Chapter 2
A Time-Dependent Analysis of Mott's Model

In this chapter we re-examine Mott's problem introducing a precise definition of the initial state and an explicit formulation of the assumptions on the physical parameters of the model. Then we state the result in a time-dependent setting and we give the details of the proof based on the analysis of some highly oscillatory integrals. Furthermore, we consider a simpler system made of a particle interacting with just one model-atom. We show that, under the given assumptions, the time evolution of the wave function of the system takes the form already outlined by Mott, clarifying the mechanism behind the validity of Mott's result.

2.1 The Three-Particle Model Revisited

In this section we reconsider the three-particle model studied by Mott. We introduce in particular: (i) a simplified Hamiltonian for the whole system, (ii) the initial state, (iii) the assumptions on the physical parameters of the model.

(i) We consider a three-particle non relativistic, spinless quantum system in dimension three made of a particle with mass M (the α-particle) and two other particles with mass m which play the role of electrons in two model-atoms with fixed nuclei. More precisely we describe such electrons as particles subject to an attractive point interaction placed at fixed positions $\boldsymbol{a}_1$, $\boldsymbol{a}_2 \in \mathbb{R}^3$, with $0 < |\boldsymbol{a}_1| < |\boldsymbol{a}_2|$.
Furthermore, the interaction between the α-particle and each atom is given by a two-body potential V. In the following, we shall always assume V to be sufficiently regular, so that all the computations we shall perform in our analysis make sense (e.g. one can choose V in the Schwartz space of smooth and rapidly decreasing functions on $\mathbb{R}^3$).
We denote by $\boldsymbol{R}$ the position coordinate of the α-particle and by $\boldsymbol{r}_1$,$\boldsymbol{r}_2$ the position coordinates of the two electrons. Therefore, the Hamiltonian of the system in $L^2(\mathbb{R}^9)$ is written as

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$$H = H_0 + \lambda V_1 + \lambda V_2, \qquad H_0 = h_0 + h_1^\gamma + h_2^\gamma \tag{2.1.1}$$

where h_0 denotes the free Hamiltonian of the α-particle

$$h_0 = -\frac{\hbar^2}{2M}\Delta_{\boldsymbol{R}} \tag{2.1.2}$$

and h_j^γ, $\gamma > 0$, $j = 1, 2$, is the point interaction Hamiltonian of strength $-(4\pi\gamma)^{-1}$ placed at $\boldsymbol{a}_j$. The parameter $\lambda > 0$ is a coupling constant and V_j is the multiplication operator by

$$V_j(\boldsymbol{R}, \boldsymbol{r}_j) = V(\delta^{-1}(\boldsymbol{R} - \boldsymbol{r}_j)), \qquad \delta > 0 \tag{2.1.3}$$

We have gathered in appendix A some basic facts on point interaction Hamiltonians. For a more detailed treatment we refer to the monograph (Albeverio et al. 2005).
Roughly speaking, the Hamiltonian h_j^γ is a self adjoint operator in $L^2(\mathbb{R}^3)$ whose domain consists of functions u sufficiently smooth for $\boldsymbol{x} \neq \boldsymbol{a}_j$ and satisfying the following singular boundary condition at $\boldsymbol{x} = \boldsymbol{a}_j$

$$\frac{\partial}{\partial r_j}(r_j u)\Big|_{\boldsymbol{x}=\boldsymbol{a}_j} = -\frac{1}{\gamma}(r_j u)\Big|_{\boldsymbol{x}=\boldsymbol{a}_j}, \qquad r_j = |\boldsymbol{x} - \boldsymbol{a}_j|, \quad \gamma > 0 \tag{2.1.4}$$

On smooth functions with compact support in $\mathbb{R}^3 \setminus \{\boldsymbol{a}_j\}$ the operator h_j^γ acts as the free Hamiltonian. An important aspect is that h_j^γ is explicitly solvable, in the sense that the spectrum is completely characterized

$$\sigma_{ac}(h_j^\gamma) = [0, \infty), \quad \sigma_{sc}(h_j^\gamma) = \emptyset, \quad \sigma_p(h_j^\gamma) = \{E_0\}, \quad E_0 = -\frac{\hbar^2}{2m\gamma^2} \tag{2.1.5}$$

where $\sigma_{ac}(h_j^\gamma), \sigma_{sc}(h_j^\gamma), \sigma_p(h_j^\gamma)$ are, respectively, the absolutely continuous, the singular continuous, and the pure point spectra of h_j^γ. Moreover, the proper and generalized eigenfunctions are

$$\zeta_j(\boldsymbol{r}) = \frac{1}{\gamma^{3/2}}\zeta^0(\gamma^{-1}(\boldsymbol{r} - \boldsymbol{a}_j)), \quad \zeta^0(\boldsymbol{x}) = \frac{1}{\sqrt{2\pi}}\frac{e^{-|\boldsymbol{x}|}}{|\boldsymbol{x}|} \tag{2.1.6}$$

$$\phi_j(\boldsymbol{r}, \boldsymbol{k}) = e^{i\boldsymbol{k}\cdot\boldsymbol{a}_j}\phi^0(\gamma^{-1}(\boldsymbol{r} - \boldsymbol{a}_j), \gamma\boldsymbol{k}), \quad \phi^0(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{(2\pi)^{3/2}}\left(e^{i\boldsymbol{y}\cdot\boldsymbol{x}} - \frac{1}{1 - i|\boldsymbol{y}|}\frac{e^{-i|\boldsymbol{y}||\boldsymbol{x}|}}{|\boldsymbol{x}|}\right) \tag{2.1.7}$$

The parameter γ has the physical meaning of a scattering length and it characterizes the effective range of the point interaction. From (2.1.6) it is also clear

that γ is a measure of the linear spread of the ground state, i.e., of the "effective diameter" of the atoms. Furthermore, in the limit $\gamma \to 0$ the Hamiltonian h_j^γ reduces to the free Hamiltonian.
The choice of point interaction Hamiltonian to modelize an atom is done for the sake of simplicity. In fact, the presence of exactly one negative eigenvalue plus an absolutely continuous spectrum coinciding with the positive real axis makes such an Hamiltonian particularly suited for a simple but non trivial description of a ionization process.
The unperturbed Hamiltonian H_0 is obviously self-adjoint and bounded from below in $L^2(\mathbb{R}^9)$. Moreover, the smoothness assumption on the interaction potential V guarantees that the perturbed Hamiltonian H is also self-adjoint and bounded from below on the same domain of H_0. In particular this implies that the dynamics generated by the Hamiltonian H is well defined.

(ii) The next step is to define the initial state for the whole system. We choose the following product state

$$\Psi_0(\boldsymbol{R}, \boldsymbol{r}_1, \boldsymbol{r}_2) = \psi(\boldsymbol{R})\zeta_1(\boldsymbol{r}_1)\zeta_2(\boldsymbol{r}_2) \tag{2.1.8}$$

where ζ_j are the bound states defined in (2.1.6) and ψ is defined as follows. Let us consider a wave packet localized in space around the origin with an average momentum along the direction $\hat{\boldsymbol{u}}$ of the unit sphere S^2. Integrating over S^2, one obtains

$$\psi(\boldsymbol{R}) = \mathcal{N}\, f(\sigma^{-1}\boldsymbol{R}) \int_{S^2} d\hat{\boldsymbol{u}}\; e^{i\frac{P_0}{\hbar}\hat{\boldsymbol{u}}\cdot\boldsymbol{R}} \tag{2.1.9}$$

where $\mathcal{N}$ is a normalization constant, $\sigma > 0$, $P_0 \equiv Mv_0 > 0$, f belongs to the Schwartz space $\mathcal{S}(\mathbb{R}^3)$ with $\|f\|_{L^2(\mathbb{R}^3)} = 1$. For concreteness we choose

$$f(\boldsymbol{x}) = \pi^{-3/4} e^{-\frac{|\boldsymbol{x}|^2}{2}} \tag{2.1.10}$$

but it will be clear in the following that the result of the analysis is independent of the specific choice of f.
Formula (2.1.9) defines an initial state for the α-particle in the form of a spherical wave concentrated in position around the origin with an isotropic average momentum P_0. Further details on such a state and on its free evolution are given in appendix B.
The choice (2.1.8) for the wave function of the whole system at time zero corresponds to the situation in which the two model-atoms are in their (unique) bound state, the α-particle is described by the spherical wave (2.1.9) and no correlation is assumed among the three particles.

(iii) The last step is to specify the hypotheses on the physical parameters of the model. We stress that such hypotheses are of crucial importance in order to correctly reproduce Mott's result in the framework of a time-dependent analysis. The assumptions are simply defined introducing the small parameter $\varepsilon > 0$ and setting the physical parameters as follows

$$\begin{aligned} &\hbar = \varepsilon^2, \qquad M = 1, \qquad \sigma = \varepsilon, \qquad m = \varepsilon, \\ &\gamma = \varepsilon, \qquad \delta = \varepsilon, \qquad \lambda = \varepsilon^2 \end{aligned} \tag{2.1.11}$$

Note that the remaining free parameters of the model v_0, $|\boldsymbol{a}_1|$, $|\boldsymbol{a}_2|$ are assumed to be of order one for $\varepsilon \to 0$. The corresponding rescaled Hamiltonian becomes

$$H^\varepsilon = H_0^\varepsilon + \varepsilon^2 V^\varepsilon, \qquad H_0^\varepsilon = h_0^\varepsilon + h_1^\varepsilon + h_2^\varepsilon \tag{2.1.12}$$

where

$$h_0^\varepsilon = -\frac{\varepsilon^4}{2}\Delta_{\boldsymbol{R}} \tag{2.1.13}$$

h_j^ε, $j = 1, 2$, are the corresponding rescaled point interaction Hamiltonians and

$$V^\varepsilon = V_1^\varepsilon + V_2^\varepsilon, \qquad V_j^\varepsilon(\boldsymbol{R}, \boldsymbol{r}_j) = V\big(\varepsilon^{-1}(\boldsymbol{R} - \boldsymbol{r}_j)\big) \tag{2.1.14}$$

Analogously, the rescaled initial state of the system is

$$\Psi_0^\varepsilon(\boldsymbol{R}, \boldsymbol{r}_1, \boldsymbol{r}_2) = \psi^\varepsilon(\boldsymbol{R})\zeta_1^\varepsilon(\boldsymbol{r}_1)\zeta_2^\varepsilon(\boldsymbol{r}_2) \tag{2.1.15}$$

$$\psi^\varepsilon(\boldsymbol{R}) = \frac{\mathcal{N}_\varepsilon}{\varepsilon^{5/2}}\, f\left(\varepsilon^{-1}\boldsymbol{R}\right) \int_{S^2} d\hat{\boldsymbol{u}}\, e^{\frac{i}{\varepsilon^2} v_0 \hat{\boldsymbol{u}}\cdot\boldsymbol{R}} \tag{2.1.16}$$

$$\zeta_j^\varepsilon(\boldsymbol{r}_j) = \frac{1}{\varepsilon^{3/2}}\zeta^0\big(\varepsilon^{-1}(\boldsymbol{r}_j - \boldsymbol{a}_j)\big) \tag{2.1.17}$$

where $\mathcal{N}_\varepsilon$ is the normalization constant, with

$$\lim_{\varepsilon\to 0} \mathcal{N}_\varepsilon = \mathcal{N}_0 \equiv \frac{v_0}{4\pi} \tag{2.1.18}$$

(see appendix B). We also note that the energy of the ground state of the two atoms now reads

$$E_0^\varepsilon = -\frac{\varepsilon}{2} \tag{2.1.19}$$

and the generalized eigenfunctions of h_j^ε are

$$\phi_j^\varepsilon(\boldsymbol{r}, \boldsymbol{k}) = e^{i\boldsymbol{k}\cdot\boldsymbol{a}_j}\phi^0(\varepsilon^{-1}(\boldsymbol{r} - \boldsymbol{a}_j), \varepsilon\boldsymbol{k}) \tag{2.1.20}$$

We briefly comment on the physical meaning of the above scaling for $\varepsilon \to 0$. We first note that the dimensionless quantity

$$\frac{\hbar}{M v_0 \sigma} \tag{2.1.21}$$

is of order ε, which means that the wavelength $\frac{\hbar}{M v_0}$ associated to the α-particle is much smaller than the spatial localization σ (high momentum regime). Analogously the quantities

$$\frac{\sigma}{|\boldsymbol{a}_j|}, \qquad \frac{\gamma}{|\boldsymbol{a}_j|}, \qquad \frac{\delta}{|\boldsymbol{a}_j|}, \qquad j = 1, 2 \tag{2.1.22}$$

are of order ε, i.e., the spatial localization of the α-particle, the "diameter" of the atoms and the effective range of the interaction are much smaller than the macroscopic distance $|\boldsymbol{a}_j|$. Moreover, we note that the ionization energy E_0 is of order ε and the coupling constant λ of order ε^2 while the initial kinetic energy of the α-particle is of order one. This guarantees that the α-particle energy loss due to the interaction with an atom is small (quasi-elastic regime) and the perturbative method can be reasonably applied.

Furthermore, it is interesting to compare the characteristic times of the system. We define, in particular, the classical flight times for $j = 1, 2$ as the time spent by a classical particle, starting from the origin with velocity v_0, to reach the atom in $\boldsymbol{a}_j$

$$\tau_j = \frac{|\boldsymbol{a}_j|}{v_0} \tag{2.1.23}$$

the characteristic "period" of the atoms

$$T_a = 2\pi \frac{\hbar}{|E_0|} = 4\pi \frac{m\gamma^2}{\hbar} \tag{2.1.24}$$

and the transit time, i.e., the time spent by the α-particle to travel the diameter of an atom

$$T_t = \frac{\gamma}{v_0} \tag{2.1.25}$$

It turns out that

$$\frac{T_t}{T_a} = O(1) \tag{2.1.26}$$

i.e., the α-particle can "see" the internal structure of the atoms. Moreover,

$$\frac{T_t}{\tau_j} = O(\varepsilon) \tag{2.1.27}$$

which implies that τ_j can be reasonably identified as the collision time of the α-particle with the atom in $\boldsymbol{a}_j$.

We conclude this section collecting some notation that will be used in the rest of this chapter.

- $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$ is a vector in $\mathbb{R}^n$, $|\boldsymbol{x}|$ the euclidean norm and $\hat{\boldsymbol{x}} = \frac{\boldsymbol{x}}{|\boldsymbol{x}|}$, $\boldsymbol{x} \neq 0$, the corresponding unit vector. The scalar product in $\mathbb{R}^n$ is denoted by $\boldsymbol{x} \cdot \boldsymbol{y}$.
- $\langle \boldsymbol{x} \rangle = (1 + |\boldsymbol{x}|^2)^{1/2}$, $\boldsymbol{x} \in \mathbb{R}^n$.
- $\underline{n} = (n_1, n_2, \dots, n_k)$ is a vector in $\mathbb{N}^k$ and, with an abuse of notation, $|n| = n_1 + n_2 + \cdots + n_k$.
- $\| \cdot \|$, $(\cdot, \cdot)$ are the norm and the scalar product in the Hilbert space of the whole system under consideration.
- For a function f defined in $\mathbb{R}^n$ we denote

$$D^{\underline{k}}_{\boldsymbol{x}} f(\boldsymbol{x}) = \frac{\partial^{|k|}}{\partial x_1^{k_1} \dots \partial x_n^{k_n}} f(\boldsymbol{x}) \tag{2.1.28}$$

  with $\underline{k} \in \mathbb{N}^n$ and $|k| = k_1 + \cdots + k_n$.
- $W^{k,1}_s(\mathbb{R}^n)$, with $n, k \in \mathbb{N}$, $s > 0$, is the weighted Sobolev space equipped with the norm

$$\| f \|_{W^{k,1}_s} = \sum_{\underline{\alpha}, |\alpha| \leq k} \int d\boldsymbol{x} \, \langle \boldsymbol{x} \rangle^s |D^{\underline{\alpha}}_{\boldsymbol{x}} f(\boldsymbol{x})| \tag{2.1.29}$$

- The Fourier transform in $\mathbb{R}^3$ of a function f is

$$\widetilde{f}(\boldsymbol{q}) = \frac{1}{(2\pi)^{3/2}} \int d\boldsymbol{x} \, e^{-i\boldsymbol{q}\cdot\boldsymbol{x}} f(\boldsymbol{x}) \tag{2.1.30}$$

- Finally C, C_k or $C_k(t)$ denote generic positive constants (possibly depending on $k \in \mathbb{N}$ and on t).

