Supporting Information for
Monochromatic X-ray source based on scattering from a magnetic nanoundulator

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Contents

Figures

I. DERIVATION OF THE SPECTRAL ANGULAR POWER OF EMITTED RADIATION FROM A SINGLE ELECTRON

We derive an analytical expression of the spectral angular power of emitted radiation for the setup shown in Fig. 1a (main text). We consider the interaction of a single electron launched parallel to the nanograting with velocity $\mathbf{v} = v\hat{z}$. The magnetic near-field generated by the nanograting has two nonzero components, B_z and B_x. We assume that the electron is launched sufficiently close to the surface of the nanograting such that the fields are periodic with the nanograting period d. Further, we assume that the electron's transverse velocity oscillations are small enough such that γ and β are approximately constant, i.e. $\dot{z} \approx v$ and $z \approx vt + z_0$. The result is that the forces on the electron due to B_z are small, and B_z can be ignored for the purpose of the derivation. Since B_x is periodic, we Fourier expand the field as $\mathbf{B}(x,y,z) = \sum_n B_n \sin\left(\frac{2\pi z}{d_n}\right)\hat{x}$, where B_n is the amplitude and $d_n = d/n$ is the period of the n-th Fourier component of B_x.

The general formula for the spectral angular distribution of the energy radiated by an electron is

$$\frac{\mathrm{d}^2 W}{\mathrm{d}\Omega \mathrm{d}\omega} = 2\varepsilon_0 c R^2 |\mathbf{E}(\omega)|^2, \tag{1}$$

where $\frac{\mathrm{d}^2 W}{\mathrm{d}\Omega \mathrm{d}\omega}$ is the energy radiated by an electron per unit solid angle $\mathrm{d}\Omega$ per unit angular frequency $\mathrm{d}\omega$, R is the distance from the electron to the observer, and $\mathbf{E}(\omega)$ is the frequency spectrum of the electric field at the observer[1]. Considering that the far field $\mathbf{E}(\omega)$ is given by

$$\mathbf{E}(\omega) = \frac{ie\omega}{4\pi\sqrt{2\pi} c\varepsilon_0 R} \int_{-\infty}^{\infty} (\mathbf{n} \times (\mathbf{n} \times \boldsymbol{\beta})) e^{i\omega(t' + \frac{R(t')}{c})} \mathrm{d}t', \tag{2}$$

where $\mathbf{n} = \frac{\mathbf{R}}{R}$ is the unit vector pointing from the electron to the observer and $\boldsymbol{\beta} = \frac{\mathbf{v}}{c}$ is the electron velocity relative to the speed of light[1], we thus have

$$\frac{\mathrm{d}^2 W}{\mathrm{d}\Omega \mathrm{d}\omega} = \frac{e^2\omega^2}{16\pi^3 c\varepsilon_0} \left| \int_{-\infty}^{\infty} (\mathbf{n} \times (\mathbf{n} \times \boldsymbol{\beta})) e^{i\omega(t' + \frac{R(t')}{c})} \mathrm{d}t' \right|^2. \tag{3}$$

Using the fact that $\mathbf{R}(t') = \mathbf{x} - \mathbf{r}(t')$, where $\mathbf{x}$ is the observer's position from the origin and $\mathbf{r}(t')$ is the electron's position from the origin, we can rewrite the term in the exponent of Eq. 3 as

$$t' + \frac{R(t')}{c} = t' + \frac{\mathbf{n}\cdot\mathbf{x}}{c} - \frac{\mathbf{n}\cdot\mathbf{r}}{c}. \tag{4}$$

