Modeling the QE and Thermal Emittance of Photocathodes*

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Introduction
The three-step model of photoemission
Derivation of QE and thermal emittance for Cu
Electron distributions for simulation codes
Summary

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Introduction

Thermal emittance has become a significant contribution to the total emittance,

\[ \varepsilon_{\text{total}} = \sqrt{\varepsilon_{\text{thermal}}^2 + \varepsilon_{\text{sc}}^2 + \varepsilon_{\text{RF}}^2 + \varepsilon_{\text{optics}}^2} \]

For Cu the experimental value is: \( \varepsilon_{\text{thermal}} \approx 0.6 \) microns/mm

In LCLS simulations the total emittance is 1 micron, for a 1.2mm radius laser on the cathode. This means the thermal emittance is approximately equal to the other sources of emittance:

\[ \varepsilon_{\text{thermal}} \approx \sqrt{\varepsilon_{\text{sc}}^2 + \varepsilon_{\text{RF}}^2 + \varepsilon_{\text{optics}}^2} \approx 0.7 \) microns

Therefore, to improve beam brightness, the thermal emittance needs to be understood and reduced. Here, the goal is to derive a realistic model, consistent for both QE and thermal emittance. Because of its success at explaining the QE of metals, the three-step model combined with the free electron gas theory of metals is used to illustrate the emission process physics.
Elements of the Three-Step Photoemission Model

Step 1: Absorption of photon
Fermi-Dirac distribution at 300 degK

\[ f_{FD}(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}} \]

\[ \phi_{eff} = \phi - \phi_{schottky} \]

Bound electrons

\( E + \hbar \omega \)

E+\hbar\omega

E

E_F

E_F+\phi_{eff}

E_F+\hbar\omega

Fermi-Dirac distribution at 300 degK

Step 2: Transport to surface
Electrons lose energy by scattering, assume e-e scattering dominates, \( F_{e-e} \) is the probability the electron makes it to the surface without scattering

\[ QE(\omega) = (1 - R(\omega)) \]

\[ \int_{E_F-\hbar\omega}^{\infty} dE \frac{N(E + \hbar \omega)(1 - f_{FD}(E + \hbar \omega))N(E)f_{FD}(E)}{E_F + \phi_{eff} - \hbar \omega} \]

\[ \int_{E_F-\hbar\omega}^{\infty} dE \frac{N(E + \hbar \omega)(1 - f_{FD}(E + \hbar \omega))N(E)f_{FD}(E)}{E_F + \phi_{eff} - \hbar \omega} \]

\[ \cos \theta_{max}(E) = \frac{1}{E_F + \phi_{eff} - \hbar \omega} \]

\[ \int_{E_F-\hbar\omega}^{\infty} dE \frac{N(E + \hbar \omega)(1 - f_{FD}(E + \hbar \omega))N(E)f_{FD}(E)}{E_F + \phi_{eff} - \hbar \omega} \]

Step 3: Escape over barrier
Escape criterion:

\[ \frac{p_{normal}^2}{2m} > E_F + \phi_{eff} \]

\[ p_{total} = \sqrt{2m(E + \hbar \omega)} \]

\[ p_{normal} = \sqrt{2m(E + \hbar \omega) \cos \theta} \]

\[ \cos \theta_{max} = \frac{p_{\perp}}{p_{total}} = \sqrt{\frac{E_F + \phi_{eff}}{E + \hbar \omega}} \]
The optical skin depth depends upon wavelength and is given by,

\[ \lambda_{opt} = \frac{\lambda}{4\pi k} \]

where \( k \) is the imaginary part of the complex index of refraction,

\[ \eta = n + ik \]

and \( \lambda \) is the free space photon wavelength.

The reflectivity is given by the Fresnel relation in terms of the real part of the index of refraction,

\[ \text{Reflectivity} = R(n_1(\omega), n_2(\omega), \theta_i) \]

Require knowledge of the complex index of refraction!
**Step 2: Transport to the Surface**

**F\textsubscript{e-e}: Probability electron at depth \(s\), absorbs a photon and escapes without scattering.**

\[
e^{-s/\lambda_{\text{opt}}} e^{-s/\lambda_{e-e}} = e^{-s/\left(\frac{1}{\lambda_{\text{opt}}} + \frac{1}{\lambda_{e-e}}\right)} = e^{-s/\lambda_{\text{eff}}}
\]

\[
P_{\text{excited}}(s) = \int_{0}^{\infty} e^{-s/\lambda_{\text{opt}}} ds = \frac{e^{-s/\lambda_{\text{opt}}}}{\lambda_{\text{opt}}}
\]

\[
F_{e-e} = \int_{0}^{\infty} f(s) ds = \frac{1}{1 + \frac{\lambda_{\text{opt}}}{\lambda_{e-e}}}
\]

