HW #10

1. Neutrino Oscillation

(a) Time evolution operator

$$e^{-i H t/\hbar} = \sum_k \frac{(-i\, t/\hbar)^k}{k!} H^k = \sum_k \frac{(-i\, t/\hbar)^k}{k!} (U E U^\dagger)^k$$

where E is the diagonal matrix of Hamiltonian eigenvalues E_n given in Eq. 1. Expanding a bit further,

$$e^{-i H t/\hbar} = \sum_k \frac{(-i\, t/\hbar)^k}{k!} (U E U^\dagger) \cdot (U E U^\dagger) \cdot \ldots. \cdot (U E U^\dagger) \cdot (U E U^\dagger)_k \,.$$

We see that apart from the ends, every $U^\dagger$ has a U to the right of it. A matrix is unitary if $U^\dagger = U^{-1}$ and $(U^\dagger)^\dagger = U$, so the expression simplifies to

$$e^{-i H t/\hbar} = U\left(\sum_k \frac{(-i\, t/\hbar)^k}{k!} E^n\right) U^\dagger = U e^{-i E t/\hbar} U^\dagger$$

$$\Longrightarrow e^{-i H t/\hbar} = U \begin{pmatrix} e^{-i E_1\, t/\hbar} & 0 & \cdots & 0 \\ 0 & e^{-i E_2\, t/\hbar} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{-i E_n\, t/\hbar} \end{pmatrix} U^\dagger$$

by the properties of matrix multiplication.

(b) Two−state transition probabilities

The probabilities are

$$P(1 \to 2) = |\langle 2 | e^{-i H t/\hbar} | 1 \rangle|^2 = |\langle 2 | U e^{-i E t/\hbar} U^\dagger | 1 \rangle|^2$$

$$P(2 \to 1) = |\langle 1 | U e^{-i E t/\hbar} U^\dagger | 2 \rangle|^2 \,.$$

We will demonstrate that there is no T−violation by showing $P(1 \to 2) - P(2 \to 1) = 0$. Let us have *Mathematica* do the work:

```
U2m = E^(I θ) ( Cos[θ] E^(I ϕ)    -Sin[θ] E^(I η)
                Sin[θ] E^(-I η)   Cos[θ] E^(-I ϕ) );
E2m = ( E1  0
        0   E2 );
amp212 = ( 0  1 ).U2m.MatrixExp[-I E2m t / ℏ].Transpose[Conjugate[U2m]].( 1
                                                                         0 );
p212 = ComplexExpand[Conjugate[amp212] * amp212];
amp221 = ( 1  0 ).U2m.MatrixExp[-I E2m t / ℏ].Transpose[Conjugate[U2m]].( 0
                                                                         1 );
p221 = ComplexExpand[Conjugate[amp221] * amp221];
TrigExpand[p212 - p221][[1, 1]]
```

```
0
```

(c) Three−state problem

Let us proceed in similar fashion as in the two−state problem above:

```
U3m = ( 1   0           0
        0   Cos[θ23]    Sin[θ23]
        0   -Sin[θ23]   Cos[θ23] ).
  ( Cos[θ13]            0   Sin[θ13] E^(-I δ)
    0                   1   0
    -Sin[θ13] E^(I δ)   0   Cos[θ13] ).( Cos[θ12]    Sin[θ12]   0
                                          -Sin[θ12]   Cos[θ12]   0
                                          0           0          1 );
E3m = ( E1  0   0
        0   E2  0
        0   0   E3 );
amp312 = ( 0  1  0 ).U3m.MatrixExp[-I E3m t / ℏ].Transpose[Conjugate[U3m]].( 1
                                                                            0
                                                                            0 );
p312 = ComplexExpand[Conjugate[amp312] * amp312];
amp321 = ( 1  0  0 ).U3m.MatrixExp[-I E3m t / ℏ].Transpose[Conjugate[U3m]].( 0
                                                                            1
                                                                            0 );
p321 = ComplexExpand[Conjugate[amp321] * amp321];
Simplify[TrigExpand[p312 - p321]][[1, 1]]
```

$$-4\,\mathrm{Cos}[\theta13]^2\,\mathrm{Sin}\left[\frac{(E1-E2)\,t}{2\,\hbar}\right]\mathrm{Sin}\left[\frac{(E1-E3)\,t}{2\,\hbar}\right]\mathrm{Sin}\left[\frac{(E2-E3)\,t}{2\,\hbar}\right]\mathrm{Sin}[\delta]\,\mathrm{Sin}[2\,\theta12]\,\mathrm{Sin}[\theta13]\,\mathrm{Sin}[2\,\theta23]$$

Indeed, when $\delta \neq 0$, the two probabilities are different.