2.2 Time-Dependent Formulation and Results

We are now in position to reformulate the problem in a full time-dependent setting. In this entire analysis, we shall always assume the validity of the hypotheses made in the previous section. As we already mentioned, under these conditions it is reasonable to consider τ_1 and τ_2, defined in (2.1.23), as the collision times of the spherical wave emerging from the origin with the first atom in $\boldsymbol{a}_1$ and the second atom in $\boldsymbol{a}_2$ respectively. Therefore, since we are interested in the probability that both atom are ionized, we shall fix

$$t > \tau_2 \tag{2.2.1}$$

The wave function of the system at time t is

$$U^\varepsilon(t)\Psi_0^\varepsilon, \qquad U^\varepsilon(t) = e^{-i\frac{t}{\varepsilon^2}H^\varepsilon} \tag{2.2.2}$$

or, using Duhamel's formula

$$U^\varepsilon(t)\Psi_0^\varepsilon = U_0^\varepsilon(t)\Psi_0^\varepsilon - i\int_0^t dt_1\; U^\varepsilon(t-t_1)\, V^\varepsilon\, U_0^\varepsilon(t_1)\Psi_0^\varepsilon \tag{2.2.3}$$

where $U_0^\varepsilon(t)$ denotes the free evolution

$$U_0^\varepsilon(t) = e^{-i\frac{t}{\varepsilon^2}H_0^\varepsilon} \tag{2.2.4}$$

Following Mott's original strategy, we shall limit our consideration to the second order approximation $\Psi_2^\varepsilon(t)$ of the state $U^\varepsilon(t)\Psi_0^\varepsilon$ which, iterating Duhamel's formula twice, is given by

$$\Psi_2^\varepsilon(t) = U_0^\varepsilon(t)\hat{\Psi}_2^\varepsilon(t) \tag{2.2.5}$$

where

$$\hat{\Psi}_2^\varepsilon(t) = \Psi_0^\varepsilon - i\int_0^t dt_1\, U_0^\varepsilon(-t_1)V^\varepsilon U_0^\varepsilon(t_1)\Psi_0^\varepsilon - \int_0^t dt_1\; U_0^\varepsilon(-t_1)V^\varepsilon U_0^\varepsilon(t_1)\int_0^{t_1} dt_2\, U_0^\varepsilon(-t_2)V^\varepsilon U_0^\varepsilon(t_2)\Psi_0^\varepsilon \tag{2.2.6}$$

Starting from $\hat{\Psi}_2^\varepsilon(t)$, one can compute the relevant object of our analysis $\mathcal{P}_2^\varepsilon(t)$, i.e., the probability that both atoms are ionized at time t up to second order in perturbation theory. In fact, applying Born's rule, we have

$$\mathcal{P}_2^\varepsilon(t) = \left(\hat{\Psi}_2^\varepsilon(t),\, E_{(0,\infty)}(h_1^\varepsilon)E_{(0,\infty)}(h_2^\varepsilon)\,\hat{\Psi}_2^\varepsilon(t)\right) \tag{2.2.7}$$

where $E_{(0,\infty)}(h_j^\varepsilon)$ is the spectral projection on the interval $(0,\infty)$ corresponding to the Hamiltonian h_j^ε. Using the eigenfunction expansion theorem for h_j^ε (see appendix A), such spectral projection is explicitly given by

$$\left(E_{(0,\infty)}(h_j^\varepsilon)g\right)(\boldsymbol{r}) = \int d\boldsymbol{k}\,\phi_j^\varepsilon(\boldsymbol{r},\boldsymbol{k})\int d\boldsymbol{r}'\,\overline{\phi_j^\varepsilon}(\boldsymbol{r}',\boldsymbol{k})g(\boldsymbol{r}') \tag{2.2.8}$$

for any $g \in L^2(\mathbb{R}^3)$. Therefore, interchanging the integration in the variables $\boldsymbol{r}_1$,$\boldsymbol{r}_2$ with the one in $\boldsymbol{k}_1$,$\boldsymbol{k}_2$, we find

$$\begin{aligned}\mathcal{P}_2^\varepsilon(t) = &\int d\boldsymbol{R}\, d\boldsymbol{r}_1 d\boldsymbol{r}_2\,\overline{\hat{\Psi}_2^\varepsilon}(t,\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2)\cdot\int d\boldsymbol{k}_1 d\boldsymbol{k}_2\,\phi_1^\varepsilon(\boldsymbol{r}_1,\boldsymbol{k}_1)\phi_2^\varepsilon(\boldsymbol{r}_2,\boldsymbol{k}_2)\\ &\int d\boldsymbol{r}_1' d\boldsymbol{r}_2'\,\overline{\phi_1^\varepsilon}(\boldsymbol{r}_1',\boldsymbol{k}_1)\overline{\phi_2^\varepsilon}(\boldsymbol{r}_2',\boldsymbol{k}_2)\hat{\Psi}_2^\varepsilon(t,\boldsymbol{R},\boldsymbol{r}_1',\boldsymbol{r}_2')\end{aligned}$$

$$= \int d\boldsymbol{R}\, d\boldsymbol{k}_1\, d\boldsymbol{k}_2 \left| \int d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, \overline{\phi_1^\varepsilon}(\boldsymbol{r}_1, \boldsymbol{k}_1) \overline{\phi_2^\varepsilon}(\boldsymbol{r}_2, \boldsymbol{k}_2) \hat{\Psi}_2^\varepsilon(\boldsymbol{R}, \boldsymbol{r}_1, \boldsymbol{r}_2, t) \right|^2 \tag{2.2.9}$$

Our aim is the characterization of $\mathcal{P}_2^\varepsilon(t)$ for a fixed time $t > \tau_2$. As expected from Mott's argument, we find that such probability is essentially zero unless $\boldsymbol{a}_2$ is "almost aligned" with $\boldsymbol{a}_1$ and the origin. The result is formulated in Theorems 2.2.1 and 2.2.2 below (see also Dell'Antonio et al 2010). In particular, in Theorem 2.2.1 we consider the case in which the angle between $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ is different from zero.

Theorem 2.2.1 *Let us fix $t > \tau_2$ and $\hat{\boldsymbol{a}}_1 \cdot \hat{\boldsymbol{a}}_2 < 1$. Then for any $k \in \mathbb{N}$ there exists a constant $C_k(t) > 0$, independent of ε, such that*

$$\mathcal{P}_2^\varepsilon(t) \leq C_k(t)\, \|\widetilde{V}\|_{W_k^{k,1}}^4 |\boldsymbol{a}_1|^{-2k} \left[\left(1 - \frac{|\boldsymbol{a}_1|}{|\boldsymbol{a}_2|}\right)^{-2k} + \left(1 - \hat{\boldsymbol{a}}_1 \cdot \hat{\boldsymbol{a}}_2\right)^{-k} \right] \varepsilon^{2k-2} \tag{2.2.10}$$

The estimate (2.2.10) shows that the ionization probability decays faster than any power of ε provided that the angle between $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ is $O(\varepsilon^\beta)$, with $0 \leq \beta < 1$. The estimate gives no information if the angle between $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ is proportional to ε, or smaller. This latter case is considered in Theorem 2.2.2 where the leading term of the asymptotic expansion for $\varepsilon \to 0$ of the ionization probability is given.

Theorem 2.2.2 *Let us fix $t > \tau_2$ and $\hat{\boldsymbol{a}}_1 \cdot \hat{\boldsymbol{a}}_2 = \cos \chi_\varepsilon$, where $\chi_\varepsilon \in [0, \chi_0 \varepsilon]$, $\chi_0 > 0$. Then, at the leading order for $\varepsilon \to 0$, we have*

$$\mathcal{P}_2^\varepsilon(t) \sim \frac{\varepsilon^6}{v_0^2 |\boldsymbol{a}_1|^4} \int d\boldsymbol{x} d\boldsymbol{y}_1 d\boldsymbol{y}_2 \left| \int d\eta_1 d\eta_2\, F(\eta_1, \eta_2, \boldsymbol{x}, \boldsymbol{y}_1, \boldsymbol{y}_2) \right|^2 \tag{2.2.11}$$

where the function F is independent of ε and it can be explicitly computed (see (2.4.64)).

The results expressed in Theorems 2.2.1, 2.2.2 can be understood on the basis of the original physical argument given by Mott. In our time-dependent setting the argument can be described as follows. At time zero the spherical wave starts to propagate in the chamber and at time τ_1 it interacts with the atom in $\boldsymbol{a}_1$. If, as a result of the interaction, such an atom is ionized then a localized wave packet emerges from $\boldsymbol{a}_1$ with momentum along the direction $\overline{O\boldsymbol{a}_1}$. In order also to obtain ionization of the atom in $\boldsymbol{a}_2$ the localized wave packet must hit the atom in $\boldsymbol{a}_2$ (at time τ_2) and this can happen only if $\boldsymbol{a}_2$ lies approximately on the line $\overline{O\boldsymbol{a}_1}$. We stress once again that such physical behavior is far from being universal and that it depends strongly on our assumptions on the physical parameters of the model.

The above heuristic argument will be made precise in a simpler model studied in Sect. 2.5.

The proof of Theorems 2.2.1, 2.2.2 makes use of a representation formula for the ionization probability $\mathcal{P}_2^\varepsilon(t)$ in terms of highly oscillatory integrals for $\varepsilon \to 0$. Such formula will be proved in the next section. Then in Sect. 2.4 we prove the results applying non-stationary and stationary phase methods to the above integrals.

2.3 Representation Formulas by Oscillatory Integrals

The aim of this section is to prove the following representation formula

$$\mathcal{P}_2^\varepsilon(t) = \frac{\mathcal{N}_\varepsilon^2}{\varepsilon^2} \int d\boldsymbol{x} d\boldsymbol{y}_1 d\boldsymbol{y}_2 \left| \alpha_{12}^\varepsilon \mathcal{G}_{12}^\varepsilon(\boldsymbol{x}, \boldsymbol{y}_1, \boldsymbol{y}_2, t) + \alpha_{21}^\varepsilon \mathcal{G}_{21}^\varepsilon(\boldsymbol{x}, \boldsymbol{y}_1, \boldsymbol{y}_2, t) \right|^2 \quad (2.3.1)$$

where for $l, j = 1, 2$, $j \neq l$ one has

$$\alpha_{lj}^\varepsilon = e^{-\frac{i}{\varepsilon}\boldsymbol{y}_l \cdot \boldsymbol{a}_1 - \frac{i}{\varepsilon}\boldsymbol{y}_j \cdot \boldsymbol{a}_2} \quad (2.3.2)$$

$$\mathcal{G}_{lj}^\varepsilon(\boldsymbol{x}, \boldsymbol{y}_1, \boldsymbol{y}_2, t) = \int_{S^2} d\hat{\boldsymbol{u}} \int_0^t dt_2 \int_0^{t_2} dt_1 \int d\boldsymbol{\eta} d\boldsymbol{\xi}\, G_{lj}(t_2, t_1, \boldsymbol{\eta}, \boldsymbol{\xi}; \boldsymbol{x}, \boldsymbol{y}_1, \boldsymbol{y}_2, t)\, e^{\frac{i}{\varepsilon}\Theta_{lj}(\hat{\boldsymbol{u}}, t_2, t_1, \boldsymbol{\eta}, \boldsymbol{\xi}; \boldsymbol{x}, \boldsymbol{y}_1, \boldsymbol{y}_2, t)} \quad (2.3.3)$$

and

$$\Theta_{lj}(\hat{\mathbf{u}}, t_2, t_1, \boldsymbol{\eta}, \boldsymbol{\xi}) = v_0 \hat{\mathbf{u}} \cdot (\mathbf{x} + t_2 \boldsymbol{\eta} + t_1 \boldsymbol{\xi}) - \mathbf{a_j} \cdot \boldsymbol{\eta} - \mathbf{a_l} \cdot \boldsymbol{\xi} + \frac{t_2}{2}(1 + |\mathbf{y_j}|^2) + \frac{t_1}{2}(1 + |\mathbf{y_l}|^2) \quad (2.3.4)$$

$$G_{lj}(t_2, t_1, \boldsymbol{\eta}, \boldsymbol{\xi}) = g(\boldsymbol{\eta}, \mathbf{y_j}) g(\boldsymbol{\xi}, \mathbf{y}_l) f(\mathbf{x} + t_2 \boldsymbol{\eta} + t_1 \boldsymbol{\xi}) e^{i\phi(t_2, t_1, \boldsymbol{\eta}, \boldsymbol{\xi})} \quad (2.3.5)$$

$$\phi(t_2, t_1, \boldsymbol{\eta}, \boldsymbol{\xi}) = \mathbf{x} \cdot (\boldsymbol{\eta} + \boldsymbol{\xi}) + \frac{t_2}{2}|\boldsymbol{\eta}|^2 + \frac{t_1}{2}|\boldsymbol{\xi}|^2 + t_2 \boldsymbol{\eta} \cdot \boldsymbol{\xi} \quad (2.3.6)$$

The function g in (2.3.5) is defined as follows

$$g(\boldsymbol{\xi}, \boldsymbol{y}) = \widetilde{V}(\boldsymbol{\xi}) h(\boldsymbol{\xi}, \boldsymbol{y}) \quad (2.3.7)$$

$$h(\boldsymbol{\xi}, \boldsymbol{y}) = \frac{1}{(2\pi)^{3/2}} \int d\boldsymbol{x}\, e^{-i\boldsymbol{\xi} \cdot \boldsymbol{x}}\, \overline{\phi^0}(\boldsymbol{x}, \boldsymbol{y})\, \zeta^0(\boldsymbol{x}), \qquad \boldsymbol{\xi}, \boldsymbol{y} \in \mathbb{R}^3 \quad (2.3.8)$$

To simplify the notation, on the r.h.s. of (2.3.4), (2.3.5), (2.3.6) we have omitted the parametric dependence on $\boldsymbol{x}, \boldsymbol{y}_1, \boldsymbol{y}_2, t$. In (2.3.1), (2.3.2), (2.3.3) we have denoted by $\boldsymbol{x}, \boldsymbol{y}_1, \boldsymbol{y}_2$ the rescaled position of the α-particle and the rescaled momenta of the electrons respectively.

The proof of (2.3.1) relies on the use of the eigenfunction expansion theorem for the Hamiltonians with point interactions h_j^ε and on the explicit form of the unitary free propagator. The computation is rather long but straightforward and it is outlined below for the sake of completeness.