Assume the electron-electron scattering length can be averaged over energy:

\[
\bar{\lambda}_{e-e} (\hbar \omega) = \frac{\int_{\phi_{\text{eff}}}^{\hbar \omega} \lambda_{e-e} (E) dE}{\int_{\phi_{\text{eff}}}^{\hbar \omega} dE} = \frac{2 \lambda_{m} E_{m}^{3/2}}{\hbar \omega \sqrt{\phi_{\text{eff}}}} \frac{1}{1 + \sqrt{\frac{\phi_{\text{eff}}}{\hbar \omega}}}
\]

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Krolikowski & Spicer, 1970

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Energy above Fermi Level (eV)

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\(\lambda_{e-e} (E') = \lambda_{e-e} (E_{m}) \left(\frac{E_{m}}{E'}\right)^{3/2}\)

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Models for QE and Thermal Emittance
Step 3: Escape Over the Barrier

Escape criterion: \[
\frac{P_{\text{normal}}^2}{2m} > E_F + \phi_{\text{eff}}
\]

\[
\cos \theta_{\text{max}} = \frac{P_{\text{normal}}}{P_{\text{total}}} = \sqrt{\frac{E_F + \phi_{\text{eff}}}{E + \hbar \omega}}
\]

\[
P_{\text{total}} = \sqrt{2m(E + \hbar \omega)}
\]

\[
P_{\text{normal}} = \sqrt{2m(E + \hbar \omega)} \cos \theta
\]

While photoemission is regarded quantum mechanical effect due to quantization of photons, emission itself is classical. I.e. electrons do not tunnel through barrier, but classically escape over it.
**Derivation of QE**

\[
\text{QE}(\omega) = (1 - R(\omega)) \frac{\int\limits_{E_F + \phi_{\text{eff}} - \hbar \omega}^{\infty} dE \ N(E + \hbar \omega)(1 - f_{FD}(E + \hbar \omega))N(E)f_{FD}(E) \int\limits_{\cos \theta_{\text{max}}(E)}^{1} d(\cos \theta)F_{e-e}(E, \omega, \theta) \int\limits_{0}^{2\pi} d\Phi}{\int\limits_{E_F - \hbar \omega}^{\infty} dE \ N(E + \hbar \omega)(1 - f_{FD}(E + \hbar \omega))N(E)f_{FD}(E) \int\limits_{-1}^{1} d(\cos \theta) \int\limits_{0}^{2\pi} d\Phi}
\]

\[
f_{FD}(E) = \frac{1}{1 + e^{(E-E_F)/k_{B}T}}
\]

Approximate F-D with step function since \(k_{B}T << E_F\)

\[
\text{The QE is then given by:}
\]

\[
\text{QE} \left(\omega\right) = \frac{1 - R(\omega) \left(\frac{E_F + \hbar \omega}{2\hbar \omega}\right)}{1 + \left(\frac{\phi_{\text{eff}}}{2\hbar \omega}\right)^{3/2}} \left[1 + \left(\frac{E_F + \hbar \omega}{E_F + \phi_{\text{eff}} - 2}\right)^{1/2} \frac{E_F + \phi_{\text{eff}}}{E_F + \hbar \omega}\right]^{-1}
\]
Measurement of the QE vs. wavelength during H-ion cleaning of copper

![Diagram of experimental setup]

- H-Ion Gun
- Micro-Leak Valve
- H-Gas Supply
- Cu Sample
- 18 Volts
- Current Meter
- Broad-Band Lamp & Scanning Monochromator
- H-Gas Supply
- H-Ion Gun Power Supply

Graph showing QE vs. wavelength for different charge values:
- initial
- 0.63mC
- 2.07mC
- 3.03mC
- 10.23mC
Fowler Plots used to determine work function

\[
\ln \left( \frac{QE}{T^2} \right) = B + \ln \left( f \left( \frac{\hbar \omega - \phi}{k_B T} \right) \right)
\]

where \( T \) is the electron temperature (assumed to be 300 degK), \( k_B \) is Boltzman’s constant, \( \hbar \omega \) is the photon energy, and \( \phi \) is the work function. \( B \) is a constant related to the electron density of states, the optical reflectivity and electron transport to the surface. The function \( f(x) \) results from integrals of the Fermi-Dirac function.

\[
f(x) = e^{x} - \frac{e^{2x}}{2} - \frac{e^{3x}}{6} - \ldots \quad \text{for } x \leq 0
\]

\[
f(x) = \frac{\pi^2}{6} + \frac{x^2}{2} - \left( e^{x} - \frac{e^{2x}}{2} - \frac{e^{3x}}{6} - \ldots \right) \quad \text{for } x \geq 0
\]