(d) [optional] CPT conservation

Again as above, substituting $U \to U^*$:

```
amp3c12 = ( 0  1  0 ).Conjugate[U3m].MatrixExp[-I E3m t / ℏ].Transpose[U3m].(1, 0, 0);
p3c12 = ComplexExpand[Conjugate[amp3c12] * amp3c12];
amp3c21 = ( 1  0  0 ).Conjugate[U3m].MatrixExp[-I E3m t / ℏ].Transpose[U3m].(0, 1, 0);
p3c21 = ComplexExpand[Conjugate[amp3c21] * amp3c21];
```

$P(1 \to 2) - P(\bar{1} \to \bar{2})$:

```
Simplify[TrigExpand[p312 - p3c12]][[1, 1]]
```

$$-4\, \mathrm{Cos}[\theta 13]^2\, \mathrm{Sin}\left[\frac{(E1 - E2)\, t}{2\, \hbar}\right] \mathrm{Sin}\left[\frac{(E1 - E3)\, t}{2\, \hbar}\right] \mathrm{Sin}\left[\frac{(E2 - E3)\, t}{2\, \hbar}\right] \mathrm{Sin}[\delta]\, \mathrm{Sin}[2\, \theta 12]\, \mathrm{Sin}[\theta 13]\, \mathrm{Sin}[2\, \theta 23]$$

$P(1 \to 2) - P(\bar{2} \to \bar{1})$:

```
TrigExpand[p312 - p3c21][[1, 1]]
```

```
0
```

2. Periodic delta−function Potential

(a) Matching conditions

Using the form of the wavefunction given in the problem,

$$\psi(-\epsilon) = A + B$$
$$\psi(+\epsilon) = e^{i k a} (A\, e^{-i \kappa a} + B\, e^{i \kappa a})$$
$$\psi'(-\epsilon) = i\, \kappa (A + B)$$
$$\psi'(+\epsilon) = i\, \kappa\, e^{i k a} (A\, e^{-i \kappa a} - B\, e^{i \kappa a})$$

The wavefunction is continuous $\psi(-\epsilon) = \psi(+\epsilon)$, but its derivative is discontinuous because of the delta−function potential, $\psi'(+\epsilon) - \psi'(-\epsilon) = \frac{2 m \lambda}{\hbar^2}\, \psi(0)$. These give the conditions

$$A + B = e^{i k a} (A\, e^{-i x a} + B\, e^{i x a})$$
$$i\, \kappa\, e^{i k a} (A\, e^{-i \kappa a} - B\, e^{i k a}) - i\, \kappa (A - B) = \frac{2 m \lambda}{\hbar^2}\, (A + B)$$

which we now solve:

```
msol = Solve[{
   A + B == E^(I k a) (A E^(-I κ a) + B E^(I κ a)), I κ E^(I k a) (A E^(-I κ a) - B E^(I κ a)) - I κ (A - B) == (2 m λ)/ℏ^2 (A + B)
  },
  {B, k}
 ];
```

Inserting the solution for k into the phase $e^{i k a}$:

```
foo1 = FullSimplify[E^(I k a) /. msol, Assumptions → {ℏ > 0, m > 0, λ > 0, κ > 0, a > 0}]
```

$$\left\{\frac{1}{2\hbar^2\kappa}\left(e^{-i a\kappa}\left(\hbar^2\left(1+e^{2 i a\kappa}\right)\kappa - i\left(-1+e^{2 i a\kappa}\right)m\lambda - 2\sqrt{e^{2 i a\kappa}\left(-\hbar^4\kappa^2+\left(\hbar^2\kappa\,\mathrm{Cos}[a\kappa]+m\lambda\,\mathrm{Sin}[a\kappa]\right)^2\right)}\right)\right),\right.$$
$$\left.\frac{1}{2\hbar^2\kappa}\left(e^{-i a\kappa}\left(\hbar^2\left(1+e^{2 i a\kappa}\right)\kappa - i\left(-1+e^{2 i a\kappa}\right)m\lambda + 2\sqrt{e^{2 i a\kappa}\left(-\hbar^4\kappa^2+\left(\hbar^2\kappa\,\mathrm{Cos}[a\kappa]+m\lambda\,\mathrm{Sin}[a\kappa]\right)^2\right)}\right)\right)\right\}$$