As a first step, we shall write the probability amplitude defined by

$$\mathcal{F}^{\varepsilon}(\boldsymbol{R},\boldsymbol{k}_1,\boldsymbol{k}_2,t)\equiv\int d\boldsymbol{r}_1\,d\boldsymbol{r}_2\,\overline{\phi_1^{\varepsilon}}(\boldsymbol{r}_1,\boldsymbol{k}_1)\overline{\phi_2^{\varepsilon}}(\boldsymbol{r}_2,\boldsymbol{k}_2)\hat{\Psi}_2^{\varepsilon}(\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2,t) \tag{2.3.9}$$

(see the r.h.s. of (2.2.9)) in terms of the free propagator generated by h_0^{ε}. Using the notation

$$U_0^{\varepsilon}(-t)V^{\varepsilon}U_0^{\varepsilon}(t)=W_1^{\varepsilon}(t)+W_2^{\varepsilon}(t)\,,\qquad W_j^{\varepsilon}(t)=e^{i\frac{t}{\varepsilon^2}h_0^{\varepsilon}}e^{i\frac{t}{\varepsilon^2}h_j^{\varepsilon}}V_j^{\varepsilon}e^{-i\frac{t}{\varepsilon^2}h_0^{\varepsilon}}e^{-i\frac{t}{\varepsilon^2}h_j^{\varepsilon}} \tag{2.3.10}$$

we rewrite the r.h.s. of (2.3.9) in the more convenient form

$$\begin{aligned}\mathcal{F}^{\varepsilon}(\boldsymbol{R},\boldsymbol{k}_1,\boldsymbol{k}_2,t)&=\int d\boldsymbol{r}_1\,d\boldsymbol{r}_2\,\overline{\phi_1^{\varepsilon}}(\boldsymbol{r}_1,\boldsymbol{k}_1)\overline{\phi_2^{\varepsilon}}(\boldsymbol{r}_2,\boldsymbol{k}_2)\Psi_0^{\varepsilon}(\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2)\\&-i\int_0^t dt_1\int d\boldsymbol{r}_1 d\boldsymbol{r}_2\,\overline{\phi_1^{\varepsilon}}(\boldsymbol{r}_1,\boldsymbol{k}_1)\overline{\phi_2^{\varepsilon}}(\boldsymbol{r}_2,\boldsymbol{k}_2)\Big[\big(W_1^{\varepsilon}(t_1)+W_2^{\varepsilon}(t_1)\big)\Psi_0^{\varepsilon}\Big](\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2)\\&-\int_0^t dt_2\int_0^{t_2}dt_1\int d\boldsymbol{r}_1 d\boldsymbol{r}_2\,\overline{\phi_1^{\varepsilon}}(\boldsymbol{r}_1,\boldsymbol{k}_1)\overline{\phi_2^{\varepsilon}}(\boldsymbol{r}_2,\boldsymbol{k}_2)\Big[\big(W_1^{\varepsilon}(t_2)+W_2^{\varepsilon}(t_2)\big)\big(W_1^{\varepsilon}(t_1)+W_2^{\varepsilon}(t_1)\big)\Psi_0^{\varepsilon}\Big](\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2)\end{aligned} \tag{2.3.11}$$

We observe that the operator $W_j^{\varepsilon}(t)$ acts non trivially only on the variables $\boldsymbol{R}$ and $\boldsymbol{r}_j$. Exploiting this fact and the orthogonality relation

$$\int d\boldsymbol{r}\,\overline{\phi_j^{\varepsilon}}(\boldsymbol{r},\boldsymbol{k})\,\zeta_j^{\varepsilon}(\boldsymbol{r})=0,\qquad j=1,2 \tag{2.3.12}$$

we obtain

$$\mathcal{F}^{\varepsilon}=\mathcal{F}_{12}^{\varepsilon}+\mathcal{F}_{21}^{\varepsilon} \tag{2.3.13}$$

and for $l,\,j=1,2,\,j\neq l$

$$\mathcal{F}_{lj}^{\varepsilon}(\boldsymbol{R},\boldsymbol{k}_1,\boldsymbol{k}_2,t)=\int_0^t dt_2\int_0^{t_2}dt_1\int d\boldsymbol{r}_1 d\boldsymbol{r}_2\,\overline{\phi_1^{\varepsilon}}(\boldsymbol{r}_1,\boldsymbol{k}_1)\overline{\phi_2^{\varepsilon}}(\boldsymbol{r}_2,\boldsymbol{k}_2)\left(W_j^{\varepsilon}(t_2)W_l^{\varepsilon}(t_1)\Psi_0^{\varepsilon}\right)(\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2) \tag{2.3.14}$$

Let us fix $l=1$, $j=2$ and let us compute $\mathcal{F}_{12}^{\varepsilon}$. Due to the specific factorized form of the initial state of the system, the action of $W_1^{\varepsilon}(t_1)$ reduces to

$$W_1^{\varepsilon}(t_1)\Psi_0^{\varepsilon}=e^{i\frac{t_1}{2\varepsilon}}\,\zeta_2^{\varepsilon}\,e^{i\frac{t_1}{\varepsilon^2}h_0^{\varepsilon}}\left(e^{i\frac{t_1}{\varepsilon}h_1^{\varepsilon}}V_1^{\varepsilon}\zeta_1^{\varepsilon}\right)e^{-i\frac{t_1}{\varepsilon^2}h_0^{\varepsilon}}\,\psi^{\varepsilon} \tag{2.3.15}$$

and therefore

$$W_2^{\varepsilon}(t_2)W_1^{\varepsilon}(t_1)\Psi_0^{\varepsilon}=e^{i\frac{t_1+t_2}{2\varepsilon}}\,e^{i\frac{t_2}{\varepsilon^2}h_0^{\varepsilon}}\left(e^{i\frac{t_2}{\varepsilon}h_2^{\varepsilon}}V_2^{\varepsilon}\zeta_2^{\varepsilon}\right)e^{-i\frac{t_2}{\varepsilon^2}h_0^{\varepsilon}}\,e^{i\frac{t_1}{\varepsilon^2}h_0^{\varepsilon}}\left(e^{i\frac{t_1}{\varepsilon}h_1^{\varepsilon}}V_1^{\varepsilon}\zeta_1^{\varepsilon}\right)e^{-i\frac{t_1}{\varepsilon^2}h_0^{\varepsilon}}\,\psi^{\varepsilon} \tag{2.3.16}$$

Using the eigenfunction expansion theorem for h_j^ε, one can explicitly write the action of the unitary group $e^{i\frac{t}{\varepsilon^2}h_j^\varepsilon}$

$$\left(e^{i\frac{t}{\varepsilon^2}h_j^\varepsilon}(V_j^\varepsilon(\boldsymbol{R},\cdot)\zeta_j^\varepsilon)\right)(\boldsymbol{r}) = e^{-i\frac{t}{2\varepsilon}}\,\widehat{V}_{j,0}^\varepsilon(\boldsymbol{R})\zeta_j^\varepsilon(\boldsymbol{r}) + \int d\boldsymbol{k}\, e^{i\frac{\varepsilon}{2}t|\boldsymbol{k}|^2}\widehat{V}_j^\varepsilon(\boldsymbol{R},\boldsymbol{k})\,\phi_j^\varepsilon(\boldsymbol{r},\boldsymbol{k}) \tag{2.3.17}$$

where

$$\widehat{V}_{j,0}^\varepsilon(\boldsymbol{R}) = \int d\boldsymbol{r}\, V_j^\varepsilon(\boldsymbol{R},\boldsymbol{r})\left|\zeta_j^\varepsilon(\boldsymbol{r})\right|^2, \qquad \widehat{V}_j^\varepsilon(\boldsymbol{R},\boldsymbol{k}) = \int d\boldsymbol{r}\,\overline{\phi_j^\varepsilon}(\boldsymbol{r},\boldsymbol{k})V(\varepsilon^{-1}(\boldsymbol{R}-\boldsymbol{r}))\zeta_j^\varepsilon(\boldsymbol{r}) \tag{2.3.18}$$

We note that

$$\int d\boldsymbol{r}\,\overline{\phi_j^\varepsilon}(\boldsymbol{r},\boldsymbol{k})\left(e^{i\frac{t}{\varepsilon^2}h_j^\varepsilon}(V_j^\varepsilon(\boldsymbol{R},\cdot)\zeta_j^\varepsilon)\right)(\boldsymbol{r}) = e^{i\frac{\varepsilon}{2}t|\boldsymbol{k}|^2}\widehat{V}_j^\varepsilon(\boldsymbol{R},\boldsymbol{k}) \tag{2.3.19}$$

The function $\widehat{V}_j^\varepsilon(\boldsymbol{R},\boldsymbol{k})$ can be more conveniently written as

$$\widehat{V}_j^\varepsilon(\boldsymbol{R},\boldsymbol{k}) = \varepsilon^{3/2}e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_j}\int d\boldsymbol{x}\,\overline{\phi^0}(\boldsymbol{x},\varepsilon\boldsymbol{k})\zeta^0(\boldsymbol{x})V\left(\varepsilon^{-1}(\boldsymbol{R}-\boldsymbol{a}_j)-\boldsymbol{x}\right) = \varepsilon^{3/2}e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_j}\int d\boldsymbol{\xi}\, g(\boldsymbol{\xi},\varepsilon\boldsymbol{k})\,e^{\frac{i}{\varepsilon}\boldsymbol{\xi}\cdot(\boldsymbol{R}-\boldsymbol{a}_j)} \tag{2.3.20}$$

where $g(\boldsymbol{\xi},\boldsymbol{y})$ has been defined in (3.3.9). Using (2.3.16), (2.3.17) and (2.3.19) in (2.3.14) we finally find

$$\mathcal{F}_{12}^\varepsilon(\boldsymbol{R},\boldsymbol{k}_1,\boldsymbol{k}_2,t) = \int_0^t dt_2\int_0^{t_2} dt_1\; e^{\frac{i}{2\varepsilon}(t_1+t_2)+i\frac{\varepsilon}{2}(t_1|\boldsymbol{k}_1|^2+t_2|\boldsymbol{k}_2|^2)}$$

$$\cdot\left(e^{i\frac{t_2}{\varepsilon^2}h_0^\varepsilon}\widehat{V}_2^\varepsilon(\cdot,\boldsymbol{k}_2)e^{-i\frac{t_2}{\varepsilon^2}h_0^\varepsilon}e^{i\frac{t_1}{\varepsilon^2}h_0^\varepsilon}\widehat{V}_1^\varepsilon(\cdot,\boldsymbol{k}_1)e^{-i\frac{t_1}{\varepsilon^2}h_0^\varepsilon}\psi^\varepsilon\right)(\boldsymbol{R}) \tag{2.3.21}$$

The next point is to write the explicit form of the last term in parenthesis in (2.3.21). Using (2.3.20) and the expression of the free propagator, we have

$$\begin{aligned}
&\left(e^{i\frac{t_1}{\varepsilon^2}h_0^\varepsilon}\widehat{V}_1^\varepsilon(\cdot,\boldsymbol{k}_1)e^{-i\frac{t_1}{\varepsilon^2}h_0^\varepsilon}\psi^\varepsilon\right)(\boldsymbol{R})\\
&= \varepsilon^{3/2}e^{-i\boldsymbol{k}_1\cdot\boldsymbol{a}_1}\int d\boldsymbol{\xi}\, g(\boldsymbol{\xi},\varepsilon\boldsymbol{k}_1)\,e^{-\frac{i}{\varepsilon}\boldsymbol{a}_1\cdot\xi}\left(e^{i\frac{t_1}{\varepsilon^2}h_0^\varepsilon}e^{\frac{i}{\varepsilon}\boldsymbol{\xi}\cdot(\cdot)}e^{-i\frac{t_1}{\varepsilon^2}h_0^\varepsilon}\psi^\varepsilon\right)(\boldsymbol{R})\\
&= \varepsilon^{3/2}e^{-i\boldsymbol{k}_1\cdot\boldsymbol{a}_1}\int d\boldsymbol{\xi}\, g(\boldsymbol{\xi},\varepsilon\boldsymbol{k}_1)\,e^{-\frac{i}{\varepsilon}\boldsymbol{a}_1\cdot\xi}\,e^{i\frac{t_1}{2}|\boldsymbol{\xi}|^2+\frac{i}{\varepsilon}\boldsymbol{\xi}\cdot\boldsymbol{R}}\,\psi^\varepsilon(\boldsymbol{R}+\varepsilon t_1\boldsymbol{\xi})
\end{aligned} \tag{2.3.22}$$

and

$$\begin{aligned}
&\left(e^{i\frac{t_2}{\varepsilon^2}h_0^\varepsilon}\widehat{V}_2^\varepsilon(\cdot,\boldsymbol{k}_2)e^{-i\frac{t_2}{\varepsilon^2}h_0^\varepsilon}\,e^{i\frac{t_1}{\varepsilon^2}h_0^\varepsilon}\widehat{V}_1^\varepsilon(\cdot,\boldsymbol{k}_1)e^{-i\frac{t_1}{\varepsilon^2}h_0^\varepsilon}\psi^\varepsilon\right)(\boldsymbol{R})\\
&\quad = \varepsilon^3 e^{-i\boldsymbol{k}_1\cdot\boldsymbol{a}_1-i\boldsymbol{k}_2\cdot\boldsymbol{a}_2}\int d\boldsymbol{\xi}d\boldsymbol{\eta}\, g(\boldsymbol{\eta},\varepsilon\boldsymbol{k}_2)g(\boldsymbol{\xi},\varepsilon\boldsymbol{k}_1)
\end{aligned} \tag{2.3.23}$$

$$\cdot\ e^{-\frac{i}{\varepsilon}(\boldsymbol{a}_1\cdot\xi+\boldsymbol{a}_2\cdot\eta)}\ e^{i\left(\frac{t_2}{2}|\eta|^2+\frac{t_1}{2}|\xi|^2+t_2\eta\cdot\xi+\frac{\boldsymbol{R}}{\varepsilon}\cdot(\eta+\xi)\right)}\psi^{\varepsilon}(\boldsymbol{R}+\varepsilon t_2\eta+\varepsilon t_1\xi)$$

Therefore, (2.3.21) can be written as

$$\begin{aligned}\mathcal{F}^{\varepsilon}_{12}(\boldsymbol{R},\boldsymbol{k}_1,\boldsymbol{k}_2,t)=\varepsilon^3 e^{-i\boldsymbol{k}_1\cdot\boldsymbol{a}_1-i\boldsymbol{k}_2\cdot\boldsymbol{a}_2}\int_0^t dt_2\int_0^{t_2}dt_1\, e^{\frac{i}{2\varepsilon}(t_1+t_2)+i\frac{\varepsilon}{2}\left(t_1|\boldsymbol{k}_1|^2+t_2|\boldsymbol{k}_2|^2\right)}\\ \cdot\int d\xi d\eta\, g(\eta,\varepsilon\boldsymbol{k}_2)g(\xi,\varepsilon\boldsymbol{k}_1)\, e^{-\frac{i}{\varepsilon}(\boldsymbol{a}_1\cdot\xi+\boldsymbol{a}_2\cdot\eta)}\\ e^{i\left(\frac{t_2}{2}|\eta|^2+\frac{t_1}{2}|\xi|^2+t_2\eta\cdot\xi+\frac{\boldsymbol{R}}{\varepsilon}\cdot(\eta+\xi)\right)}\psi^{\varepsilon}(\boldsymbol{R}+\varepsilon t_2\eta+\varepsilon t_1\xi)\end{aligned}\tag{2.3.24}$$

The last step is to introduce the explicit expression of ψ^{ε} (see (2.1.16)) in (2.3.24). We obtain

$$\begin{aligned}\mathcal{F}^{\varepsilon}_{12}(\boldsymbol{R},\boldsymbol{k}_1,\boldsymbol{k}_2,t)=\varepsilon^{1/2}\mathcal{N}_{\varepsilon}e^{-i\boldsymbol{k}_1\cdot\boldsymbol{a}_1-i\boldsymbol{k}_2\cdot\boldsymbol{a}_2}\int_{S^2}d\hat{\boldsymbol{u}}\int_0^t dt_2\int_0^{t_2}dt_1\int d\xi d\eta\, g(\eta,\varepsilon\boldsymbol{k}_2)g(\xi,\varepsilon\boldsymbol{k}_1)\\ \cdot f(\varepsilon^{-1}\boldsymbol{R}+t_2\eta+t_1\xi)\, e^{i\left[\frac{t_2}{2}|\eta|^2+\frac{t_1}{2}|\xi|^2+t_2\eta\cdot\xi+\varepsilon^{-1}\boldsymbol{R}\cdot(\eta+\xi)\right]}\\ \cdot\ e^{\frac{i}{\varepsilon}\left[v_0\hat{\boldsymbol{u}}\cdot(\varepsilon^{-1}\boldsymbol{R}+t_2\eta+t_1\xi)-\boldsymbol{a}_1\cdot\xi-\boldsymbol{a}_2\cdot\eta+\frac{t_1}{2}(1+|\varepsilon\boldsymbol{k}_1|^2)+\frac{t_2}{2}(1+|\varepsilon\boldsymbol{k}_2|^2)\right]}\end{aligned}\tag{2.3.25}$$

Defining the rescaled variables $\boldsymbol{x}=\varepsilon^{-1}\boldsymbol{R}$, $\boldsymbol{y}_1=\varepsilon\boldsymbol{k}_1$, $\boldsymbol{y}_2=\varepsilon\boldsymbol{k}_2$, formula (2.3.25) reduces to

$$\mathcal{F}^{\varepsilon}_{12}(\varepsilon\boldsymbol{x},\varepsilon^{-1}\boldsymbol{y}_1,\varepsilon^{-1}\boldsymbol{y}_2,t)=\varepsilon^{1/2}\mathcal{N}_{\varepsilon}\,\alpha^{\varepsilon}_{12}\,\mathcal{G}^{\varepsilon}_{12}(\boldsymbol{x},\boldsymbol{y}_1,\boldsymbol{y}_2,t)\tag{2.3.26}$$

where $\alpha^{\varepsilon}_{12}$ and $\mathcal{G}_{12}$ are defined in (2.3.2), (2.3.3). A completely analogous computation can be done for $\mathcal{F}^{\varepsilon}_{21}$. Then, the representation formula (2.3.1) follows.

2.4 Proof of Mott's Result

We start from the representation formula (2.3.1). The two terms $\mathcal{G}^{\varepsilon}_{lj}$ appearing in (2.3.1) correspond to the possible "graphs" in the second order perturbative expansion. In particular $\mathcal{G}^{\varepsilon}_{12}$ corresponds to the graph in which the atom in $\boldsymbol{a}_1$ is ionized before the atom in $\boldsymbol{a}_2$ and $\mathcal{G}^{\varepsilon}_{21}$ to the opposite case.