Since $\mathbf{x}$ is fixed, we can ignore the $\frac{\mathbf{n}\cdot\mathbf{x}}{c}$ term, since this becomes an overall phase shift in Eq. 3. We now have

$$\frac{\mathrm{d}^2 W}{\mathrm{d}\Omega \mathrm{d}\omega} = \frac{e^2\omega^2}{16\pi^3 c\varepsilon_0} \left| \int_{-T/2}^{T/2} (\mathbf{n} \times (\mathbf{n} \times \boldsymbol{\beta})) e^{i\omega(t' - \frac{\mathbf{n}\cdot\mathbf{r}}{c})} \mathrm{d}t' \right|^2, \tag{5}$$

where we have replaced the integration limits $-\infty$ to ∞ with $-T/2$ to $T/2$, where $T = \frac{Nd}{v}$ is the electron's total interaction time with the nanograting and N is the number of periods in the nanograting. We proceed by deriving expressions for $\mathbf{r}$ and $\boldsymbol{\beta}$ using the relativistic Lorentz force law $\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$, where $\mathbf{p} = \gamma m \mathbf{v}$. Then the equations of motion for the electron are

$$\ddot{x} = \frac{-e}{\gamma m}(\dot{y}B_z - \dot{z}B_y) = 0, \tag{6}$$

$$\ddot{y} = \frac{-e}{\gamma m}(\dot{z}B_x - \dot{x}B_z) = -\frac{ev}{\gamma m}\sum_{n=1}^{\ell} B_n \sin\left(\frac{2\pi z}{d_n}\right) = -\sum_{n=1}^{\ell} \frac{evB_n}{\gamma m} \sin\left(\frac{2\pi vt}{d_n}\right). \tag{7}$$

Integrating the equation for $\ddot{y}$, we find

$$\dot{y} = \sum_{n=1}^{\ell} \frac{eB_n d_n}{2\pi\gamma m} \cos\left(\frac{2\pi z}{d_n}\right) = \sum_{n=1}^{\ell} \frac{K_n c}{\gamma} \cos(W_n t), \tag{8}$$

$$y = \sum_{n=1}^{\ell} \frac{K_n c}{\gamma W_n} \sin(W_n t), \tag{9}$$

where $K_n = \frac{eB_nd_n}{2\pi mc}$ is the magnetic deflection parameter and $W_n = \frac{2\pi\beta c}{d_n}$ the angular frequency of oscillation due to the n-th Fourier component. We can now write the expressions for $\mathbf{n}$, $\mathbf{r}$, and $\boldsymbol{\beta}$ (assuming that $\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}t} = 0$, which is true in the far field case):

$$\mathbf{n} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}, \quad \mathbf{r} = \begin{pmatrix} 0 \\ \sum\limits_{n=1}^{\ell} \frac{K_n c}{\gamma W_n}\sin(W_n t) \\ \beta c t \end{pmatrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} 0 \\ \sum\limits_{n=1}^{\ell} \frac{K_n}{\gamma}\cos(W_n t) \\ \beta \end{pmatrix}. \tag{10}$$

We then have

$$\begin{aligned} \mathbf{n}\times(\mathbf{n}\times\boldsymbol{\beta}) &= \begin{pmatrix} \beta\sin\theta\cos\theta\cos\phi \\ \beta\sin\theta\sin\phi\cos\theta \\ -\beta\sin^2\theta \end{pmatrix} + \frac{1}{\gamma}\begin{pmatrix} \sin^2\theta\sin\phi\cos\phi \\ -\sin^2\theta\cos^2\phi - \cos^2\theta \\ \sin\theta\sin\phi\cos\theta \end{pmatrix}\sum_{n=1}^{\ell} K_n\cos(W_n t) \\ &= \mathbf{A} + \mathbf{B}\sum_{n=1}^{\ell} K_n\cos(W_n t), \end{aligned} \tag{11}$$

where we have separated the vector into time-independent and time-dependent components due to the factors of $\cos(W_n t)$. For the phase in Eq. 5 we have

$$t - \frac{\mathbf{n}\cdot\mathbf{r}}{c} = (1-\beta\cos\theta)t - \frac{\sin\theta\sin\phi}{\gamma}\sum_{n=1}^{\ell}\frac{K_n\sin(W_n t)}{W_n}. \tag{12}$$