Making the suggested substitution $d = \hbar^2 / m\lambda$:

```
phase = Expand[Simplify[foo1 /. λ → ℏ^2 / (m * d), Assumptions → {ℏ > 0, d > 0, κ > 0, a > 0}]]
```

$$\left\{\frac{1}{2}e^{-i a\kappa}+\frac{1}{2}e^{i a\kappa}+\frac{i\,e^{-i a\kappa}}{2 d\kappa}-\frac{i\,e^{i a\kappa}}{2 d\kappa}-\frac{e^{-i a\kappa}\sqrt{e^{2 i a\kappa}\left(d^2\kappa^2\,\mathrm{Cos}[a\kappa]^2+\mathrm{Sin}[a\kappa]^2+d\kappa\left(-d\kappa+\mathrm{Sin}[2 a\kappa]\right)\right)}}{d\kappa},\right.$$
$$\left.\frac{1}{2}e^{-i a\kappa}+\frac{1}{2}e^{i a\kappa}+\frac{i\,e^{-i a\kappa}}{2 d\kappa}-\frac{i\,e^{i a\kappa}}{2 d\kappa}+\frac{e^{-i a\kappa}\sqrt{e^{2 i a\kappa}\left(d^2\kappa^2\,\mathrm{Cos}[a\kappa]^2+\mathrm{Sin}[a\kappa]^2+d\kappa\left(-d\kappa+\mathrm{Sin}[2 a\kappa]\right)\right)}}{d\kappa}\right\}$$

We can read off the expressions for the two roots:

$$e^{i k a} = \cos\kappa a + \frac{1}{\kappa d}\sin\kappa a \pm \sqrt{\cos^2\kappa a + \frac{1}{(\kappa d)^2}\sin^2\kappa a - 1 + \frac{1}{\kappa d}\sin 2\kappa a}\,.$$

Recognizing that $\sin 2\kappa a = 2\sin\kappa a\cdot\cos\kappa a$, we may factor the radicand and pull out a $\sqrt{-1}$ to give

$$e^{i k a} = \cos\kappa a + \frac{1}{\kappa d}\sin\kappa a \pm i\sqrt{1-\left(\cos\kappa a + \frac{1}{\kappa d}\sin\kappa a\right)^2}$$

as desired.

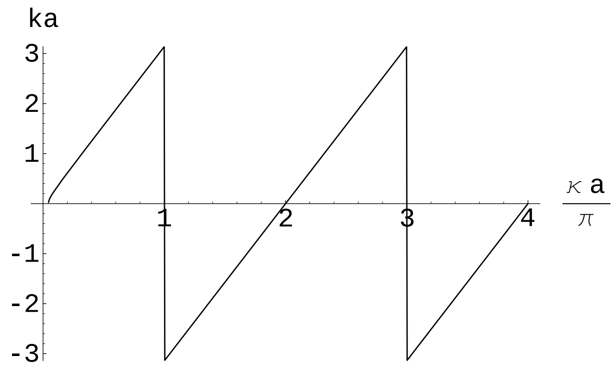
(b) Zero potential limit

In the limit $d \to \infty$, which is nothing but a free particle without a potential, we have

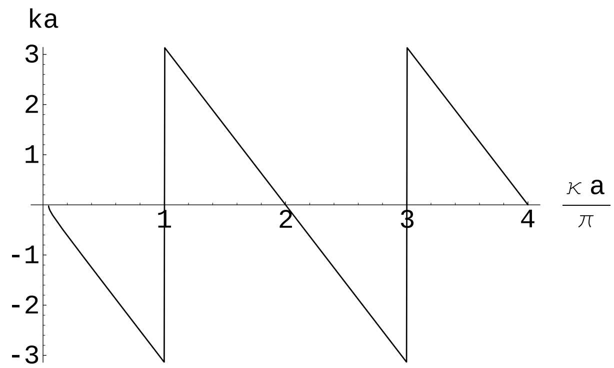
$$e^{i k a} = \cos\kappa a \pm i\sqrt{1-\cos^2\kappa a} = e^{\pm i\kappa a},$$

and so $\kappa = \pm\left(k + \frac{2\pi n}{a}\right)$; equivalently, k is the momentum modulo $\frac{2\pi n}{a}$. Therefore, κ and hence the energy grow continuously as a function of k. This can be seen numerically with a d that is large enough:

