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Emission, Emittance and Entropy of High Intensity Electron Beams

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14. ABSTRACT Abstract The interaction of intense electromagnetic fields, such as those produced by present day and future lasers, with electric charges in matter is of both fundamental and practical interest. An important area of current research is that of controlling electron emission from metals on the femto-second scale. We propose to carry out analytical and numerical investigations of the dynamics of electrons interacting with a strong laser field. To do this we will: A. expand our present work solving the time dependent Schrodinger equation describing photoemission following the turning on of a monochromatic laser field with a femtosecond periods to include a constant electric field, two colored laser fields and carrier-envelope-phase effects. B. Work on the general problem of tunneling times using results obtained from the exact solution of the Schrodinger equation. One of our tools will be the study of the Wigner distribution function. This is ongoing work in collaboration with Dr. Don Shiffler from the Air Force Research Laboratory in Kirtland. C. Study the effect of Coulomb interactions leading to space change limitations on the current, Schottky reduction of barrier height, emittance of beams and other relevant plasma non equilibrium transport properties will also be pursued.			
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Non-perturbative Solution of the 1d Schrödinger Equation Describing Photoemission from a Sommerfeld model Metal by an Oscillating Field

1 Physical setting

The emission of electrons from a metal surface induced by the application of an external electric field is a problem of continuing theoretical and practical interest . It was first fully analyzed for the constant electric field using the “new mechanics” by Fowler and Nordheim in 1928 . They considered the Sommerfeld model of quasi-free electrons confined to a metal occupying the entire half-space $x < 0$ by an effective step potential U . The metal is filled with electrons up to a Fermi level \mathcal{E}_F , neglecting the small number of thermal electrons at room temperatures. This gives the work function $W := U - \mathcal{E}_F$, i.e. W is the minimum amount of energy necessary to take an electron out of the metal.

Applying a constant external electric field E for $x > 0$, see Figure 1, an electron in the Fermi sea moving in the positive x -direction, described by a plane wave e^{ikx} , $k > 0$, can then tunnel out of the metal (we use units in which $\hbar = m = e = 1$).

To describe this system FN considered the Schrödinger equation

$$i\partial_t\psi = -\frac{1}{2}\partial_x^2\psi + \Theta(x)(U - Ex)\psi \quad (1.1)$$

where $\Theta(x)$ is the Heaviside function, equal to 1 if $x > 0$ and 0 otherwise. To compute the stationary current observed after the field has been on for a while, FN made the Ansatz that $\psi(x, t)$ is a generalized eigenfunction of (1.1)

$$\psi(x, t) = e^{-\frac{ik^2}{2}t}\phi_E(x) \quad (1.2)$$

with ϕ_E satisfying the equation

$$\frac{k^2}{2}\phi_E = \frac{1}{2}\partial_x^2\phi_E - \Theta(x)(U - Ex)\phi_E. \quad (1.3)$$

The requirement that there be only one incoming wave from the left, given by e^{ikx} , $k > 0$, for $x < 0$ and only outgoing electrons for $x > 0$, as well as that $\phi_E(x)$ and its derivative be continuous at $x = 0$, and that $\phi_E(x)$ be bounded as $|x| \rightarrow \infty$, gave $\phi_E(x) = e^{ikx} + R_0e^{-ikx}$ for $x < 0$ and an Airy function expression for $x > 0$.

The FN computation is still the basic ingredient for the analysis of constant field currents experiments at present . Their analysis does not consider the initial state of the system when the field is turned on. To check the validity of the FN ansatz (1.2) we recently revisited the FN setup by solving (1.1) for general initial values of $\psi(x, 0)$. We showed that for all $\psi(x, 0)$ representing an incoming beam e^{ikx} plus some square integrable function, $\psi(x, t)$ converges to the FN solution when $t \rightarrow \infty$. The asymptotic approach behaves like $t^{-\frac{3}{2}}$. We considered in particular the initial state corresponding to a solution of (1.3) when $E = 0$:

$$\psi(x, 0) = \phi_0(x) = \begin{cases} e^{ikx} + R_0e^{-ikx} & \text{for } x \leq 0 \\ T_0e^{-\sqrt{2U-k^2}x} & \text{for } x > 0 \end{cases}, \quad R_0 = \frac{ik + \sqrt{2U - k^2}}{ik - \sqrt{2U - k^2}}, \quad T_0 = \frac{2ik}{ik - \sqrt{2U - k^2}}. \quad (1.4)$$