Since we always assume $|\boldsymbol{a}_1|<|\boldsymbol{a}_2|$, we expect that the contribution of $\mathcal{G}^{\varepsilon}_{21}$ is negligible. In fact, we shall see that the phase Θ_{21} has no critical points in the integration region and then, by standard integration by parts, we prove that the contribution of the oscillatory integral $\mathcal{G}^{\varepsilon}_{21}$ is proportional to ε^k, for any $k\in\mathbb{N}$ (step (i)).

The estimate of the term $\mathcal{G}_{12}^{\varepsilon}$ is more delicate and we have to distinguish the non aligned from the aligned case. It turns out that the phase Θ_{12} has no critical points in the first case and then the contribution of $\mathcal{G}_{12}^{\varepsilon}$ is proportional to ε^k, for any $k \in \mathbb{N}$. This leads to the proof of Theorem 2.2.1 (step (ii)).

On the other hand, in the aligned case the phase Θ_{12} has a manifold of critical points parametrized by a vector in $\mathbb{R}^2$. By a careful application of the stationary phase method to $\mathcal{G}_{12}^{\varepsilon}$, we compute the leading term of the asymptotic expansion for $\varepsilon \to 0$, and conclude the proof of Theorem 2.2.2 (step (iii)).

In the following we give the details of the proof of the above statements.

(i) Estimate of $\mathcal{G}_{21}^{\varepsilon}$.
The first point is to show that the gradient of phase Θ_{21} with respect to the variables $\boldsymbol{\eta}, \boldsymbol{\xi}$ doesn't vanish in the integration region. Taking into account that the phase is explicitly given by

$$\Theta_{21} = v_0 \hat{\boldsymbol{u}} \cdot (\boldsymbol{x} + t_2 \boldsymbol{\eta} + t_1 \boldsymbol{\xi}) - \boldsymbol{a}_1 \cdot \boldsymbol{\eta} - \boldsymbol{a}_2 \cdot \boldsymbol{\xi} + \frac{t_2}{2}(1 + |\boldsymbol{y}_1|^2) + \frac{t_1}{2}(1 + |\boldsymbol{y}_2|^2) \tag{2.4.1}$$

one has

$$|\nabla_{\boldsymbol{\eta}\boldsymbol{\xi}} \Theta_{21}|^2 = \sum_{k=1}^{3} \left[\left(\frac{\partial \Theta_{21}}{\partial \eta_k} \right)^2 + \left(\frac{\partial \Theta_{21}}{\partial \xi_k} \right)^2 \right] = \left(v_0 t_2 \hat{\boldsymbol{u}} - \boldsymbol{a}_1 \right)^2 + \left(v_0 t_1 \hat{\boldsymbol{u}} - \boldsymbol{a}_2 \right)^2$$

$$\geq v_0^2 \left[(t_2 - \tau_1)^2 + (t_1 - \tau_2)^2 \right] \tag{2.4.2}$$

In the region $\{(t_2, t_1) \in \mathbb{R}^2 \mid 0 \leq t_2 \leq t,\ 0 \leq t_1 \leq t_2\}$ the r.h.s. of (2.4.2) takes its minimum for $t_2 = t_1 = \frac{\tau_1 + \tau_2}{2}$. Then

$$|\nabla_{\boldsymbol{\eta}\boldsymbol{\xi}} \Theta_{21}|^2 \geq \frac{v_0^2}{2}(\tau_1 - \tau_2)^2 = \frac{v_0^2 \tau_2^2}{2} \left(1 - \frac{\tau_1}{\tau_2} \right)^2 = \frac{|\boldsymbol{a}_2|^2}{2} \left(1 - \frac{|\boldsymbol{a}_1|}{|\boldsymbol{a}_2|} \right)^2 \tag{2.4.3}$$

Thus we have obtained the estimate

$$|\nabla_{\boldsymbol{\eta}\boldsymbol{\xi}} \Theta_{21}| \geq \Delta_{21} \tag{2.4.4}$$

where

$$\Delta_{21} \equiv \frac{|\boldsymbol{a}_2|}{\sqrt{2}} \left(1 - \frac{|\boldsymbol{a}_1|}{|\boldsymbol{a}_2|} \right) \tag{2.4.5}$$

Note that our assumption $|\boldsymbol{a}_1| < |\boldsymbol{a}_2|$ guarantees that Δ_{21} is a positive constant.

The estimate (2.4.4) allows to control $\mathcal{G}_{21}^{\varepsilon}$ for $\varepsilon \to 0$ using standard non stationary phase methods (Fedoryuk 1971; Hörmander 1983; Bleinstein and Handelsman 1975). In fact, recalling the identity

$$a\, e^{ib} = -i\ \mathrm{div}\left(e^{ib}\frac{\nabla b}{|\nabla b|^2}\, a\right) + i\, e^{ib}\ \mathrm{div}\left(\frac{\nabla b}{|\nabla b|^2}\, a\right) \tag{2.4.6}$$

and integrating by parts in the integral with respect to the variables $\boldsymbol{\zeta} = (\zeta_1, \ldots, \zeta_6) \equiv (\eta_1, \eta_2, \eta_3, \xi_1, \xi_2, \xi_3)$ we have

$$\mathcal{G}_{21}^{\varepsilon} = i\varepsilon \int_{S^2} d\hat{\boldsymbol{u}} \int_0^t dt_2 \int_0^{t_2} dt_1 \int d\boldsymbol{\zeta}\, (T_{\boldsymbol{\zeta}} G_{21})\, e^{\frac{i}{\varepsilon}\Theta_{21}} \tag{2.4.7}$$

where the operator $T_{\boldsymbol{\zeta}}$ acts as follows

$$T_{\boldsymbol{\zeta}} G_{21} = \frac{1}{|\nabla_{\boldsymbol{\zeta}} \Theta_{21}|^2} \sum_{j=1}^{6} \frac{\partial \Theta_{21}}{\partial \zeta_j} \frac{\partial G_{21}}{\partial \zeta_j} \tag{2.4.8}$$

We recall that Θ_{21} is linear in $\boldsymbol{\zeta}$. As a consequence, only the derivatives of G_{21} in (2.4.8) are functions of $\boldsymbol{\zeta}$. Therefore, the operator $T_{\boldsymbol{\zeta}}^k$, $k \in \mathbb{N}$, is given by

$$T_{\boldsymbol{\zeta}}^k G_{21} = \frac{1}{|\nabla_{\boldsymbol{\zeta}} \Theta_{21}|^{2k}} \sum_{\underline{m}, |m|=k} \left(\frac{\partial \Theta_{21}}{\partial \zeta_1}\right)^{m_1} \cdots \left(\frac{\partial \Theta_{21}}{\partial \zeta_6}\right)^{m_6} D_{\boldsymbol{\zeta}}^{\underline{m}} G_{21} \tag{2.4.9}$$

Integrating by parts k times in (2.4.7) and using estimate (2.4.4) we have

$$\begin{aligned} \left|\mathcal{G}_{21}^{\varepsilon}\right| &= \left|(i\varepsilon)^k \int_{S^2} d\hat{\boldsymbol{u}} \int_0^t dt_2 \int_0^{t_2} dt_1 \int d\boldsymbol{\zeta}\, (T_{\boldsymbol{\zeta}}^k G_{21})\, e^{\frac{i}{\varepsilon}\Theta_{21}}\right| \\ &\le 4\pi \frac{\varepsilon^k}{\Delta_{21}^k} \int_0^t dt_2 \int_0^{t_2} dt_1 \int d\boldsymbol{\zeta} \sum_{\underline{m}, |m|=k} \left|D_{\boldsymbol{\zeta}}^{\underline{m}} G_{21}\right| \end{aligned} \tag{2.4.10}$$

From (2.4.10) one obtains the following estimate of the L^2-norm squared of $\mathcal{G}_{21}^{\varepsilon}(\boldsymbol{x}, \boldsymbol{y}_1, \boldsymbol{y}_2, t)$

$$\begin{aligned} \int d\boldsymbol{x} d\boldsymbol{y}_1 d\boldsymbol{y}_2 \left|\mathcal{G}_{21}^{\varepsilon}\right|^2 &\le \frac{4\pi^2 t^4 \varepsilon^{2k}}{\Delta_{21}^{2k}} \\ &\times \sup_{t_2, t_1, t_2', t_1'} \int d\boldsymbol{\zeta} d\boldsymbol{\zeta}' \left[\int d\boldsymbol{x} d\boldsymbol{y}_1 d\boldsymbol{y}_2 \left(\sum_{\underline{m}, |m|=k} \left|D_{\boldsymbol{\zeta}}^{\underline{m}} G_{21}\right|\right)^2\right]^{1/2} \\ &\cdot \left[\int d\boldsymbol{x} d\boldsymbol{y}_1 d\boldsymbol{y}_2 \left(\sum_{\underline{m}', |m'|=k} \left|D_{\boldsymbol{\zeta}'}^{\underline{m}'} G_{21}\right|\right)^2\right]^{1/2} \end{aligned} \tag{2.4.11}$$

where we have interchanged the integration order and used the Schwartz inequality.

The next step is the estimate of the derivatives of G_{21}. We have

$$\begin{aligned}
&\sum_{\underline{m},|m|=k} \left| D_{\zeta}^{m} G_{21} \right| \\
&\leq C_k \sum_{\underline{n},|n|\leq k} |D_{\eta}^{n} g(\boldsymbol{\eta}, \boldsymbol{y}_1)| \sum_{\underline{l},|l|\leq k} |D_{\xi}^{l} g(\boldsymbol{\xi}, \boldsymbol{y}_2)| \sum_{\underline{p},|p|\leq k} |D_{\boldsymbol{x}}^{p} f(\boldsymbol{x} + t_2\boldsymbol{\eta} + t_1\boldsymbol{\xi})| \\
&\cdot \sum_{i=1}^{k} (|\boldsymbol{x}| + t|\boldsymbol{\eta}| + t|\boldsymbol{\xi}|)^i
\end{aligned} \tag{2.4.12}$$

Note that

$$\begin{aligned}
\sum_{i=1}^{k} (|\boldsymbol{x}| + t|\boldsymbol{\eta}| + t|\boldsymbol{\xi}|)^i &\leq \sum_{i=1}^{k} (|\boldsymbol{x} + t_2\boldsymbol{\eta} + t_1\boldsymbol{\xi}| + 2t|\boldsymbol{\eta}| + 2t|\boldsymbol{\xi}|)^i \\
&\leq C_k(t) \langle \boldsymbol{x} + t_2\boldsymbol{\eta} + t_1\boldsymbol{\xi} \rangle^k \langle \boldsymbol{\eta} \rangle^k \langle \boldsymbol{\xi} \rangle^k
\end{aligned} \tag{2.4.13}$$

for some positive $C_k(t)$. Then, recalling definition (3.3.9), we obtain the following estimate of the derivatives of G_{21}

$$\begin{aligned}
&\sum_{\underline{m},|m|=k} \left| D_{\zeta}^{m} G_{21} \right| \\
&\leq C_k(t) \langle \boldsymbol{\eta} \rangle^k \sum_{\underline{n},|n|\leq k} |D_{\eta}^{n} \widetilde{V}(\boldsymbol{\eta})| \langle \boldsymbol{\xi} \rangle^k \sum_{\underline{l},|l|\leq k} |D_{\xi}^{l} \widetilde{V}(\boldsymbol{\xi})| \langle \boldsymbol{x} + t_2\boldsymbol{\eta} + t_1\boldsymbol{\xi} \rangle^k \\
&\sum_{\underline{p},|p|\leq k} |D_{\boldsymbol{x}}^{p} f(\boldsymbol{x} + t_2\boldsymbol{\eta} + t_1\boldsymbol{\xi})| \cdot \sum_{\underline{q},|q|\leq k} |D_{\eta}^{q} h(\boldsymbol{\eta}, \boldsymbol{y}_1)| \sum_{\underline{r},|r|\leq k} |D_{\xi}^{r} h(\boldsymbol{\xi}, \boldsymbol{y}_2)|
\end{aligned} \tag{2.4.14}$$

Using (2.4.14), we then have (see (2.4.11))

$$\begin{aligned}
&\left[\int d\boldsymbol{x} d\boldsymbol{y}_1 d\boldsymbol{y}_2 \left(\sum_{\underline{m},|m|=k} \left| D_{\zeta}^{m} G_{21} \right| \right)^2 \right]^{1/2} \leq C_k(t) \langle \boldsymbol{\eta} \rangle^k \sum_{\underline{n},|n|\leq k} |D_{\eta}^{n} \widetilde{V}(\boldsymbol{\eta})| \langle \boldsymbol{\xi} \rangle^k \sum_{\underline{l},|l|\leq k} |D_{\xi}^{l} \widetilde{V}(\boldsymbol{\xi})| \\
&\cdot \sum_{\underline{p},|p|\leq k} \left(\int d\boldsymbol{x} \langle \boldsymbol{x} \rangle^{2k} |D_{\boldsymbol{x}}^{p} f(\boldsymbol{x})|^2 \right)^{1/2} \sum_{\underline{q},|q|\leq k} \left(\int d\boldsymbol{y}_1 |D_{\eta}^{q} h(\boldsymbol{\eta}, \boldsymbol{y}_1)|^2 \right)^{1/2} \sum_{\underline{r},|r|\leq k} \left(\int d\boldsymbol{y}_2 |D_{\xi}^{r} h(\boldsymbol{\xi}, \boldsymbol{y}_2)|^2 \right)^{1/2}
\end{aligned} \tag{2.4.15}$$

In order to estimate the last two terms in (2.4.15), we first note that

$$D_{\eta}^{q} h(\boldsymbol{\eta}, \boldsymbol{y}) = \frac{(-i)^{|q|}}{(2\pi)^{3/2}} \int d\boldsymbol{x}\, e^{-i\boldsymbol{\eta}\cdot\boldsymbol{x}}\, x_1^{q_1} x_2^{q_2} x_3^{q_3}\, \zeta_0(\boldsymbol{x})\, \overline{\phi^0}(\boldsymbol{x}, \boldsymbol{y}) \tag{2.4.16}$$

where $q_1 + q_2 + q_3 = |q|$ (see definition (2.3.8)). As a consequence of the eigenfunction expansion theorem for a point interaction Hamiltonian, we know that the integral kernel $\overline{\phi^0}(\boldsymbol{x}, \boldsymbol{y})$ defines a bounded operator in $L^2(\mathbb{R}^3)$, with norm less or equal to one. Hence

$$\sup_{\boldsymbol{\eta}} \int d\boldsymbol{y}\, |D^q_{\boldsymbol{\eta}} h(\boldsymbol{\eta}, \boldsymbol{y})|^2 \leq \frac{1}{(2\pi)^3} \int d\boldsymbol{x}\ \left| x_1^{q_1} x_2^{q_2} x_3^{q_3}\ \zeta_0(\boldsymbol{x}) \right|^2 < C \tag{2.4.17}$$

for some constant $C > 0$. Using (2.4.17) and the fact that the function f is a gaussian, the estimate (2.4.15) reduces to

$$\left[\int d\boldsymbol{x} d\boldsymbol{y}_1 d\boldsymbol{y}_2 \Big(\sum_{\underline{m}, |m|=k} \left| D^m_{\boldsymbol{\zeta}} G_{21} \right| \Big)^2 \right]^{1/2} \leq C_k(t)\, \langle \boldsymbol{\eta} \rangle^k \sum_{\underline{n}, |n| \leq k} |D^n_{\boldsymbol{\eta}} \widetilde{V}(\boldsymbol{\eta})|\, \langle \boldsymbol{\xi} \rangle^k \sum_{\underline{l}, |l| \leq k} |D^l_{\boldsymbol{\xi}} \widetilde{V}(\boldsymbol{\xi})| \tag{2.4.18}$$

Taking into account of (2.4.18) and (2.4.11), we have

$$\begin{aligned} \int d\boldsymbol{x} d\boldsymbol{y}_1 d\boldsymbol{y}_2\, |\mathcal{G}^\varepsilon_{21}|^2 &\leq C_k(t) \frac{\varepsilon^{2k}}{\Delta_{21}^{2k}} \int d\boldsymbol{\eta} d\boldsymbol{\xi} d\boldsymbol{\eta}' d\boldsymbol{\xi}'\, \langle \boldsymbol{\eta} \rangle^k \sum_{\underline{n}, |n| \leq k} |D^n_{\boldsymbol{\eta}} \widetilde{V}(\boldsymbol{\eta})|\, \langle \boldsymbol{\xi} \rangle^k \sum_{\underline{l}, |l| \leq k} |D^l_{\boldsymbol{\xi}} \widetilde{V}(\boldsymbol{\xi})| \\ &\cdot \langle \boldsymbol{\eta}' \rangle^k \sum_{\underline{n}', |n'| \leq k} |D^{n'}_{\boldsymbol{\eta}'} \widetilde{V}(\boldsymbol{\eta}')|\, \langle \boldsymbol{\xi}' \rangle^k \sum_{\underline{l}', |l'| \leq k} |D^{l'}_{\boldsymbol{\xi}'} \widetilde{V}(\boldsymbol{\xi}')| \\ &= C_k(t)\, \|\widetilde{V}\|^4_{W^{k,1}_k} |\boldsymbol{a}_2|^{-2k} \left(1 - \frac{|\boldsymbol{a}_1|}{|\boldsymbol{a}_2|} \right)^{-2k} \varepsilon^{2k} \end{aligned} \tag{2.4.19}$$

where we have used the two definitions (2.1.29) and (2.4.5). The above estimate concludes the proof of step (i).