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Models for QE and Thermal Emittance

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Stanford Linear Accelerator Center
Comparison with Experimental QE for Copper

![Graph showing Quantum Efficiency vs. Wavelength]

<table>
<thead>
<tr>
<th>Fermi Energy</th>
<th>7eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Work Function</td>
<td>4.31eV</td>
</tr>
<tr>
<td>$\phi_{\text{schottky}}$ @50MV/m</td>
<td>0.268eV</td>
</tr>
<tr>
<td>e-e scattering length @8.6eV</td>
<td>22 angstroms</td>
</tr>
</tbody>
</table>
Some comments on QE and “Thermal” Emittance

So for metals there is excellent agreement between the free electron gas model and experiment, but what about the thermal emittance?

The QE and the thermal emittance are connected and are given by a common, consistent theory.

But the problem is both theoretical and experimental:
   No combined QE and thermal emittance measurements.
   Techniques for these measurements now exist!
   No QE vs. wavelength at high field to verify the QE theory!
   Measure QE in RF gun at 3-laser wavelengths?

*Since there is no “temperature” for photoemission at ambient temperatures, the emittance isn’t really “thermal”. It should be called “photoelectric emittance” instead.
Definition of the Photoelectric Emittance

The normalized rms transverse emittance in trace-coordinates is defined without any correlation [Lawson, “The Physics of Beams”] as

\[ \varepsilon_N = \beta \gamma \sigma_x \sigma_{x^\prime} \]

\[ \sigma_{x^\prime} = \frac{\sigma_{p_x}}{p_{total}} = \frac{\sqrt{\left\langle p_x^2 \right\rangle}}{\beta \gamma mc} \]

\[ \varepsilon_N = \sigma_x \frac{\sqrt{\left\langle p_x^2 \right\rangle}}{mc} = \frac{R_{cathode}}{2} \frac{\sqrt{\left\langle p_x^2 \right\rangle}}{mc} \]

For a uniform radial distribution of radius \( R_{cathode} \):

\[ \sigma_x = \frac{R_{cathode}}{2} \]

\[ \left\langle p_x^2 \right\rangle = \frac{\iiint g(E, \theta, \varphi) p_x^2 dE d(\cos \theta) d\varphi}{\iiint g(E, \theta, \varphi) dE d(\cos \theta) d\varphi} \]

Where \( g(E, \theta, \varphi) \) is the electron distribution function at the cathode surface.
Derivation of the Photoelectric Emittance

The rms transverse momentum can be computed from the three-step model of photoemission in a manner similar to the quantum efficiency.

\[ p_x = \sqrt{2m(E + \hbar \omega)} \sin \theta \cos \varphi \]

\[ E = \frac{p_{total}^2}{2m} \]

\[
\begin{align*}
\langle p_x^2 \rangle &= \int_{E_F - \hbar \omega}^{\infty} dE \ N(E + \hbar \omega)(1 - f_{FD}(E + \hbar \omega))N(E)f_{FD}(E) \\
&\quad \times \left( \int_{0}^{1} d(\cos \varphi) \right) \left( \int_{0}^{2\pi} d\varphi \right) \frac{p_x^2}{p_{total}}
\end{align*}
\]

\[
\begin{align*}
\langle p_{p}^2 \rangle &= \frac{2m}{E_{F} + \phi_{eff} - \hbar \omega} \int_{E_{F}}^{E_{F} + \phi_{eff} - \hbar \omega} dE \ \int_{0}^{2\pi} d(\cos \theta) \sin^2 \theta \cos^2 \varphi \\
&\quad \times \left( \int_{0}^{1} d(\cos \theta) \right) \left( \int_{0}^{2\pi} d\varphi \right) \cos \theta_{max}
\end{align*}
\]

\[ E_N = R_{cathode} \sqrt{\frac{E_F + \hbar \omega}{12mc^2} \left[ \frac{1 - 2r^{1/2} + 2r^{3/2} - r^2}{1 - 2r^{1/2} + r} \right]^{1/2}} \]

\[ r = \frac{E_F + \phi_{eff}}{E_F + \hbar \omega} \]

\[ \phi_{eff} = \phi - \phi_{schottky} \]
Affect of External Field on Photoelectric Emittance

The Schottky Effect

\[ \varepsilon_N = R_{\text{cathode}} \sqrt{\frac{E_F + \hbar \omega}{12mc^2} \left[ 1 - 2r^{1/2} + 2r^{3/2} - r^2 \right]}^{1/2} \]

\[ \varepsilon_N = \sigma \sqrt{\frac{\hbar \omega - \phi_{\text{eff}}}{3mc^2}} = \frac{R_{\text{cathode}}}{2} \sqrt{\frac{\hbar \omega - \phi_{\text{eff}}}{3mc^2}} \]