Eq. 5 now becomes

$$\begin{aligned} \frac{\mathrm{d}^2W}{\mathrm{d}\Omega\mathrm{d}\omega} &= \frac{e^2\omega^2}{16\pi^3 c\varepsilon_0}\left|\int_{-T/2}^{T/2}(\mathbf{A}+\mathbf{B}\sum_{n=1}^{\ell}K_n\cos(W_n t))\exp\left[i\omega(1-\beta\cos\theta)t - \sum_{m=1}^{\ell}\frac{i\omega\sin\theta\sin\phi K_m\sin(W_m t)}{\gamma W_m}\right]\mathrm{d}t\right|^2 \\ &= \frac{e^2\omega^2}{16\pi^3 c\varepsilon_0}\left|\int_{-T/2}^{T/2}(\mathbf{A}+\mathbf{B}\sum_{n=1}^{\ell}K_n\cos(W_n t))\exp\left[i\omega(1-\beta\cos\theta)t + \sum_{m=1}^{\ell}i\xi_m\sin(W_m t)\right]\mathrm{d}t\right|^2, \end{aligned} \tag{13}$$

where $\xi_m = \frac{-K_m\omega\sin\theta\sin\phi}{W_m\gamma}$ is the amplitude of oscillation in the y direction normalized to the y component of the wave vector $k_y = \frac{\omega\sin\theta\sin\phi}{c}$. For the dimensions of interest, ξ_m and K_m are small, and we proceed by approximating $\exp\left[\sum\limits_{m=1}^{\ell} i\xi_m\sin(W_m t)\right]$ as $1+\sum\limits_{m=1}^{\ell} i\xi_m\sin(W_m t)$ and by dropping terms of order K_nK_m. We have

$$\begin{aligned} &\frac{e^2\omega^2}{16\pi^3 c\varepsilon_0}\left|\int_{-T/2}^{T/2}(\mathbf{A}+\mathbf{B}\sum_{n=1}^{\ell}K_n\cos(W_n t))e^{i\omega(1-\beta\cos\theta)t}\left(1+\sum_{m=1}^{\ell}i\xi_m\sin(W_m t)\right)\mathrm{d}t\right|^2 \\ &= \frac{e^2\omega^2}{16\pi^3 c\varepsilon_0}\left|\int_{-T/2}^{T/2}\mathbf{A}e^{i\omega(1-\beta\cos\theta)t}\mathrm{d}t + \sum_{n=1}^{\ell}\int_{-T/2}^{T/2}\mathbf{B}K_n\cos(W_n t)e^{i\omega(1-\beta\cos\theta)t}\mathrm{d}t\right. \\ &\qquad\left. + \sum_{m=1}^{\ell}\int_{-T/2}^{T/2}i\mathbf{A}\xi_m\sin(W_m t)e^{i\omega(1-\beta\cos\theta)t}\mathrm{d}t + \sum_{n,m=1}^{\ell}\mathcal{O}(K_nK_m)\right|^2. \end{aligned} \tag{14}$$

The first term of the expression does not contribute radiation and can be dropped. To see this, we can directly evaluate the integral and consider the limit as the interaction time $T\to\infty$:

$$\begin{aligned} &\lim_{T\to\infty}\int_{-T/2}^{T/2}e^{i\omega(1-\beta\cos\theta)t}\mathrm{d}t \\ &= \lim_{T\to\infty}T\,\mathrm{sinc}\left(\frac{T\omega(1-\beta\cos\theta)}{2}\right) \\ &= \delta\left(\frac{\omega(1-\beta\cos\theta)}{2}\right). \end{aligned} \tag{15}$$