(ii) Estimate of $\mathcal{G}^\varepsilon_{12}$ in the non aligned case.
Here we consider the case $\hat{\boldsymbol{a}}_1 \cdot \hat{\boldsymbol{a}}_2 < 1$. Without loss of generality, we fix

$$\hat{\boldsymbol{a}}_1 = (0, 0, 1)\,, \qquad \hat{\boldsymbol{a}}_2 = (\sin\chi, 0, \cos\chi)\,, \qquad \chi \in (0, \pi] \tag{2.4.20}$$

and we define the following two subsets of S^2

$$\mathcal{C}_1 = \left\{ \hat{\boldsymbol{u}} \in S^2 \,|\, \hat{u}_1^2 + \hat{u}_2^2 < \sin^2 \frac{\chi}{2} \right\}, \qquad \mathcal{C}_2 = S^2 \setminus \mathcal{C}_1 \tag{2.4.21}$$

Note that $\hat{\boldsymbol{a}}_j \in \mathcal{C}_j$, $j = 1, 2$, but $\hat{\boldsymbol{a}}_j \notin \mathcal{C}_k$, for $j \neq k$. Let us write $\mathcal{G}^\varepsilon_{12}$ (see (2.3.3)) as the sum of the two contributions from $\mathcal{C}_1$ and $\mathcal{C}_2$, i.e.

$$\mathcal{G}_{12}^{\varepsilon} = \mathcal{G}_{12}^{\varepsilon,1} + \mathcal{G}_{12}^{\varepsilon,2} \tag{2.4.22}$$

$$\mathcal{G}_{12}^{\varepsilon,j} = \int_{\mathcal{C}_j} d\hat{\boldsymbol{u}} \int_0^t dt_2 \int_0^{t_2} dt_1 \int d\boldsymbol{\eta} d\boldsymbol{\xi}\, G_{12}\, e^{\frac{i}{\varepsilon}\Theta_{12}} \tag{2.4.23}$$

where the phase Θ_{12} is explicitly given by

$$\Theta_{12} = v_0 \hat{\boldsymbol{u}} \cdot (\boldsymbol{x} + t_2\boldsymbol{\eta} + t_1\boldsymbol{\xi}) - \boldsymbol{a}_2 \cdot \boldsymbol{\eta} - \boldsymbol{a}_1 \cdot \boldsymbol{\xi} + \frac{t_2}{2}(1 + |\boldsymbol{y}_2|^2) + \frac{t_1}{2}(1 + |\boldsymbol{y}_1|^2) \tag{2.4.24}$$

We represent a unit vector $\hat{\boldsymbol{u}} \in S^2$ as $\hat{\boldsymbol{u}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, $\theta \in [0, \pi]$, $\phi \in [0, 2\pi)$. Therefore for $\hat{\boldsymbol{u}} \in \mathcal{C}_1$ one has

$$\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{a}}_2 = \sin\theta\cos\phi\sin\chi + \cos\theta\cos\chi \le \cos(\chi - \theta) \le \cos\frac{\chi}{2} \tag{2.4.25}$$

and the gradient of Θ_{12} with respect to the variable $\boldsymbol{\eta}$ satisfies

$$\begin{aligned} &\left|\nabla_{\boldsymbol{\eta}}\Theta_{12}\right|^2 = v_0^2\left(t_2^2 + \tau_2^2 - 2\,t_2\tau_2\,\hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{a}}_2\right) \ge v_0^2\left(t_2^2 + \tau_2^2 - 2\,t_2\tau_2\,\cos\frac{\chi}{2}\right) \\ &\ge v_0^2 \min_{x\ge 0}\left(x^2 + \tau_2^2 - 2\,x\,\tau_2\cos\frac{\chi}{2}\right) = v_0^2\tau_2^2\sin^2\frac{\chi}{2} \ge v_0^2\tau_1^2\sin^2\frac{\chi}{2} \\ &= \frac{|\boldsymbol{a}_1|^2}{2}(1 - \cos\chi) = \frac{|\boldsymbol{a}_1|^2}{2}\left(1 - \hat{\boldsymbol{a}}_1\cdot\hat{\boldsymbol{a}}_2\right) \equiv \Delta_{12}^2 \end{aligned} \tag{2.4.26}$$

where Δ_{12} is a strictly positive constant. Analogously, for $\hat{\boldsymbol{u}} \in \mathcal{C}_2$ one has

$$\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{a}}_1 = \cos\theta \le \cos\frac{\chi}{2} \tag{2.4.27}$$

and the gradient of Θ_{12} with respect to the variable $\boldsymbol{\xi}$ satisfies

$$\left|\nabla_{\boldsymbol{\xi}}\Theta_{12}\right|^2 = v_0^2\left(t_1^2 + \tau_1^2 - 2\,t_1\tau_1\,\hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{a}}_1\right) \ge \Delta_{12}^2 \tag{2.4.28}$$

Using estimates (2.4.26), (2.4.28) and applying non stationary phase methods along the same line of the previous case one can show that the contributions of $\mathcal{G}_{12}^{\varepsilon,1}$ and of $\mathcal{G}_{12}^{\varepsilon,2}$ can be made arbitrarily small for $\varepsilon \to 0$. More precisely, one can prove the estimate

$$\int d\boldsymbol{x} d\boldsymbol{y}_1 d\boldsymbol{y}_2 \left|\mathcal{G}_{12}^{\varepsilon}\right|^2 \le C_k(t)\,\|\widetilde{V}\|_{W_k^{k,1}}^4 |\boldsymbol{a}_1|^{-2k}\left(1 - \hat{\boldsymbol{a}}_1\cdot\hat{\boldsymbol{a}}_2\right)^{-k}\varepsilon^{2k} \tag{2.4.29}$$

Taking into account formulas (2.3.1), (2.4.19), (2.4.29) we conclude the proof of Theorem 2.2.1.

(iii) Analysis of $\mathcal{G}_{12}^{\varepsilon}$ in the aligned case.
Here we analyze $\mathcal{G}_{12}^{\varepsilon}$ in the case $\hat{\boldsymbol{a}}_1 \cdot \hat{\boldsymbol{a}}_2 = \cos\chi_\varepsilon$, with $\chi_\varepsilon \in [0, \chi_0\varepsilon]$, $\chi_0 > 0$. It turns out that, in this case, the phase of the oscillatory integral $\mathcal{G}_{12}^{\varepsilon}$ has stationary points. This implies that the ionization probability $\mathcal{P}_2^{\varepsilon}(t)$ cannot be made arbitrarily small for $\varepsilon \to 0$ and the leading term of its asymptotic expansion in powers of ε can be computed.

We fix the unit vectors $\hat{\boldsymbol{a}}_1, \hat{\boldsymbol{a}}_2$ as follows

$$\hat{\boldsymbol{a}}_1 = (0, 0, 1), \qquad \hat{\boldsymbol{a}}_2 = (\sin\chi_\varepsilon, 0, \cos\chi_\varepsilon) \tag{2.4.30}$$

We also fix the angle θ_0, $0 < \theta_0 < \frac{\pi}{2}$, and define the subset of S^2

$$\mathcal{C}_0 = \left\{ \hat{\boldsymbol{u}} \in S^2 \,|\, \hat{u}_1^2 + \hat{u}_2^2 < \sin^2\theta_0 \right\} \tag{2.4.31}$$

Note that for ε sufficiently small one has $\hat{\boldsymbol{a}}_1, \hat{\boldsymbol{a}}_2 \in \mathcal{C}_0$. In order to characterize the asymptotic behavior of $\mathcal{G}_{12}^{\varepsilon}$ for $\varepsilon \to 0$, we decompose $\mathcal{G}_{12}^{\varepsilon}$ in a "non-stationary part" $\mathcal{G}_{12}^{\varepsilon,n}$ (corresponding to $\hat{\boldsymbol{u}} \in S^2 \setminus \mathcal{C}_0$) and a "stationary part" $\mathcal{G}_{12}^{\varepsilon,s}$ (corresponding to $\hat{\boldsymbol{u}} \in \mathcal{C}_0$)

$$\mathcal{G}_{12}^{\varepsilon} = \mathcal{G}_{12}^{\varepsilon,n} + \mathcal{G}_{12}^{\varepsilon,s} \tag{2.4.32}$$

$$\mathcal{G}_{12}^{\varepsilon,n} = \int_{S^2\setminus\mathcal{C}_0} d\hat{\boldsymbol{u}} \int_0^t dt_2 \int_0^{t_2} dt_1 \int d\boldsymbol{\eta} d\boldsymbol{\xi}\, G_{12}^{\varepsilon}\, e^{\frac{i}{\varepsilon}\Theta} \tag{2.4.33}$$

$$\mathcal{G}_{12}^{\varepsilon,s} = \int_{\mathcal{C}_0} d\hat{\boldsymbol{u}} \int_0^t dt_2 \int_0^{t_2} dt_1 \int d\boldsymbol{\eta} d\boldsymbol{\xi}\, G_{12}^{\varepsilon}\, e^{\frac{i}{\varepsilon}\Theta} \tag{2.4.34}$$

where

$$G_{12}^{\varepsilon} = G_{12}\, e^{i\delta_\varepsilon}, \qquad \delta_\varepsilon = -\frac{\sin\chi_\varepsilon}{\varepsilon}\,|\boldsymbol{a}_2|\eta_1 + \frac{1-\cos\chi_\varepsilon}{\varepsilon}\,|\boldsymbol{a}_2|\eta_3 \tag{2.4.35}$$

$$\Theta = v_0\hat{\boldsymbol{u}}\cdot(\boldsymbol{x} + t_2\boldsymbol{\eta} + t_1\boldsymbol{\xi}) - \hat{\boldsymbol{a}}_1\cdot(|\boldsymbol{a}_2|\boldsymbol{\eta} + |\boldsymbol{a}_1|\boldsymbol{\xi}) + \frac{t_2}{2}(1+|\boldsymbol{y}_2|^2) + \frac{t_1}{2}(1+|\boldsymbol{y}_1|^2) \tag{2.4.36}$$

We shall analyze the asymptotic behavior of the two oscillatory integrals $\mathcal{G}_{12}^{\varepsilon,n}$ and $\mathcal{G}_{12}^{\varepsilon,s}$ separately.

We first show that the phase Θ has no stationary points in $S^2 \setminus \mathcal{C}_0$ and then the contribution of $\mathcal{G}_{12}^{\varepsilon,n}$ is negligible for $\varepsilon \to 0$. For $\hat{\boldsymbol{u}} \in S^2 \setminus \mathcal{C}_0$ we have $-1 \le \hat{u}_3 < \cos\theta_0$ and

$$\begin{aligned} |\nabla_{\boldsymbol{\eta}\boldsymbol{\xi}}\Theta|^2 &= \left(v_0 t_2\hat{\boldsymbol{u}} - |\boldsymbol{a}_2|\hat{\boldsymbol{a}}_1\right)^2 + \left(v_0 t_1\hat{\boldsymbol{u}} - |\boldsymbol{a}_1|\hat{\boldsymbol{a}}_1\right)^2 \\ &= v_0^2\Big[t_1^2 + t_2^2 + \tau_1^2 + \tau_2^2 - 2\hat{u}_3\,(\tau_1 t_1 + \tau_2 t_2)\Big] \end{aligned}$$

$$
\begin{aligned}
&> v_0^2\Big[t_1^2 + t_2^2 + \tau_1^2 + \tau_2^2 - 2\cos\theta_0\,(\tau_1 t_1 + \tau_2 t_2)\Big] \\
&\geq v_0^2 \min_{x,y\geq 0}\Big[x^2 + y^2 + \tau_1^2 + \tau_2^2 - 2\cos\theta_0\,(\tau_1 x + \tau_2 y)\Big] \\
&= v_0^2\,(\tau_1^2 + \tau_2^2)\sin^2\theta_0 \equiv (|\boldsymbol{a}_1|^2 + |\boldsymbol{a}_2|^2)\sin^2\theta_0 \qquad (2.4.37)
\end{aligned}
$$

The r.h.s. of (2.4.37) is a strictly positive constant. Then, proceeding as in the previous cases, it is now possible to show that the contribution of $\mathcal{G}_{12}^{\varepsilon,n}$ is negligible for $\varepsilon \to 0$. This means that the ionization probability in the aligned case can be written as

$$
\mathcal{P}_2^{\varepsilon}(t) = \frac{\mathcal{N}_{\varepsilon}^2}{\varepsilon^2}\int d\boldsymbol{x}\,d\boldsymbol{y}_1\,d\boldsymbol{y}_2\,\left|\mathcal{G}_{12}^{\varepsilon,s}(\boldsymbol{x},\boldsymbol{y}_1,\boldsymbol{y}_2,t)\right|^2 + \mathcal{R}_k(\varepsilon) \qquad (2.4.38)
$$

where $\mathcal{R}_k(\varepsilon) = O(\varepsilon^{2k-2})$ for any $k \in \mathbb{N}$.

Let us analyze $\mathcal{G}_{12}^{\varepsilon,s}$. It turns out that, for $\hat{\boldsymbol{u}} \in \mathcal{C}_0$, the phase Θ has a manifold of critical points in the integration region, parametrized by a vector in $\mathbb{R}^2$. Indeed, let us fix the variables $(\eta_1,\eta_2) \in \mathbb{R}^2$ as parameters and let us write $\mathcal{G}_{12}^{\varepsilon,s}$ as follows

$$
\mathcal{G}_{12}^{\varepsilon,s} = \int d\eta_1 d\eta_2\,\mathcal{I}^{\varepsilon}(\eta_1,\eta_2) \qquad (2.4.39)
$$

$$
\mathcal{I}^{\varepsilon}(\eta_1,\eta_2) = \int_{\Omega} d\boldsymbol{q}\,\frac{G_{12}^{\varepsilon}(\boldsymbol{q};\eta_1,\eta_2)}{\sqrt{1-\mu^2-\nu^2}}\,e^{\frac{i}{\varepsilon}\Theta(\boldsymbol{q};\eta_1,\eta_2)} \qquad (2.4.40)
$$

where $\boldsymbol{q} \equiv (\mu,\nu,t_2,t_1,\eta_3,\boldsymbol{\xi})$ and

$$
\Omega = \Big\{\boldsymbol{q} \equiv (\mu,\nu,t_2,t_1,\eta_3,\boldsymbol{\xi}) \mid \mu^2+\nu^2 < \sin^2\theta_0,\ t_2 \in [0,t],\ t_1 \in [0,t_2],\ \eta_3 \in \mathbb{R},\ \boldsymbol{\xi} \in \mathbb{R}^3\Big\} \qquad (2.4.41)
$$

Note that in (2.4.41) we have represented the unit vector $\hat{\boldsymbol{u}} \in \mathcal{C}_0$ in the form

$$
\hat{\boldsymbol{u}} = (\mu,\ \nu,\ \sqrt{1-\mu^2-\nu^2}), \qquad (\mu,\nu) \in \mathbb{R}^2, \qquad \mu^2+\nu^2 < \sin^2\theta_0 \qquad (2.4.42)
$$

By a direct computation, one can verify that for each value of the parameters $(\eta_1,\eta_2) \in \mathbb{R}^2$ the phase $\Theta(\boldsymbol{q};\eta_1,\eta_2)$, $\boldsymbol{q} \in \Omega$, has exactly one critical point given by

$$
\boldsymbol{q}_0 \equiv (0,0,\ \tau_2,\ \tau_1,\ \eta_3^0,\ \xi_1^0,\ \xi_2^0,\ \xi_3^0) \qquad (2.4.43)
$$

where

$$
\begin{aligned}
&\eta_3^0 = -\frac{1+|\boldsymbol{y}_2|^2}{2v_0}, \quad \xi_1^0 = -\frac{x_1+\tau_2\eta_1}{\tau_1}, \quad \xi_2^0 = -\frac{x_2+\tau_2\eta_2}{\tau_1}, \qquad (2.4.44)\\
&\xi_3^0 = -\frac{1+|\boldsymbol{y}_1|^2}{2v_0}
\end{aligned}
$$

Moreover one has

$$\Theta^0 \equiv \Theta(\boldsymbol{q}_0; \eta_1, \eta_2) = x_3 + \frac{\tau_1}{v_0}(1 + |\boldsymbol{y}_1|^2) + \frac{\tau_2}{v_0}(1 + |\boldsymbol{y}_2|^2) \tag{2.4.45}$$

and

$$|D^2\Theta^0| \equiv |D^2_{\boldsymbol{q}}\Theta(\boldsymbol{q}_0; \eta_1, \eta_2)| = t^4\tau_1^4 \tag{2.4.46}$$

It is relevant that both the phase and the Hessian of the phase at the critical point are strictly positive and do not depend on the parameters (η_1, η_2). This fact is crucial to apply the stationary phase theorem (Fedoryuk 1971; Hörmander 1983; Bleinstein and Handelsman 1975) to the oscillatory integral $\mathcal{I}^\varepsilon(\eta_1, \eta_2)$ and to derive its asymptotic expansion for $\varepsilon \to 0$.

