Solution of time-dependent Schrödinger equation for field emission

Ian Jauslin

joint with Ovidiu Costin, Rodica Costin, and Joel L. Lebowitz

Field emission
Emitter

\[ V(x) = U \Theta(x) \]
Semi-classical model

\[ V_t(x) = \Theta(x)(U - E_t x), \quad E_t = e_0 + e_1 \cos(\omega t) \]
Triangular barrier

\[ V(x) = \Theta(x)(U - Ex) \]
Field emission through a triangular barrier

- [Millikan, Lauritsen, 1928]: experimental plot of the logarithm of the current against $1/E$
Field emission through a triangular barrier

- [Fowler, Nordheim, 1928]: predicted that the current is, for small $E$,

$$J \approx C e^{-\frac{a}{E}}$$

- ([Rokhlenko, 2011]: studied the range of applicability of the approximation, and found more accurate approximations for larger fields.)
Fowler-Nordheim equation

- Schrödinger equation

\[ i\partial_t \psi = -\Delta \psi + \Theta(x)(U - Ex)\psi \]

- Fowler-Nordheim: quasi-stationary solution: \( \psi_{FN}(x, t) = e^{-ik^2t}\varphi_{FN}(x) \)

\[ \varphi_{FN}(x) = \begin{cases} 
  e^{ikx} + R_E e^{-ikx} & x < 0 \\
  T_E Ai(e^{-\frac{i\pi}{3}}(E^\frac{1}{3}x - E^{-\frac{2}{3}}(U - k^2))) & x > 0
\end{cases} \]

\( R_E \) and \( T_E \) are chosen so that \( \varphi_{FN} \) and \( \partial \varphi_{FN} \) are continuous at \( x = 0 \).
Fowler-Nordheim equation
Initial value problem

- Initial condition:

\[ \psi(x, 0) = \begin{cases} 
  e^{ikx} + R_0 e^{-ikx} & x < 0 \\
  T_0 e^{-\sqrt{U-k^2}x} & x > 0 
\end{cases} \]

\( R_0 \) and \( T_0 \) ensure that \( \psi \) and \( \partial \psi \) are continuous.

- Behaves asymptotically like \( \psi_{\text{FN}} \):

\[ \psi(x, t)e^{ik^2t} \xrightarrow{t \to \infty} \varphi_{\text{FN}}(x) \]
Initial value problem

- Laplace transform:

\[ \hat{\psi}_p(x) := \int_0^\infty dt \, e^{-pt} \psi(x,t) \]

- Schrödinger equation:

\[ (-\Delta + \Theta(x)V(x) - ip)\psi_p(x) = -i\psi(x,0), \quad V(x) := U - Ex \]
Solution in Laplace space

- For simplicity, $R_0 \equiv T_0 \equiv 0$.
- Solution:

\[ \hat{\psi}_p(x) = \begin{cases} 
  C_1(p)e^{-ipx} - \frac{ie^{ikx}}{-ip + k^2} & \text{if } x < 0 \\
  C_2(p)\varphi_p(x) & \text{if } x > 0 
\end{cases} \]

with

\[ (-\Delta + V(x) - ip)\varphi_p(x) = 0 \]
\[ \varphi_p(x) = \text{Ai} \left( e^{-\frac{i\pi}{3}} \left( E^{\frac{1}{3}}x - E^{-\frac{2}{3}}(U - ip) \right) \right) \]
Solution in Laplace space

- $C_1$ and $C_2$ ensure that $\hat{\psi}_p(x)$ and $\partial\hat{\psi}_p(x)$ are continuous at $x = 0$:

$$C_1(p) = \frac{i(ik\varphi_p(0) - \partial\varphi_p(0))}{(-ip + k^2)(\sqrt{-ip}\varphi_p(0) - \partial\varphi_p(0))}$$

$$C_2(p) = -\frac{i}{(\sqrt{-ip} + ik)(\sqrt{-ip}\varphi_p(0) - \partial\varphi_p(0))}.$$
Poles in Laplace plane
Asymptotic behavior

• As $t \to \infty$:

$$\psi(x, t) = \psi_{FN}(x, t) + \left(\frac{t}{\tau_E(x)}\right)^{-\frac{3}{2}} + O(t^{-\frac{5}{2}}).$$

• If $k < 0$ (reflected wave), then there is no pole on the imaginary axis, so there is no contribution as $t \to \infty$.

• Similarly, the transmitted wave in the initial condition does not contribute.
Laser field

- Time dependent potential:

\[ V_t(x) = \Theta(x)(U - \epsilon \omega \cos(\omega t)x) \]

- Magnetic gauge:

\[ \Psi(x, t) := \psi(x, t)e^{-ix\Theta(x)A(t)}, \quad A(t) := \int_0^t ds \epsilon \omega \cos(\omega s) = \epsilon \sin(\omega t) \]

satisfies

\[ i\partial_t \Psi(x, t) = \left( (-i\nabla + \Theta(x)A(t))^2 + \Theta(x)U \right) \Psi(x, t) \]
Periodic solution

- A solution:

\[ \Psi(x, t) = \begin{cases} 
\Psi_I(x, t) + \Psi_R(x, t) & \text{if } x < 0 \\
\Psi_T(x, t) & \text{if } x > 0 
\end{cases} \]

\[ \Psi_I(x, t) = e^{ikx} \exp(-ik^2 t) \]

\[ \Psi_R(x, t) = \sum_{M \in \mathbb{Z}} R_M e^{iq_M x} \exp(-iq_M^2 t) \]

\[ \Psi_T(x, t) = \sum_{M \in \mathbb{Z}} T_M e^{ip_M x} \exp\left(-iUt - i \int_0^t d\tau \left(p_M + A(\tau)\right)^2 \right) \]
• Choose $q_M$ and $p_M$ to make the solution periodic (up to the phase $e^{ik^2 t}$):

$$q_M = \pm \sqrt{k^2 + M\omega}, \quad p_M = \pm \sqrt{k^2 - U + M\omega - U_V}$$

and

$$U_V := \frac{\omega}{2\pi} \int_0^{2\pi} d\tau \ A^2(\tau) = \frac{\epsilon^2}{2}.$$