The result is a delta function which only has a nonzero contribution at $\omega = 0$, and the term contributes no radiation. For the remaining terms, we expand $\cos(W_n t)$ and $\sin(W_m t)$ in terms of complex exponentials. We have

$$\frac{e^2\omega^2}{16\pi^3 c\varepsilon_0}\left|\frac{1}{2}\sum_{n=1}^{\ell}\int_{-T/2}^{T/2}\Big[\mathbf{B}K_n(e^{it[\omega(1-\beta\cos\theta)+W_n]}+e^{it[\omega(1-\beta\cos\theta)-W_n]}) + \mathbf{A}\xi_n(e^{it[\omega(1-\beta\cos\theta)+W_n]}-e^{it[\omega(1-\beta\cos\theta)-W_n]})\Big]\mathrm{d}t\right|^2. \tag{16}$$

Any terms containing exponentials of the form $e^{it[\omega(1-\beta\cos\theta)+W_n]}$ do not contribute radiation and can be dropped. To see this, we again directly evaluate the integral of the exponential and take the limit as $T \to \infty$:

$$\lim_{T\to\infty}\int_{-T/2}^{T/2} e^{it[\omega(1-\beta\cos\theta)+W_n]}\mathrm{d}t = \delta\bigg(\frac{\omega(1-\beta\cos\theta)+W_n}{2}\bigg). \tag{17}$$

The delta function is only nonzero for negative ω and thus has no contribution to the single-sided spectrum. Finally, we simplify the expression by evaluating the remaining integrals, which leaves us with

$$\frac{\mathrm{d}^2W}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{e^2\omega^2T^2}{64\pi^3c\varepsilon_0}\left|\sum_{n=1}^{\ell}(\mathbf{B}K_n - \mathbf{A}\xi_n)\,\mathrm{sinc}\left(\frac{T[\omega(1-\beta\cos\theta)-W_n]}{2}\right)\right|^2, \tag{18}$$

where we have simplified Eq. 5 to this form. Dividing Eq. 18 by T yields the final form for the spectral angular distribution of the power radiated by an electron:

$$\boxed{\frac{\mathrm{d}^2P}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{e^2\omega^2T}{64\pi^3c\varepsilon_0}\left|\sum_{n=1}^{\ell}(\mathbf{B}K_n - \mathbf{A}\xi_n)\,\mathrm{sinc}\left(\frac{T[\omega(1-\beta\cos\theta)-W_n]}{2}\right)\right|^2.} \tag{19}$$

II. SPECTRAL ANGULAR POWER OF EMITTED RADIATION FROM A BUNCHED ELECTRON BEAM

The radiation power of the source can be enhanced by using a bunched electron beam. Here we consider the interaction of a bunched electron beam with the nanograting, where the beam is sent parallel to the nanograting with uniform initial velocity $\mathbf{v} = v\hat{z}$. We consider a beam which is one electron thick, consisting of M electrons which are equally spaced along z by a distance Δz. The spectral angular power of radiation is then given by

$$\frac{\mathrm{d}^2P_{\text{tot}}}{\mathrm{d}\Omega\mathrm{d}\omega} = M[1+(M-1)\left|f\right|^2]\frac{\mathrm{d}^2P_{\text{sing}}}{\mathrm{d}\Omega\mathrm{d}\omega}], \tag{20}$$

where

$$f = \frac{1}{Q}\int\rho(\mathbf{r})\exp(\mathbf{k}\cdot\mathbf{r})\mathrm{d}\mathbf{r}. \tag{21}$$

Here $\frac{\mathrm{d}^2P_{\text{sing}}}{\mathrm{d}\Omega\mathrm{d}\omega}$ is the spectral angular radiation power due to a single electron (given by Eq. 19), f is the Fourier transform of the charge distribution $\rho(\mathbf{r})$, Q is the total charge, and $\mathbf{k}$ is the wave vector for the radiation[2]. In this case, $\rho(\mathbf{r}) = \sum_{n=0}^{M-1} -e\delta(z-n\Delta z)$, and $Q = -Me$. Then for $\left|f\right|^2$ we have

$$\begin{aligned}\left|f\right|^2 &= \left|\frac{1}{-Me}\int\sum_{n=0}^{M-1}-e\delta(z-n\Delta z)\exp(ik_zz)\mathrm{d}z\right|^2 \\ &= \left|\frac{1}{M}\sum_{n=0}^{M-1}\exp\bigg(\frac{i\omega\cos(\theta)n\Delta z}{c}\bigg)\right|^2 \\ &= \frac{1}{M^2}\frac{\sin^2\left(\frac{M\omega\cos(\theta)\Delta z}{2c}\right)}{\sin^2\left(\frac{\omega\cos(\theta)\Delta z}{2c}\right)}.\end{aligned} \tag{22}$$