However, we prefer a more elementary approach which, in our opinion, makes both the proof and the result more transparent.

Using the specific form of the phase Θ and an appropriate change of the integration variables, we rewrite $\mathcal{I}^\varepsilon(\eta_1, \eta_2)$ in a more convenient form for the derivation of the asymptotic expansion for $\varepsilon \to 0$. More precisely, let us denote

$$\boldsymbol{p} = (\mu, \nu, t_2, t_1), \qquad \boldsymbol{k} = (\eta_3, \xi_1, \xi_2, \xi_3) \tag{2.4.47}$$

and let us represent the phase Θ as

$$\Theta = B(\boldsymbol{p}; \eta_1, \eta_2) + \boldsymbol{A}(\boldsymbol{p}) \cdot \boldsymbol{k} \tag{2.4.48}$$

where

$$B(\boldsymbol{p}; \eta_1, \eta_2) = v_0\mu(x_1 + t_2\eta_1) + v_0\nu(x_2 + t_2\eta_2) + v_0\sqrt{1-\mu^2-\nu^2}\, x_3 + \frac{t_2}{2}(1+|\boldsymbol{y}_2|^2) + \frac{t_1}{2}(1+|\boldsymbol{y}_1|^2) \tag{2.4.49}$$

$$\boldsymbol{A}(\boldsymbol{p}) = v_0 \left(t_2\sqrt{1-\mu^2-\nu^2} - \tau_2,\ \mu t_1,\ \nu t_1, t_1\sqrt{1-\mu^2-\nu^2} - \tau_1 \right) \tag{2.4.50}$$

Note that the critical point of the phase is (see (2.4.43), (2.4.44))

$$\boldsymbol{q}^0 = (\boldsymbol{p}^0, \boldsymbol{k}^0(\eta_1, \eta_2)), \qquad \boldsymbol{p}^0 = (0, 0, \tau_2, \tau_1), \qquad \boldsymbol{k}^0(\eta_1, \eta_2) = (\eta_3^0, \xi_1^0, \xi_2^0, \xi_3^0) \tag{2.4.51}$$

With the above notation the oscillatory integral $\mathcal{I}^\varepsilon(\eta_1, \eta_2)$ can be written as

$$\mathcal{I}^\varepsilon(\eta_1, \eta_2) = \int_D d\boldsymbol{p}\, \frac{e^{\frac{i}{\varepsilon}B(\boldsymbol{p};\eta_1,\eta_2)}}{\sqrt{1-\mu^2-\nu^2}} \int d\boldsymbol{k}\, G^\varepsilon_{12}(\boldsymbol{p}, \boldsymbol{k}; \eta_1, \eta_2)\, e^{\frac{i}{\varepsilon}\boldsymbol{A}(\boldsymbol{p})\cdot\boldsymbol{k}} \tag{2.4.52}$$

where D is the domain of integration corresponding to the variables $\boldsymbol{p}$ and

$$G^\varepsilon_{12}(\boldsymbol{p}, \boldsymbol{k}; \eta_1, \eta_2) \equiv G^\varepsilon_{12}(t_2, t_1, \boldsymbol{\eta}, \boldsymbol{\xi}) \tag{2.4.53}$$

The next crucial point is the change of coordinates

$$\boldsymbol{p} = L_\varepsilon \boldsymbol{z} \tag{2.4.54}$$

defined by

$$\mu = \frac{\varepsilon}{v_0\tau_1} z_1, \quad \nu = \frac{\varepsilon}{v_0\tau_1} z_2, \quad t_2 = \tau_2 + \frac{\varepsilon}{v_0} z_3, \quad t_1 = \tau_1 + \frac{\varepsilon}{v_0} z_4 \tag{2.4.55}$$

Hence

$$\mathcal{I}^\varepsilon(\eta_1,\eta_2) = \frac{\varepsilon^4}{v_0^4\tau_1^2} \int_{D_\varepsilon} d\boldsymbol{z} \, \frac{e^{\frac{i}{\varepsilon} B(L_\varepsilon \boldsymbol{z};\eta_1,\eta_2)}}{\sqrt{1 - \frac{\varepsilon^2}{v_0^2\tau_1^2}(z_1^2+z_2^2)}} \int d\boldsymbol{k} \, G_{12}^\varepsilon(L_\varepsilon \boldsymbol{z}, \boldsymbol{k}; \eta_1, \eta_2) \, e^{\frac{i}{\varepsilon} \boldsymbol{A}(L_\varepsilon \boldsymbol{z})\cdot \boldsymbol{k}} \tag{2.4.56}$$

where D_ε is the domain of integration corresponding to the variables $\boldsymbol{z}$

$$D_\varepsilon = \left\{ \boldsymbol{z} \in \mathbb{R}^4 \,|\, z_1^2 + z_2^2 < \frac{v_0^2\tau_1^2}{\varepsilon^2} \sin^2\theta_0, \; -\frac{v_0\tau_2}{\varepsilon} < z_3 < \frac{v_0}{\varepsilon}(t-\tau_2), \; -\frac{v_0\tau_1}{\varepsilon} < z_4 < \frac{v_0}{\varepsilon}(\tau_2 - \tau_1) + z_3 \right\} \tag{2.4.57}$$

We note that for $\varepsilon \to 0$ one has $L_\varepsilon \boldsymbol{z} \to \boldsymbol{p}^0$ (see (2.4.51)) and $D_\varepsilon \to \mathbb{R}^4$. Moreover a Taylor expansion of $\boldsymbol{A}(L_\varepsilon \boldsymbol{z})$ and $B(L_\varepsilon \boldsymbol{z}; \eta_1, \eta_2)$ around $\varepsilon = 0$ gives

$$\boldsymbol{A}(L_\varepsilon \boldsymbol{z}) = \varepsilon \boldsymbol{z} + \boldsymbol{A}_\varepsilon^{(2)}(\boldsymbol{z}) \tag{2.4.58}$$

$$B(L_\varepsilon \boldsymbol{z}; \eta_1, \eta_2) = \Theta^0 - \varepsilon \boldsymbol{k}^0(\eta_1,\eta_2)\cdot \boldsymbol{z} + B_\varepsilon^{(2)}(\boldsymbol{z}; \eta_1, \eta_2), \tag{2.4.59}$$

where $\boldsymbol{k}^0(\eta_1,\eta_2)$ is defined in (2.4.51) and $\boldsymbol{A}_\varepsilon^{(2)}(\boldsymbol{z})$, $B_\varepsilon^{(2)}(\boldsymbol{z}; \eta_1, \eta_2)$ are explicitly known functions of order ε^2 for $\varepsilon \to 0$. Taking into account (2.4.58), (2.4.59), we have

$$\mathcal{I}^\varepsilon(\eta_1,\eta_2) = \frac{\varepsilon^4}{v_0^4\tau_1^2} e^{\frac{i}{\varepsilon}\Theta^0} \int_{D_\varepsilon} d\boldsymbol{z} \, \frac{e^{-i\boldsymbol{k}^0(\eta_1,\eta_2)\cdot \boldsymbol{z}} \, e^{\frac{i}{\varepsilon} B_\varepsilon^{(2)}(\boldsymbol{z};\eta_1,\eta_2)}}{\sqrt{1 - \frac{\varepsilon^2}{v_0^2\tau_1^2}(z_1^2+z_2^2)}} \int d\boldsymbol{k} \, G_{12}^\varepsilon(L_\varepsilon \boldsymbol{z}, \boldsymbol{k}; \eta_1, \eta_2) \, e^{i\boldsymbol{z}\cdot\boldsymbol{k}} \, e^{\frac{i}{\varepsilon} A_\varepsilon^{(2)}(\boldsymbol{z})\cdot \boldsymbol{k}} \tag{2.4.60}$$

A Taylor expansion of the integrand in the r.h.s. (2.4.60), together with an estimate of the error done replacing the domain D_ε with $\mathbb{R}^4$, allows to obtain an expansion of $\mathcal{I}^\varepsilon(\eta_1,\eta_2)$ for $\varepsilon \to 0$, with an explicitly computable remainder. This means that the asymptotic expansion at any order in ε can be derived in a rather straightforward way (for an analogous computation see e.g. Finco and Teta 2011).

Here we are interested in the leading term for $\varepsilon \to 0$ of $\mathcal{I}^\varepsilon(\eta_1,\eta_2)$. From (2.4.60) one immediately obtains

$$\mathcal{I}^{\varepsilon}(\eta_1,\eta_2) \sim \frac{\varepsilon^4}{v_0^4\tau_1^2}\, e^{\frac{i}{\varepsilon}\Theta^0} \int d\boldsymbol{z}\, e^{-i\boldsymbol{k}^0(\eta_1,\eta_2)\cdot\boldsymbol{z}} \int d\boldsymbol{k}\, G_{12}^0(L_0\boldsymbol{z},\boldsymbol{k};\eta_1,\eta_2)\, e^{i\boldsymbol{z}\cdot\boldsymbol{k}}$$
$$= \frac{(2\pi)^4\varepsilon^4}{v_0^4\tau_1^2}\, e^{\frac{i}{\varepsilon}\Theta^0} G_{12}^0(\boldsymbol{p}^0,\boldsymbol{k}^0(\eta_1,\eta_2);\eta_1,\eta_2) \tag{2.4.61}$$

where $G_{12}^0 = G_{12}^{\varepsilon}|_{\varepsilon=0}$. From (2.4.61) and (2.4.39) we also have the leading term for $\varepsilon \to 0$ of $\mathcal{G}_{12}^{\varepsilon,s}$

$$\mathcal{G}_{12}^{\varepsilon,s} \sim \frac{(2\pi)^4\varepsilon^4}{v_0^4\tau_1^2}\, e^{\frac{i}{\varepsilon}\Theta^0} \int d\eta_1 d\eta_2\, G_{12}^0(\boldsymbol{p}^0,\boldsymbol{k}^0(\eta_1,\eta_2);\eta_1,\eta_2) \tag{2.4.62}$$

We recall that $\mathcal{G}_{12}^{\varepsilon,s}$ is a function of $\boldsymbol{x}$, $\boldsymbol{y}_1$, $\boldsymbol{y}_2$ and t. On the other hand, it is clear from (2.4.62) that the leading term of $\mathcal{G}_{12}^{\varepsilon,s}$ for $\varepsilon \to 0$ does not depend on t. Using (2.4.62), (2.4.38) and restoring the dependence on $\boldsymbol{x}$, $\boldsymbol{y}_1$, $\boldsymbol{y}_2$, we finally obtain the leading term for $\varepsilon \to 0$ of the ionization probability

$$\mathcal{P}_2^{\varepsilon}(t) \sim \frac{\varepsilon^6}{v_0^2|\boldsymbol{a}_1|^4} \int d\boldsymbol{x} d\boldsymbol{y}_1 d\boldsymbol{y}_2 \left| 4\pi^3 \int d\eta_1 d\eta_2\, G_{12}^0(\boldsymbol{p}^0,\boldsymbol{k}^0(\eta_1,\eta_2);\eta_1,\eta_2,\boldsymbol{x},\boldsymbol{y}_1,\boldsymbol{y}_2)\right|^2$$
$$= \frac{\varepsilon^6}{v_0^2|\boldsymbol{a}_1|^4} \int d\boldsymbol{x} d\boldsymbol{y}_1 d\boldsymbol{y}_2 \left| \int d\eta_1 d\eta_2\, F(\eta_1,\eta_2,\boldsymbol{x},\boldsymbol{y}_1,\boldsymbol{y}_2)\right|^2 \tag{2.4.63}$$

where we have defined

$$F(\eta_1,\eta_2,\boldsymbol{x},\boldsymbol{y}_1,\boldsymbol{y}_2) = 4\pi^3 G_{12}^0(\boldsymbol{p}^0,\boldsymbol{k}^0(\eta_1,\eta_2);\eta_1,\eta_2,\boldsymbol{x},\boldsymbol{y}_1,\boldsymbol{y}_2) \tag{2.4.64}$$

This concludes the proof of Theorem 2.2.2.

2.5 Asymptotic Dynamics in Presence of One Model-Atom

Let us consider a simpler model of a non relativistic quantum system made of only two spinless particles in dimension three of masses M and m. The latter is bound by an harmonic potential of frequency ω around the equilibrium position $\boldsymbol{a}$. The first particle plays the role of the α-particle while the harmonically bounded particle plays the role of an electron in a very simplified version of model-atom with fixed nucleus. The interaction between the test particle and the harmonic oscillator is described, as in the previous sections, by a smooth two-body potential V.

Denoting by $\boldsymbol{R}$ the position coordinate of the α-particle and by $\boldsymbol{r}$ the position coordinate of the harmonic oscillator, the Hamiltonian of the system in $L^2(\mathbb{R}^6)$ is given by

$$H = H_0 + \lambda V \tag{2.5.1}$$

where

$$H_0 = h_0 + h_\omega, \qquad h_0 = -\frac{\hbar^2}{2M}\Delta_{\boldsymbol{R}}, \qquad h_\omega = -\frac{\hbar^2}{2m}\Delta_{\boldsymbol{r}} + \frac{1}{2}m\omega^2(\boldsymbol{r}-\boldsymbol{a})^2 \quad (2.5.2)$$

$\lambda > 0$ is a coupling constant and V is the multiplication operator by

$$V(\boldsymbol{R}, \boldsymbol{r}) = V(\delta^{-1}(\boldsymbol{R} - \boldsymbol{r})), \qquad \delta > 0 \quad (2.5.3)$$

We want to analyze the evolution of this system when the initial state is the same as the one considered in the previous case, i.e., a product state of a spherical wave for the α-particle and the ground state for the oscillator. Under the same kind of assumptions made in Sect. 2.1, we shall describe the asymptotic form of the wave function of the system for $t > \tau$, where τ is the collision time

$$\tau = \frac{|\boldsymbol{a}|}{v_0} \quad (2.5.4)$$

and v_0 is the velocity of the α-particle. It turns out that such asymptotic form is the sum of two terms, describing two rather different behaviors of the system. The first term corresponds to the situation in which the oscillator remains in the ground state and the α-particle is described by a (slightly deformed) spherical wave, freely evolving in space. The second (smaller) term corresponds to the situation in which the oscillator is in an excited state and the α-particle is described by the free evolution of a wave packet, well concentrated in position and momentum, emerging from the excited oscillator with an average momentum direction along the line joining the origin with the center of the oscillator $\boldsymbol{a}$.

This result is a rigorous version of the heuristic idea expressed by Mott in his paper, explaining the outcome of Mott's analysis in the three-particle model. Indeed, according to the results outlined above, when a collision with the first atom produces excitation the α-particle is localized around the atom and acquires a momentum with direction aligned with $\overline{O\boldsymbol{a}_1}$. As a consequence, the second atom will be excited only if it lies on the same line.