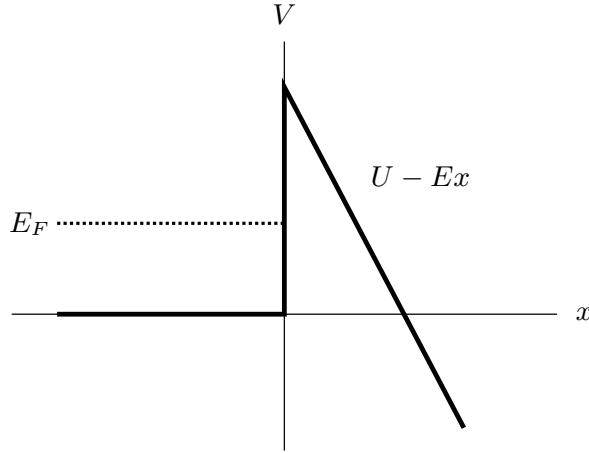


Figure 1: The potential considered by Fowler and Nordheim. $x < 0$ corresponds to the region inside the metal and $x > 0$ corresponds to the vacuum outside.

Time-periodic electric field and the photoelectric effect. In the present work, we consider a setup similar to that of FN, except that the external field E is taken to be periodic in time with period $\frac{2\pi}{\omega}$. More precisely, we consider solutions of the equation

$$i\partial_t\psi = -\frac{1}{2}\partial_x^2\psi + \Theta(x)(U - Ex\cos\omega t)\psi, \quad t > 0 \quad (1.5)$$

with an initial value $\psi(x, 0)$. Physically, this can represent, depending on ω , a great variety of situations ranging from an alternating field produced by a mechanical generator to one produced by shining a laser on the metal surface.

For small values of ω the situation is in some ways similar to the constant field case with electrons tunneling through the (oscillating) barrier, although the limit $\omega \rightarrow 0$ in (1.5) is very singular. For large ω , the situation is expected to be similar to that of the photoelectric effect, where light shining on a metal surface causes the almost instantaneous emission of electrons with a well-defined maximum kinetic energy K , given by the Einstein formula $K = \omega - W$ (recall that $\hbar = 1$ in our units). Here of course we do not consider discrete photons, since (1.5) represents the electric field classically. It is expected however that the discrete jumps will show up as resonances. Something like this is indeed the case for weak fields. For large fields one has to add to W the ponderomotive energy of the electron in the oscillating field. There is a vast physical literature on this topic.

2 Mathematical setting.

From a mathematical point of view, the existence of solutions of (1.5) with appropriate physical initial conditions which remain bounded and behave in a physical way for all x and t is not obvious. In the physics literature, Faisal et al. considered periodic solutions of (1.5) for general periodic fields $E(t) = E(t + 2\pi/\omega)$

and, in analogy to the work of FN sought solutions of (1.5) in the form ¹

$$\psi(x, t) = e^{-\frac{1}{2}ik^2t}\phi(x, t) \tag{2.1}$$

where $\phi(x, t)$ is periodic in time and has a single incoming wave e^{ikx} for $x < 0$, $k > 0$. The continuity conditions at $x = 0$ then lead to an infinite set of linear equations for the Fourier coefficients of ϕ . The existence of solutions for this infinite system was not proven. What Faisal & al. did was to truncate the infinite set of equations and solve the truncated system numerically.