The power spectrum due to $\frac{\mathrm{d}^2 P_{\mathrm{sing}}}{\mathrm{d}\Omega \mathrm{d}\omega}$ will be enhanced whenever the bunching resonant enhancement condition $|f|^2 = 1$ holds, which occurs when $\omega \cos\theta = \frac{2cm\pi}{\Delta z}$ for integers m. Finally, $\frac{\mathrm{d}^2 P_{\mathrm{tot}}}{\mathrm{d}\Omega \mathrm{d}\omega}$ can be written as

$$\boxed{\frac{\mathrm{d}^2 P_{\mathrm{tot}}}{\mathrm{d}\Omega \mathrm{d}\omega} = \left[M + \left(\frac{M-1}{M}\right) \frac{\sin^2\left(\frac{M\omega\cos(\theta)\Delta z}{2c}\right)}{\sin^2\left(\frac{\omega\cos(\theta)\Delta z}{2c}\right)}\right] \frac{\mathrm{d}^2 P_{\mathrm{sing}}}{\mathrm{d}\Omega \mathrm{d}\omega}.} \tag{23}$$

III. RADIATION DUE TO BREHMSSTRAHLUNG

In addition to inverse-Compton radiation, we expect that bremsstrahlung radiation will be prevalent in our system due to free electrons colliding with the sample. Here, we estimate the power of bremsstrahlung radiation due to a single electron and compare it to the power of inverse-Compton radiation. We use the parameters of the reference nanograting used throughout the main text, where $\mu = 1.4 \times 10^6$A/m, $d = 150$ nm, $a = 110$ nm, $h = 40$ nm and $N = 31^3$. The ferromagnetic material of the nanograting is composed of $Fe_{81}Ga_{19}$, and the substrate is GaAs. We take the substrate thickness to be on the order of $1\,\mu\mathrm{m}$, which is much larger than the ferromagnetic material height. In this case, we expect most of the energy loss due to bremsstrahlung radiation to come from the substrate material.

Here we estimate the power of bremsstrahlung radiation due to a single electron with a kinetic energy of 5 MeV colliding with the sample. The radiative stopping power for a 5 MeV electron in GaAs is 2.704×10^{-1} MeV cm^2 g^{-1}[4]. Multiplying this value by the density of GaAs (5.31 g cm^{-3}[4]) and the velocity of the electron ($v \approx c$) yields the approximate energy loss per second of the electron. Since the spectral width of bremsstrahlung radiation is approximately equal to the electron's kinetic energy[5], we can estimate the power per unit angular frequency of bremsstrahlung by dividing the energy loss per second by the electron's kinetic energy. Then the power per unit angular frequency of bremsstrahlung is approximately 1.38×10^{-9} W eV^{-1}. The power per unit angular frequency per unit solid angle of bremsstrahlung is given by the power per unit angular frequency divided by 4π, which is 1.10×10^{-10} W eV^{-1} sr^{-1}.