This section is devoted to give a quantitative description of the evolution of the two-particle system wave function. In the next section we shall give a brief outline of the proof. For a detailed analysis, in the general case of N harmonic oscillators, we refer to (Recchia and Teta, 2013).

Let us consider the initial state

$$\Psi_0(\boldsymbol{R}, \boldsymbol{r}) = \psi(\boldsymbol{R})\varphi_{\underline{0}}(\boldsymbol{r}) \quad (2.5.5)$$

where $\psi(\boldsymbol{R})$ is the spherical wave defined in (2.1.9) and $\varphi_{\underline{0}}$ is the ground state of the harmonic oscillator centered in $\boldsymbol{a}$. The eigenfunctions of the harmonic oscillator are denoted by

$$\varphi_{\underline{n}}(\boldsymbol{r}) = \gamma^{-3/2}\phi_{\underline{n}}(\gamma^{-1}(\boldsymbol{r}-\boldsymbol{a})), \quad \gamma = \sqrt{\frac{\hbar}{m\omega}}, \quad \phi_{\underline{n}}(\boldsymbol{x}) \equiv \phi_{n_1}(x_1)\phi_{n_2}(x_2)\phi_{n_3}(x_3) \tag{2.5.6}$$

where $\underline{n} = (n_1, n_2, n_3) \in \mathbb{N}^3$ and ϕ_{n_k} is the Hermite function of order n_k. In particular the ground state corresponds to $\underline{n} = \underline{0} = (0, 0, 0)$.

We assume that the physical parameters characterizing the system have the same order of magnitude considered in Sect. 2.1. More precisely, we introduce once again a small parameter $\varepsilon > 0$ and fix

$$\hbar = \varepsilon^2 \qquad M = 1 \qquad \sigma = \varepsilon \qquad m = \varepsilon \qquad \omega = \varepsilon^{-1} \qquad \delta = \varepsilon \qquad \lambda = \varepsilon^2 \tag{2.5.7}$$

Under this scaling the Hamiltonian becomes

$$H^\varepsilon = H_0^\varepsilon + \varepsilon^2 V^\varepsilon \tag{2.5.8}$$

where

$$H_0^\varepsilon = h_0^\varepsilon + h^\varepsilon, \qquad h_0^\varepsilon = -\frac{\varepsilon^4}{2}\Delta_{\boldsymbol{R}}, \qquad h^\varepsilon = \varepsilon^{-1}\left[-\frac{\varepsilon^4}{2}\Delta_{\boldsymbol{r}} + \frac{1}{2}(\boldsymbol{r}-\boldsymbol{a})^2\right] \tag{2.5.9}$$

and

$$V^\varepsilon(\boldsymbol{R}, \boldsymbol{r}) = V\left(\varepsilon^{-1}(\boldsymbol{R}-\boldsymbol{r})\right) \tag{2.5.10}$$

The rescaled initial state of the system is

$$\Psi_0^\varepsilon(\boldsymbol{R}, \boldsymbol{r}) = \psi^\varepsilon(\boldsymbol{R})\varphi_{\underline{0}}^\varepsilon(\boldsymbol{r}) \tag{2.5.11}$$

$$\varphi_{\underline{n}}^\varepsilon(\boldsymbol{r}) = \frac{1}{\varepsilon^{3/2}}\phi_{\underline{n}}\left(\varepsilon^{-1}(\boldsymbol{r}-\boldsymbol{a})\right) \qquad \underline{n} \in \mathbb{N}^3 \tag{2.5.12}$$

and ψ^ε has been defined in (2.1.16). We note that under this scaling the energy levels of the harmonic oscillator are

$$E_{\underline{n}}^\varepsilon = \varepsilon\left(|n| + \frac{3}{2}\right), \qquad |n| = n_1 + n_2 + n_3 \tag{2.5.13}$$

We are now ready to study the solution of the Schrödinger equation of the system with initial datum Ψ_0^ε

$$\mathcal{U}^\varepsilon(t)\Psi_0^\varepsilon, \qquad \mathcal{U}^\varepsilon(t) = e^{-i\frac{t}{\varepsilon^2}H^\varepsilon} \tag{2.5.14}$$

for $t > \tau$. In particular we shall perform a perturbative analysis, computing the first correction to the free evolution of the system

$$\mathcal{U}_0^\varepsilon(t)\Psi_0^\varepsilon\,, \qquad \mathcal{U}_0^\varepsilon(t) = e^{-i\frac{t}{\varepsilon^2}H_0^\varepsilon} \tag{2.5.15}$$

for $\varepsilon \to 0$. In order to formulate the result, we fix a reference frame such that

$$\hat{\boldsymbol{a}} = (0, 0, 1) \tag{2.5.16}$$

and we introduce the following definition

Definition 2.1 *Let $P^\varepsilon = P^\varepsilon(\boldsymbol{R}, \boldsymbol{r})$ be the function*

$$P^\varepsilon(\boldsymbol{R}, \boldsymbol{r}) = \sum_{\underline{n}} P_{\underline{n}}^\varepsilon(\boldsymbol{R})\, \varphi_{\underline{n}}^\varepsilon(\boldsymbol{r}) \tag{2.5.17}$$

where $P_{\underline{n}}^\varepsilon$ is the wave packet for the α-particle given by

$$P_{\underline{n}}^\varepsilon(\boldsymbol{R}) \equiv P_{\underline{n}}^\varepsilon(R_1, R_2, R_3) = \frac{C_{\underline{n}}^\varepsilon}{\varepsilon^{3/2}}\, \mathcal{F}_{\underline{n}}\left(\frac{R_1}{\varepsilon}, \frac{R_2}{\varepsilon}, 0\right) e^{-\frac{1}{2\varepsilon^2}\left(R_3 - \mathcal{Z}_{\underline{n}}^\varepsilon\right)^2 + \frac{i}{\varepsilon^2} v_{\underline{n}}^\varepsilon R_3} \tag{2.5.18}$$

$$C_{\underline{n}}^\varepsilon = \frac{2\pi^{5/4}}{i|\boldsymbol{a}|^2}\, e^{\frac{i}{\varepsilon}|n|\tau + i\frac{|n|^2\tau}{2v_0^2}} \tag{2.5.19}$$

$$\mathcal{F}_{\underline{n}}(\boldsymbol{y}) \equiv \mathcal{F}_{\underline{n}}(y_1, y_2, y_3) = e^{-i\frac{|y|^2}{2\tau}} \left(\widetilde{\phi_{\underline{n}}\phi_{\underline{0}}} \cdot \widetilde{V}\right)\left(-\frac{y_1}{\tau}, -\frac{y_2}{\tau}, -\frac{y_3}{\tau} - \frac{|n|}{v_0}\right) \tag{2.5.20}$$

$$\mathcal{Z}_{\underline{n}}^\varepsilon = \frac{|n|\tau}{v_0}\varepsilon \tag{2.5.21}$$

$$v_{\underline{n}}^\varepsilon = v_0 - \frac{|n|}{v_0}\varepsilon \tag{2.5.22}$$

The wave packet $P_{\underline{n}}^\varepsilon$ will be the crucial object emerging from our analysis. It is written as the product of two different wave packets. The first one is a two-dimensional wave packet in the variables R_1, R_2, belonging to a plane orthogonal to the direction $\hat{\boldsymbol{a}}$, and it is well concentrated around the origin both in position and momentum for $\varepsilon \to 0$. The second one is a one-dimensional wave packet in the variable R_3, i.e. the coordinate along the direction $\hat{\boldsymbol{a}}$. For $\varepsilon \to 0$ such wave packet is well concentrated in position around $\mathcal{Z}_{\underline{n}}^\varepsilon$ and in momentum around $v_{\underline{n}}^\varepsilon$. This means that the whole wave packet $P_{\underline{n}}^\varepsilon$ is concentrated in position around $\mathcal{Z}_{\underline{n}}^\varepsilon \hat{\boldsymbol{a}}$ and in momentum around $v_{\underline{n}}^\varepsilon \hat{\boldsymbol{a}}$. As a consequence, its free evolution computed at time $t = \tau$

$$\left(e^{-i\frac{\tau}{\varepsilon^2}h_0^\varepsilon} P_{\underline{n}}^\varepsilon\right)(\boldsymbol{R}) \tag{2.5.23}$$

is a wave packet, localized in position around $\boldsymbol{a}$ and in momentum around $v_{\underline{n}}^\varepsilon \hat{\boldsymbol{a}}$. In fact, from (2.5.21) and (2.5.22), the average position at $t = \tau$ is

$$\mathcal{Z}^{\varepsilon}_{\underline{n}}\,\hat{\boldsymbol{a}} + v^{\varepsilon}_{\underline{n}}\,\hat{\boldsymbol{a}}\,\tau = \boldsymbol{a} \tag{2.5.24}$$

while the momentum is a conserved quantity for the free dynamics.

In conclusion, (2.5.23) is the precise expression of the wave packet described in the introductory remarks of the section. Its role in the asymptotic evolution of the wave function of the system is specified in the following theorem.

Theorem 2.5.2 *Let us fix $t > \tau$. Then there exists $C(t) > 0$, independent of ε, such that*

$$\mathcal{U}^{\varepsilon}(t)\Psi^{\varepsilon}_0 = \mathcal{U}^{\varepsilon}_0(t)\Psi^{\varepsilon}_0 + \varepsilon^2\,\mathcal{U}^{\varepsilon}_0(t)P^{\varepsilon} + \mathcal{E}^{\varepsilon}(t) \tag{2.5.25}$$

where

$$\|\mathcal{E}^{\varepsilon}(t)\| \leq C(t)\,\varepsilon^3 \tag{2.5.26}$$

Let us briefly comment on the above result. Theorem 2.5.2 provides the required approximate dynamics of the system for $t > \tau$ and ε small. Using the expressions for the free propagator $\mathcal{U}^{\varepsilon}_0(t)$, the initial state Ψ^{ε}_0 and the function P^{ε}, formula (2.5.25) can be rewritten as

$$\begin{aligned}\left(\mathcal{U}^{\varepsilon}(t)\Psi^{\varepsilon}_0\right)(\boldsymbol{R},\boldsymbol{r}) &= e^{-i\frac{t}{\varepsilon^2}E^{\varepsilon}_{\underline{0}}}\left[\left(e^{-i\frac{t}{\varepsilon^2}h^{\varepsilon}_0}\psi^{\varepsilon}\right)(\boldsymbol{R}) + \varepsilon^2\left(e^{-i\frac{t}{\varepsilon^2}h^{\varepsilon}_0}P^{\varepsilon}_{\underline{0}}\right)(\boldsymbol{R})\right]\varphi^{\varepsilon}_{\underline{0}}(\boldsymbol{r}) \\ &+ \varepsilon^2\sum_{\underline{n}\neq\underline{0}} e^{-i\frac{t}{\varepsilon^2}E^{\varepsilon}_{\underline{n}}}\left(e^{-i\frac{t}{\varepsilon^2}h^{\varepsilon}_0}P^{\varepsilon}_{\underline{n}}\right)(\boldsymbol{R})\,\varphi^{\varepsilon}_{\underline{n}}(\boldsymbol{r}) + \mathcal{E}^{\varepsilon}(t)\end{aligned} \tag{2.5.27}$$

In the previous formula the approximate wave function has been written as the sum of two terms, corresponding to two different possible "histories" of the system. In the first one, the oscillator remains in its ground state and the α-particle is described by the sum

$$\left(e^{-i\frac{t}{\varepsilon^2}h^{\varepsilon}_0}\psi^{\varepsilon}\right)(\boldsymbol{R}) + \varepsilon^2\left(e^{-i\frac{t}{\varepsilon^2}h^{\varepsilon}_0}P^{\varepsilon}_{\underline{0}}\right)(\boldsymbol{R}) \tag{2.5.28}$$

i.e., the free evolution of the initial spherical wave slightly deformed by the free evolution of the small wave packet $P^{\varepsilon}_{\underline{0}}$, emerging from the oscillator. The second term is a sum over all possible excited states of the oscillator. Corresponding to each term of the sum, the α-particle is described by ε^2 times

$$\left(e^{-i\frac{t}{\varepsilon^2}h^{\varepsilon}_0}P^{\varepsilon}_{\underline{n}}\right)(\boldsymbol{R}) \tag{2.5.29}$$

i.e., the free evolution for $t > \tau$ of the wave packet $P^{\varepsilon}_{\underline{n}}$, $\underline{n} \neq \underline{0}$. As we already remarked, each wave packet emerges at $t = \tau$ from the excited oscillator with momentum $v^{\varepsilon}_{\underline{n}}\,\hat{\boldsymbol{a}}$. Therefore, for $t > \tau$, the wave packet will be concentrated around the uniform classical motion

$$\boldsymbol{R}(t) = \boldsymbol{a} + \left(v_0 - \frac{|n|}{v_0}\,\varepsilon\right)(t-\tau)\,\hat{\boldsymbol{a}} \tag{2.5.30}$$

We also note that the wave packet $P_{\underline{0}}^{\varepsilon}$ is produced by an elastic collision between the α-particle with momentum v_0 (recall that $M = 1$) and the oscillator and therefore its momentum is unaffected, i.e., $v_{\underline{0}}^{\varepsilon} = v_0$. On the other hand, the wave packet $P_{\underline{n}}^{\varepsilon}$, $\underline{n} \neq \underline{0}$, is produced by a (weak) inelastic collision with an energy loss $\Delta E = \varepsilon|n|$. In this case, after the collision, the momentum of the α-particle is

$$\sqrt{2\left(\frac{v_0^2}{2} - \Delta E\right)} = v_0\sqrt{1 - \frac{2|n|}{v_0^2}\,\varepsilon} = v_0 - \frac{|n|}{v_0}\,\varepsilon + O(\varepsilon^2) \tag{2.5.31}$$

coinciding with $v_{\underline{n}}^{\varepsilon}$ at first order in ε.

2.6 Outline of the Proof

The proof of Theorem 2.5.2 requires several intermediate steps. In this section we describe only the line of reasoning, referring to (Recchia and Teta, 2013) for a detailed proof.

We start with Duhamel's formula to represent the solution of the Schrödinger equation

$$\mathcal{U}^{\varepsilon}(t)\Psi_0^{\varepsilon} = \mathcal{U}_0^{\varepsilon}(t)\Psi_0^{\varepsilon} - i\int_0^t ds\, \mathcal{U}^{\varepsilon}(t-s)\, V^{\varepsilon}\, \mathcal{U}_0^{\varepsilon}(s)\Psi_0^{\varepsilon} \tag{2.6.1}$$

Iterating twice we obtain

$$\mathcal{U}^{\varepsilon}(t)\Psi_0^{\varepsilon} = \mathcal{U}_0^{\varepsilon}(t)\Psi_0^{\varepsilon} + \mathcal{U}_0^{\varepsilon}(t) I^{\varepsilon}(t)\Psi_0^{\varepsilon} + \mathcal{R}^{\varepsilon}(t) \tag{2.6.2}$$

where we have denoted

$$I^{\varepsilon}(t) = -i\int_0^t ds\, \mathcal{U}_0^{\varepsilon}(-s)\, V^{\varepsilon}\, \mathcal{U}_0^{\varepsilon}(s) \tag{2.6.3}$$

$$\mathcal{R}^{\varepsilon}(t) = \mathcal{U}_0^{\varepsilon}(t) J^{\varepsilon}(t)\Psi_0^{\varepsilon} - i\int_0^t ds\, \mathcal{U}^{\varepsilon}(t-s)\, V^{\varepsilon}\, \mathcal{U}_0^{\varepsilon}(s) J^{\varepsilon}(s)\Psi_0^{\varepsilon} \tag{2.6.4}$$

$$J^{\varepsilon}(t) = -\int_0^t ds \int_0^s d\sigma\, \mathcal{U}_0^{\varepsilon}(-s)\, V^{\varepsilon}\, \mathcal{U}_0^{\varepsilon}(s) \mathcal{U}_0^{\varepsilon}(-\sigma)\, V^{\varepsilon}\, \mathcal{U}_0^{\varepsilon}(\sigma) \tag{2.6.5}$$

In order to isolate the relevant contribution coming from the term $I^{\varepsilon}(t)\Psi_0^{\varepsilon}$ for $\varepsilon \to 0$, it is convenient to introduce the "portion around $\hat{\boldsymbol{a}}$" of the initial spherical wave

$$\psi_0^\varepsilon(\boldsymbol{R}) = \frac{\mathcal{N}_\varepsilon}{\varepsilon^{5/2}} f\left(\varepsilon^{-1}\boldsymbol{R}\right) \int_{\mathcal{C}_0} d\hat{\boldsymbol{u}}\, e^{\frac{i}{\varepsilon^2} v_0 \hat{\boldsymbol{u}}\cdot\boldsymbol{R}} \tag{2.6.6}$$

where $\mathcal{C}_0$ has been defined in (2.4.31), and correspondingly

$$\Psi_{0,0}^\varepsilon(\boldsymbol{R}, \boldsymbol{r}) = \psi_0^\varepsilon(\boldsymbol{R})\varphi_{\underline{0}}^\varepsilon(\boldsymbol{r}) \tag{2.6.7}$$

Taking into account definition (2.6.7), we rewrite (2.6.2) as follows

$$\mathcal{U}^\varepsilon(t)\Psi_0^\varepsilon = \mathcal{U}_0^\varepsilon(t)\Psi_0^\varepsilon + \mathcal{U}_0^\varepsilon(t)I^\varepsilon(t)\Psi_{0,0}^\varepsilon + \mathcal{U}_0^\varepsilon(t)I^\varepsilon(t)\left(\Psi_0^\varepsilon - \Psi_{0,0}^\varepsilon\right) + \mathcal{R}^\varepsilon(t) \tag{2.6.8}$$

In order to prove Theorem 2.5.2, one has to show that $I^\varepsilon(t)\Psi_{0,0}^\varepsilon = \varepsilon^2 P^\varepsilon + O(\varepsilon^3)$ and also that the last two terms of (2.6.8) are $O(\varepsilon^3)$.