During this award, we rigorously analyzed the full time evolution of (1.5) both for L^2 initial conditions as well as for an incoming beam e^{ikx} as in (1.4) plus other terms which do not contribute to the long time behavior. We then find that for L^2 initial conditions $\psi(x, t)$ decays pointwise at least a rate $O(t^{-1/2})$. For this, we first obtain a RAGE-type theorem for this time-dependent potential. In the case the initial condition contains an incoming wave as in (1.4) (plus possible L^2 perturbations), the solution converges at least at a rate $O(t^{-1/2})$ to the ansatz derived by Faisal et al. . It follows from our result that the infinite system of equations obtained by Faisal & al. has a solution. We limit our analysis to time-periodic fields of the form in (1.5) but expect our results to extend to general periodic fields.

To obtain these results we derive an integral equation for $\psi(x, 0) := \psi_0(x)$, which we show to have a unique solution. We also obtain a set of formulas that recover the full wave function $\psi(x, t)$ from ψ_0 . The properties of ψ_0 , and therefore of ψ , are derived from the integral equation that it solves. By far the most delicate analysis concerns the long time behavior of the solution of the Schrödinger equation.

Behind the apparent simplicity of the potential in (1.5) lie a number of significant mathematical difficulties making the analysis particularly challenging. Among them: lack of smoothness, and the fact that the Hamiltonian is unbounded in a time dependent way both in physical domain and in momentum space (owing to the unboundedness of the potential energy term). As a result, the classical PDE toolkit does not apply and the type of results that we need do not seem, as far as we know, to be in the literature. To overcome these difficulties, we develop new methods, which we combine with the spectral measure theory of the underlying unbounded operators.

3 Main Results

Denote

$$\mathcal{D} = H^2(\mathbb{R} \setminus \{0\}) \cap H^1(\mathbb{R}) \cap \{f \mid xf \in L^2(\mathbb{R})\} \tag{3.1}$$

Theorem 1. (a) *The Hamiltonians $\mathcal{H}_t := -\frac{1}{2}\partial_x^2\psi + \Theta(x)(U - Ex \cos \omega t)\psi$, densely defined on C_0^∞ have a self-adjoint extension on \mathcal{D} for each fixed t .*

(b) *The evolution of $\psi(x, t)$ is given by a unitary group if $\psi(x, 0) \in \mathcal{D}$.*

Theorem 2. *If the initial state $\psi(x, 0) := f$ is in \mathcal{D} , then (1.5) has a unique solution $\psi(\cdot, t) \in \mathcal{D}$, and ψ is continuously differentiable in $t > 0$.*

Theorem 3. [Long Time Behavior] (i) *For initial conditions in a dense subset of \mathcal{D} we have: for any compact set $A \subset \mathbb{R}$ the long time behavior is²*

$$\int_A |\psi(x, t)|^2 dx = O(t^{-1}) \quad \text{as } t \rightarrow \infty \tag{3.2}$$

¹Using the magnetic rather than the length gauge.

²We believe that the actual behavior below is $O(t^{-3})$, but this results from difficult to calculate cancellations occurring in algebraically cumbersome expressions.

(ii) If the initial condition $\psi(\cdot, 0)$ is in $L^2(\mathbb{R})$, we have

$$\lim_{t \rightarrow \infty} \psi(x, t) = 0 \quad (3.3)$$

uniformly in x in compact sets in \mathbb{R} .

Theorem 4. [Wave Initial Condition] For the initial state (1.4) equation (1.5) has a unique solution that is bounded, and

$$\psi(x, t) \sim e^{-ik^2 t/2} \phi(x, t) \quad \text{as } t \rightarrow \infty$$

where ϕ is time-periodic of period $2\pi/\omega$.

Remark 5. In the proof of this theorem, we will make an additional simplifying assumption: $U + \frac{E^2}{4\omega^2}$ is not an integer multiple of ω , and neither is $U + \frac{E^2}{4\omega^2} - \frac{k^2}{2}$. We do this because these cases have a slightly different singularity structure, which would require small changes in the proof, which we will not belabour. These exceptional cases correspond to a marginal situation in which absorbing an integer number of photons raises the energy of the electron to exactly the ionization value.

Remark 6. Faisal, Kamiński and Sączuk computed the periodic solutions of the Schrödinger equation (1.5) with an incoming plane wave. By Theorem 4, the solution they computed must be the asymptotic solution ϕ .