For copper:

\[ \phi_{\text{eff}} = \phi - \phi_{\text{schottky}} \]

\[ \phi_{\text{schottky}} = 3.7947 \times 10^{-5} \sqrt{E(V/m)} \text{ eV} \]
Electron Kinematics at the Surface for Free Electron Gas Model

\[ \frac{p_{z,in}^2}{2m} \geq E_F + \phi \quad p_{z,in} \geq \sqrt{2m(E_F + \phi)} \]
\[ p_{total,in} = \sqrt{2m(E + \hbar \omega)} \quad p_{total,out} = \sqrt{2m(E + \hbar \omega - E_F - \phi)} \]
\[ p_{x,in} = p_{x,out} \]
\[ p_{x,in} = p_{total,in} \sin \theta_{in} = p_{total,out} \sin \theta_{out} = p_{x,out} \]
\[ \sin \theta_{out} = \frac{E + \hbar \omega}{\sqrt{E + \hbar \omega - E_F - \phi}} \]

Therefore, the electrons are refracted at the surface.

On the metal side, the maximum angle of emission is

\[ p_z = \sqrt{2m(E + \hbar \omega) \cos \theta_{in}} \geq \sqrt{2m(E_F + \phi)} \]

\[ \cos \theta_{max,in} = \frac{E_F + \phi}{\sqrt{E + \hbar \omega}} \quad \sin \theta_{max,in} = \frac{E + \hbar \omega - E_F - \phi}{\sqrt{E + \hbar \omega}} \]

On vacuum side, the maximum angle is:

\[ \sin \theta_{max,out} = \sin \theta_{max,in} \frac{E + \hbar \omega}{\sqrt{E + \hbar \omega - E_F - \phi}} = 1 \quad \Rightarrow \quad \theta_{max,out} = 90\text{deg} \]

*Maximum external angle of emission is 90deg, corresponding to total internal reflection.
Initial Distributions for Simulation Codes

Therefore electron energy and angular distribution at the cathode surface can be computed and used for the initial conditions in simulation codes. In the case of the noble metals, this model provides nearly first-principle, physically realistic distributions.

Here the free electron gas distribution is compared with an initial distribution commonly used in simulation codes such as General Particle Tracer (GPT).

Simulation codes assume all the electrons have the same energy, $E$, and the electrons are uniformly emitted in the two cylindrical angles $\theta$ and $\Phi$. Or to be precise,

\[ \theta \text{ is uniform on the interval } [0, \frac{\pi}{2}] \]
\[ \Phi \text{ is uniform on the interval } [0, 2\pi] \]
\[ \beta = \sqrt{\frac{2E}{mc^2}} ; \quad \beta_x = \beta \sin \theta \cos \Phi ; \quad \beta_z = \beta \cos \theta ; \quad \beta_{xy} = \beta \sin \theta \]
Initial distributions based on 3-step model using free-electron gas for the EDOS
Escaping Electron Energy Distribution
Models for QE and Thermal Emittance

Internal Energy

External Energy

Internal Angle (deg)

External Angle (deg)

Internal beta

External beta
Fermi-Dirac distribution energy-angle scatter plots

Incident Electrons

Emitted Electrons
Fermi Gas Angular Distribution

Simulation Angular Distribution, e.g. GPT
Comparison of energy-angle scatter plots

Fermi-Dirac

GPT

at fixed azimuth angle, $\phi$
Comparison with Typical Simulation Distribution

\[ \theta \text{ is uniform on the interval } \left[ 0, \frac{\pi}{2} \right] \]
\[ \Phi \text{ is uniform on the interval } \left[ 0, 2\pi \right] \]

\[ \beta = \sqrt{\frac{2E}{mc^2}} \; ; \; \beta_x = \beta \sin \theta \cos \Phi \; ; \; \beta_z = \beta \cos \theta \]

Work in progress to compare distributions using GPT

\[ \theta, \beta, \Phi \]
\[ \pi \; \pi \]
\[ \cos \theta \; \cos \sin \theta \; \cos \theta \]
\[ \cos \Phi \; \cos \theta \; \cos \theta \]
Summary:

- Apply surface science physics to electron simulations and use to motivate cathode R&D
- Future work will compare simulations for F-D and uniform distributions
- Optical parameters are essential for calculations, esp. the complex index of refraction
- Experiments are needed to confirm distributions:
  - PEEM etc.
- Begin investigating other cathode types: semi-conductor, diamond-amplified, meta-materials etc.
- Experimental and theory should be developed together
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And a Final Comment:
Fabrication of S1-cathode over a structured substrate

Need to study:
1. Compatibility with copper or other metallic substrate
2. Vacuum requirements and long term stability: Approach for installation in gun
4. Temporal response