The first step is to obtain convenient representation formulas for the relevant quantities $I^\varepsilon(t)\Psi_{0,0}^\varepsilon$, $I^\varepsilon(t)(\Psi_0^\varepsilon - \Psi_{0,0}^\varepsilon)$ and $J^\varepsilon(t)\Psi_0^\varepsilon$. This can be done following the same line of reasoning of Sect. 2.3. For each quantity we perform a series expansion with respect to the eigenfunctions of the harmonic oscillator and we obtain formulas for the expansion coefficients in terms of highly oscillatory integrals. Such representation formulas allow to exploit stationary and non stationary phase methods to characterize the asymptotic behavior of each quantity for $\varepsilon \to 0$. In the case of $I^\varepsilon(t)\Psi_{0,0}^\varepsilon$, we obtain

$$\left(I^\varepsilon(t)\Psi_{0,0}^\varepsilon\right)(\varepsilon\boldsymbol{x}, \boldsymbol{r}) = \sum_{\underline{n}} \mathcal{I}_{\underline{n}}^\varepsilon(t, \boldsymbol{x})\varphi_{\underline{n}}^\varepsilon(\boldsymbol{r}) \tag{2.6.9}$$

where

$$\mathcal{I}_{\underline{n}}^\varepsilon(t, \boldsymbol{x}) = \frac{\mathcal{N}_\varepsilon}{i\varepsilon^{5/2}} \int_\Lambda d\mu d\nu ds \int d\boldsymbol{\xi}\, F_{\underline{n}}(\boldsymbol{\xi}, \mu, \nu, s; \boldsymbol{x})\, e^{\frac{i}{\varepsilon}\Phi_{\underline{n}}(\boldsymbol{\xi},\mu,\nu,s;\boldsymbol{x})} \tag{2.6.10}$$

$$F_{\underline{n}}(\boldsymbol{\xi}, \mu, \nu, s; \boldsymbol{x}) = \frac{e^{i\boldsymbol{\xi}\cdot\boldsymbol{x} + i\frac{s}{2}\boldsymbol{\xi}^2}}{\sqrt{1-\mu^2-\nu^2}}\, g_{\underline{n},\underline{0}}(\boldsymbol{\xi})\, f(\boldsymbol{x} + s\,\boldsymbol{\xi}) \tag{2.6.11}$$

$$g_{\underline{n},\underline{m}}(\boldsymbol{\xi}) = \widetilde{\phi_{\underline{n}}\phi_{\underline{m}}}(\boldsymbol{\xi})\tilde{V}(\boldsymbol{\xi}) \tag{2.6.12}$$

$$\Phi_{\underline{n}}(\boldsymbol{\xi}, \mu, \nu, s; x) = -|\boldsymbol{a}|\xi_3 + v_0\left[\mu(x_1 + s\xi_1) + \nu(x_2 + s\xi_2) + \sqrt{1-\mu^2-\nu^2}(x_3 + s\xi_3)\right] + |n|s \tag{2.6.13}$$

and the integration region Λ is given by

$$\Lambda = \left\{(\mu, \nu, s) \in \mathbb{R}^3 \,|\, \mu^2 + \nu^2 < \sin^2\theta_0,\ 0 < s < t\right\} \tag{2.6.14}$$

Analogous representations can be derived also for $I^\varepsilon(t)(\Psi_0^\varepsilon - \Psi_{0,0}^\varepsilon)$ and $J^\varepsilon(t)\Psi_0^\varepsilon$.

The next step is to compute the asymptotic expansion of the oscillatory integral $\mathcal{I}_{\underline{n}}^\varepsilon(t, \boldsymbol{x})$ for $\varepsilon \to 0$. One can easily verify that for $t > \tau$ the phase $\Phi_{\underline{n}}$ in the oscillatory

integral has exactly one, non degenerate, critical point in the integration region given by $(\mu, \nu, s) = z^c, \boldsymbol{\xi} = \boldsymbol{\xi}^c$, where

$$z^c = (0, 0, \tau) \qquad \boldsymbol{\xi}^c = \left(-\frac{x_1}{\tau}, -\frac{x_2}{\tau}, -\frac{|n|}{v_0}\right) \tag{2.6.15}$$

As it was done in Sect. 2.4, case (iii), we can directly compute the leading term of the expansion using an elementary approach, essentially based on a change of coordinates in the oscillatory integral. In fact, defining

$$\boldsymbol{\mathcal{A}}(\mu, \nu, s) = v_0 \left(\mu s, \nu s, \sqrt{1-\mu^2-\nu^2}\, s - \tau\right) \tag{2.6.16}$$

$$\mathcal{B}_{\underline{n}}(\mu, \nu, s; \boldsymbol{x}) = v_0 x_1 \mu + v_0 x_2 \nu + v_0 x_3 \sqrt{1-\mu^2-\nu^2} + |n| s \tag{2.6.17}$$

the phase can be represented as

$$\Phi_{\underline{n}}(\boldsymbol{\xi}, \mu, \nu, s; \boldsymbol{x}) = \boldsymbol{\mathcal{A}}(\mu, \nu, s) \cdot \boldsymbol{\xi} + \mathcal{B}_{\underline{n}}(\mu, \nu, s; \boldsymbol{x}) \tag{2.6.18}$$

and the oscillatory integral is written as

$$\mathcal{I}^{\varepsilon}_{\underline{n}}(t, \boldsymbol{x}) = \frac{\mathcal{N}_\varepsilon}{i\varepsilon^{5/2}} \int_\Lambda d\mu d\nu ds\, e^{\frac{i}{\varepsilon}\mathcal{B}_{\underline{n}}(\mu,\nu,s;\boldsymbol{x})} \int d\boldsymbol{\xi}\; F_{\underline{n}}(\boldsymbol{\xi}, \mu, \nu, s; \boldsymbol{x})\; e^{\frac{i}{\varepsilon}\boldsymbol{\mathcal{A}}(\mu,\nu,s)\cdot\boldsymbol{\xi}} \tag{2.6.19}$$

Let us introduce the following linear change of coordinates

$$(\mu, \nu, s) = \mathcal{L}_\varepsilon(z_1, z_2, z_3) \equiv \mathcal{L}_\varepsilon z \tag{2.6.20}$$

$$\mu = \frac{\varepsilon}{v_0\tau} z_1, \qquad \nu = \frac{\varepsilon}{v_0\tau} z_2, \qquad s = \tau + \frac{\varepsilon}{v_0} z_3 \tag{2.6.21}$$

Hence

$$\mathcal{I}^{\varepsilon}_{\underline{n}}(t, \boldsymbol{x}) = \frac{\mathcal{N}_\varepsilon \sqrt{\varepsilon}}{i v_0^3 \tau^2} \int_{\Lambda_\varepsilon} dz\, e^{\frac{i}{\varepsilon}\mathcal{B}_{\underline{n}}(\mathcal{L}_\varepsilon z;\boldsymbol{x})} \int d\boldsymbol{\xi}\; F_{\underline{n}}(\boldsymbol{\xi}, \mathcal{L}_\varepsilon z; \boldsymbol{x})\; e^{\frac{i}{\varepsilon}\boldsymbol{\mathcal{A}}(\mathcal{L}_\varepsilon z)\cdot\boldsymbol{\xi}} \tag{2.6.22}$$

where the integration region Λ_ε is given by

$$\Lambda_\varepsilon = \left\{ z \in \mathbb{R}^3 \,|\, z_1^2 + z_2^2 < \frac{v_0^2\tau^2}{\varepsilon^2} \sin^2\theta_0,\; -\frac{v_0\tau}{\varepsilon} < z_3 < \frac{v_0}{\varepsilon}(t-\tau) \right\} \tag{2.6.23}$$

We note that, for $\varepsilon \to 0$, one has $\mathcal{L}_\varepsilon z \to z^c$ and $\Lambda_\varepsilon \to \mathbb{R}^3$. Let us expand $\mathcal{A}(\mathcal{L}_\varepsilon z)$ and $\mathcal{B}(\mathcal{L}_\varepsilon z; \boldsymbol{x})$ around $\varepsilon = 0$. One has

$$\mathcal{A}(\mathcal{L}_\varepsilon z) = \varepsilon z + \mathcal{A}^{(2)}_\varepsilon(z) \tag{2.6.24}$$

$$\mathcal{B}_{\underline{n}}(\mathcal{L}_\varepsilon z;\boldsymbol{x}) = v_0 x_3 + |n|\tau - \varepsilon\,\boldsymbol{\xi}^c\cdot z + \mathcal{B}^{(2)}_\varepsilon(z;\boldsymbol{x}) \tag{2.6.25}$$

where $\mathcal{A}^{(2)}_\varepsilon(z)$ and $\mathcal{B}^{(2)}_\varepsilon(z;\boldsymbol{x})$ are explicitly known functions of order $O(\varepsilon^2)$ for $\varepsilon\to 0$. Taking into account of (2.6.24) and (2.6.25), we write

$$\mathcal{I}^\varepsilon_{\underline{n}}(t,\boldsymbol{x}) = \frac{\mathcal{N}_\varepsilon\sqrt{\varepsilon}}{i\,v_0^3\tau^2}\,e^{\frac{i}{\varepsilon}(v_0 x_3+|n|\tau)}\int_{\Lambda_\varepsilon} dz\, e^{-i\boldsymbol{\xi}^c\cdot z+\frac{i}{\varepsilon}\mathcal{B}^{(2)}_\varepsilon(z;\boldsymbol{x})}\int d\boldsymbol{\xi}\; F_{\underline{n}}(\boldsymbol{\xi},\mathcal{L}_\varepsilon z;\boldsymbol{x})\; e^{iz\cdot\xi+\frac{i}{\varepsilon}\mathcal{A}^{(2)}_\varepsilon(z)} \tag{2.6.26}$$

From the above expression it is now possible to derive the asymptotic expansion for $\varepsilon\to 0$, with an explicit remainder. In particular, we are interested in the leading term and therefore we easily obtain

$$\begin{aligned}\mathcal{I}^\varepsilon_{\underline{n}}(t,\boldsymbol{x}) &= \frac{\mathcal{N}_0\sqrt{\varepsilon}}{i\,v_0^3\tau^2}\,e^{\frac{i}{\varepsilon}(v_0x_3+|n|\tau)}\int dz\, e^{-i\boldsymbol{\xi}^c\cdot z}\int d\boldsymbol{\xi}\; F_{\underline{n}}(\boldsymbol{\xi},z^c;\boldsymbol{x})\,e^{iz\cdot\xi} + Q^\varepsilon_{\underline{n}}(t,\boldsymbol{x})\\ &= \frac{2\pi^2\sqrt{\varepsilon}}{i|\boldsymbol{a}|^2}\,e^{\frac{i}{\varepsilon}(v_0x_3+|n|\tau)}\,F_{\underline{n}}(\boldsymbol{\xi}^c,z^c;\boldsymbol{x}) + Q^\varepsilon_{\underline{n}}(t,\boldsymbol{x})\end{aligned} \tag{2.6.27}$$

where we have used $\mathcal{N}_0 = (4\pi)^{-1}v_0$ and we have denoted by $Q^\varepsilon_{\underline{n}}(t,\boldsymbol{x})$ the remainder.

The next point is to find the explicit expression for the leading term. From (2.6.11), (2.6.12) and (2.6.15) we have

$$\begin{aligned}F_{\underline{n}}(\boldsymbol{\xi}^c,z^c;\boldsymbol{x}) &= e^{i\boldsymbol{\xi}^c\cdot\boldsymbol{x}+i\frac{\tau}{2}(\xi^c)^2}\,g_{\underline{n},\underline{0}}(\boldsymbol{\xi}^c)\,f(\boldsymbol{x}+\tau\boldsymbol{\xi}^c)\\ &= e^{i\frac{|n|^2\tau}{2v_0^2}}\,e^{-i\frac{x_1^2+x_2^2}{2\tau}}\,g_{\underline{n},\underline{0}}\left(-\frac{x_1}{\tau},-\frac{x_2}{\tau},-\frac{|n|}{v_0}\right)f\left(0,0,x_3-\frac{|n|\tau}{v_0}\right)e^{-i\frac{|n|}{v_0}x_3}\\ &= e^{i\frac{|n|^2\tau}{2v_0^2}}\,\mathcal{F}_{\underline{n}}(x_1,x_2,0)\;\pi^{-3/4}\,e^{-\frac{1}{2}\left(x_3-\frac{|n|\tau}{v_0}\right)^2-i\frac{|n|}{v_0}x_3}\end{aligned} \tag{2.6.28}$$

where, in the last line, we have used (2.5.20) and (2.1.10). Substituting (2.6.28) in (2.6.27) and using the Definition 2.5.1, we finally find

$$\begin{aligned}\mathcal{I}^\varepsilon_{\underline{n}}(t,\boldsymbol{x}) &= \sqrt{\varepsilon}\,C^\varepsilon_{\underline{n}}\,\mathcal{F}_{\underline{n}}(x_1,x_2,0)\;e^{-\frac{1}{2}\left(x_3-\frac{|n|\tau}{v_0}\right)^2+\frac{i}{\varepsilon}\left(v_0-\frac{|n|}{v_0}\varepsilon\right)x_3} + Q^\varepsilon_{\underline{n}}(t,\boldsymbol{x})\\ &= \varepsilon^2\,P^\varepsilon_{\underline{n}}(\varepsilon\,\boldsymbol{x}) + Q^\varepsilon_{\underline{n}}(t,\boldsymbol{x})\end{aligned} \tag{2.6.29}$$

As a result of the analysis performed above, we succeeded in isolating the first non trivial correction to the free dynamics of the system. In particular, using (2.6.8), (2.6.9) and (2.6.29), we can derive the following representation for the solution of the Schrödinger equation

$$\mathcal{U}^\varepsilon(t)\Psi^\varepsilon_0 \;=\; \mathcal{U}^\varepsilon_0(t)\Psi^\varepsilon_0 \;+\; \varepsilon^2\,\mathcal{U}^\varepsilon_0(t)P^\varepsilon \;+\; \mathcal{E}(t) \tag{2.6.30}$$

where the remainder $\mathcal{E}(t)$ is explicitly given by

$$\mathcal{E}(t) = \mathcal{U}_0^\varepsilon(t) \sum_{\underline{n}} Q_{\underline{n}}^\varepsilon(t) \varphi_{\underline{n}}^\varepsilon + \mathcal{U}_0^\varepsilon(t) I^\varepsilon(t) \left(\Psi_0^\varepsilon - \Psi_{0,0}^\varepsilon\right) + \mathcal{R}^\varepsilon(t) \qquad (2.6.31)$$

and $Q_{\underline{n}}^\varepsilon(t)$ denotes the function implicitly defined in (2.6.27). The last technical, and rather long, step of the proof is the estimate of the remainder. Using the representation formulas in terms of oscillatory integrals and repeated integration by parts (see Recchia and Teta 2013 for details), one obtains estimate (2.5.26), concluding the proof of Theorem 2.5.2.

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