i.e. when the projectile velocity approaches the orbiting velocity of the electron to be excited. In this case one finds $\lambda(v)$ by replacing ψ_{i0} in (2.4) by the corresponding initial state.

To summarize, by introducing a velocity-dependent variational parameter into the unperturbed Hamiltonian we have found a description of how to combine the molecular and the atomic limit by using only first order perturbation theory. One must, however, keep in mind that the transition amplitude can only then be calculated by the first order formula (2.2) if there is no strong coupling to neighbouring shells. Otherwise higher order terms are necessary but an expansion in the new basis set belonging to $H_0(\lambda)$ may have a faster convergence than that corresponding to the molecular or atomic limit.

I would like to thank P.A. Amundsen for interesting discussions and the Bergen group for their great hospitality during my stay in Norway.

References

1. Meyerhof, W.E., Taulbjerg, K.: Ann. Rev. Nucl. Sci. **27**, 279 (1977)
2. Briggs, J.S., Taulbjerg, K.: Topics in Modern Physics, Sellin, I. (ed.). Berlin: Springer 1978
3. Bang, J., Hansteen, J.M.: K. Dan. Vid. Selsk. Mat. Fys. Medd. **31** No. 13 (1959)
4. Kleber, M.: J. Phys. B **11**, 1069 (1978)
5. McDowell, M.R.C., Coleman, J.P.: Introduction to the Theory of Ion-Atom Collisions, p. 117, 123. Amsterdam-London: North Holland 1970
6. Morgan, T.J., Geddes, J., Gilbody, H.B.: J. Phys. B **6**, 2118 (1973)
7. Jakubassa, D.H.: Z. Physik A **285**, 249 (1978)
8. Lægsgaard, E., Andersen, J.U., Lund, M.: Electronic and Atomic Collisions, Watel, G. (ed.), p. 353. Amsterdam-New York-Oxford: North Holland 1978

Doris H. Jakubassa
on leave from the Technische
Universität München,
present address:
Institute of Physics
University of Aarhus
8 Aarhus C, Denmark