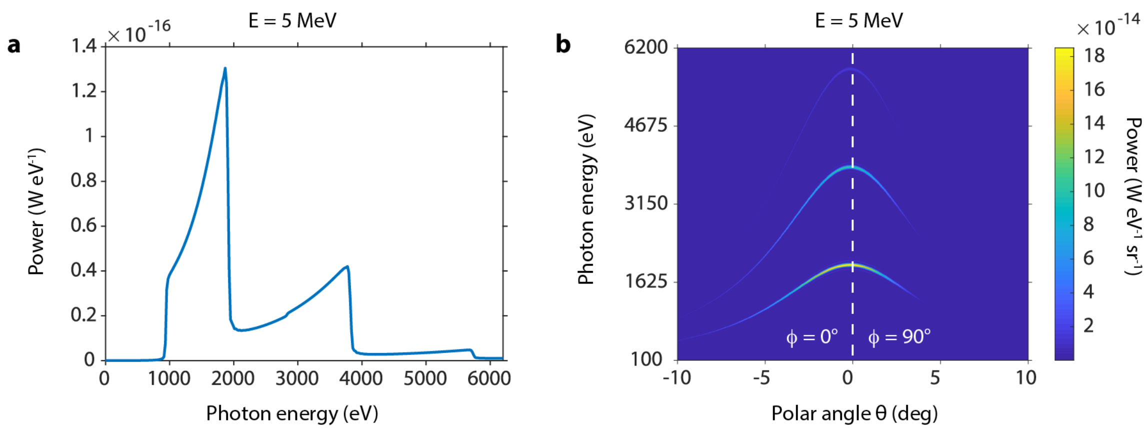

FIG. S1. **Inverse-Compton power spectra due to a single electron with a kinetic energy of 5 MeV. a**, Analytical results of the spectral radiation power integrated over all solids angles from a single electron, in units of W eV^{-1}. **b**, Analytical results of the spectral angular radiation power from a single electron, in units of W eV^{-1} sr^{-1}.

We now compare the power of bremsstrahlung radiation estimated above to that of inverse-Compton radiation. We calculate the inverse-Compton radiation using the analytical formula in Eq. 2 of the main text. The calculation is carried out using the parameters of the reference nanograting and an electron with a kinetic energy of 5 MeV, launched in the z direction with initial height $x_0 = 1$ nm above the nanograting surface. In Fig. S1a, we plot the power per unit angular frequency (W eV^{-1}) of inverse-Compton radiation integrated over all solid angles. The spectrum peaks at photon energies of 1.87 keV and 3.77 keV, with powers of 1.31×10^{-16} W eV^{-1} and 4.21×10^{-17} W eV^{-1} respectively. In Fig. S1b, we plot the power per unit angular frequency per unit solid angle (W eV^{-1} sr^{-1}) of inverse-Compton radiation (Fig. 2d in the main text). The angular spectrum peaks at photon energies of 1.91 keV and 3.82 keV, with powers of 1.82×10^{-13} W eV^{-1} sr^{-1} and 1.07×10^{-13} W eV^{-1} sr^{-1}.

Although bremsstrahlung results in a broad frequency spectrum, the energy transfer from electrons to photons in bremsstrahlung is more efficient than in inverse-Compton scattering. By the above calculations, the power of bremsstrahlung integrated over all solid angles is at least seven orders of magnitude larger than the peak powers of inverse-Compton radiation integrated over all solid angles. However, since inverse-Compton is more directional than bremsstrahlung, the power per unit solid angle of bremsstrahlung is only three orders of magnitude larger than that of inverse-Compton. Therefore, it is critical that bremsstrahlung is minimized in the system as much as possible. The experimental setup should be chosen such that the electron beam collides minimally with the sample. For an electron beam with a conical profile, the setup should be arranged similarly to Fig. 3b in the main text. In choosing the initial height of the electron beam, there will be a tradeoff between bremsstrahlung and inverse-Compton radiation: lowering the initial height allows electrons to interact closer to the nanograting surface which enhances inverse-Compton, but it also increases the chance that electrons collide with the nanograting which enhances bremsstrahlung. Other ways to lessen the effects of bremsstrahlung include minimizing the thickness of the substrate and choosing substrate materials with smaller radiative stopping powers, since the spectral power is approximately proportional to the radiative stopping power. Finally, inverse-Compton radiation can be enhanced by increasing the length of the nanograting along z, since the power of inverse-Compton scales with the electron interaction time (Eq. 2 in the main text), and bunching the electron beam, as detailed in the main text.

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