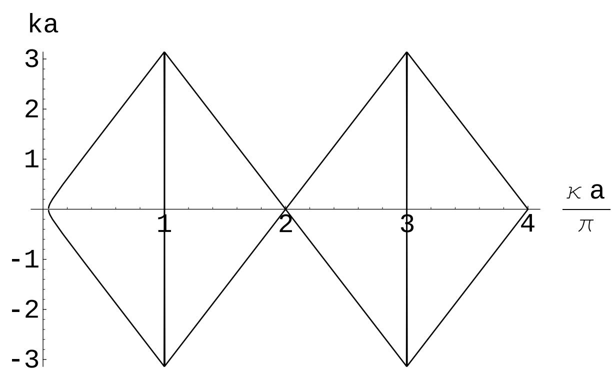
```
kplot1 = Plot[-I / a * Log[phase[[1]]] /. {a → 1, d → 100} /. κ → π * x,
  {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κ a / π", "ka"}];
```




```
kplot2 = Plot[-I / a * Log[phase[[2]]] /. {a → 1, d → 100} /. κ → π * x,
  {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κ a / π", "ka"}];
```




```
Show[kplot1, kplot2];
```



As we can see, no band gaps −− every κ has a real k.

(c) Weak potential

Looking at the equation

$$e^{i k a} = \cos\kappa a + \frac{1}{\kappa d}\sin\kappa a \pm i\sqrt{1 - \left(\cos\kappa a + \frac{1}{\kappa d}\sin\kappa a\right)^2}\ ,$$

if the argument of the square root is negative, the l.h.s. becomes pure real and cannot satisfy the equation for a real k. Therefore there is no solution when $\left|\cos\kappa a + \frac{1}{\kappa d}\sin\kappa a\right| > 1$. When d is finite but large, the combination exceeds unity for $\kappa a = n\pi + \epsilon$ $(\epsilon > 0)$. This can be seen by expanding it in terms of ϵ,

$$\cos(n\pi + \epsilon) = (-1)^n \left(1 - \frac{\epsilon^2}{2} + O(\epsilon^4)\right), \sin(n\pi + \epsilon) = (-1)^n\,(\epsilon + O(\epsilon^3)),$$

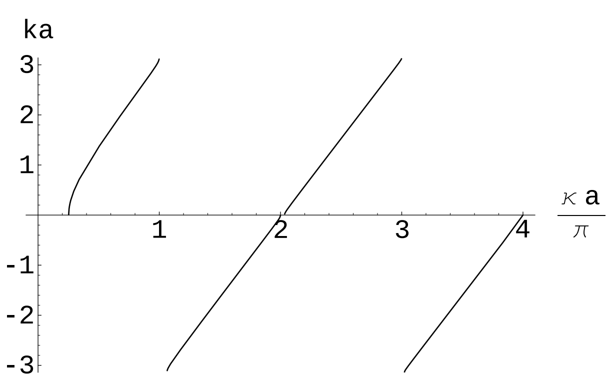
$$\Longrightarrow \cos\kappa a + \frac{1}{\kappa d}\sin\kappa a = (-1)^n \left(1 + \frac{1}{\kappa d}\epsilon - \frac{\epsilon^2}{2} + O(\epsilon^3)\right).$$

The magnitude exceeds unity for $0 < \epsilon < 2/\kappa d \simeq 2a/n\pi d$. The gap must exist just above $\kappa = n\pi/a$ for any n, while the gap becomes smaller for large n. So there exists a band gap at $\kappa = \pm\pi/a$.

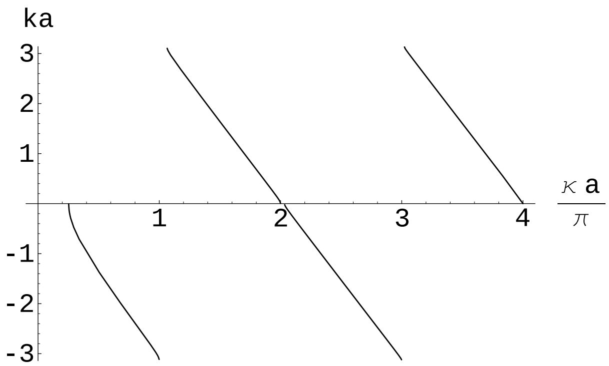
(d) Plots for weak and strong potentials

Let us plot for the given cases as we did in (b), first the weak $d = 3a$:

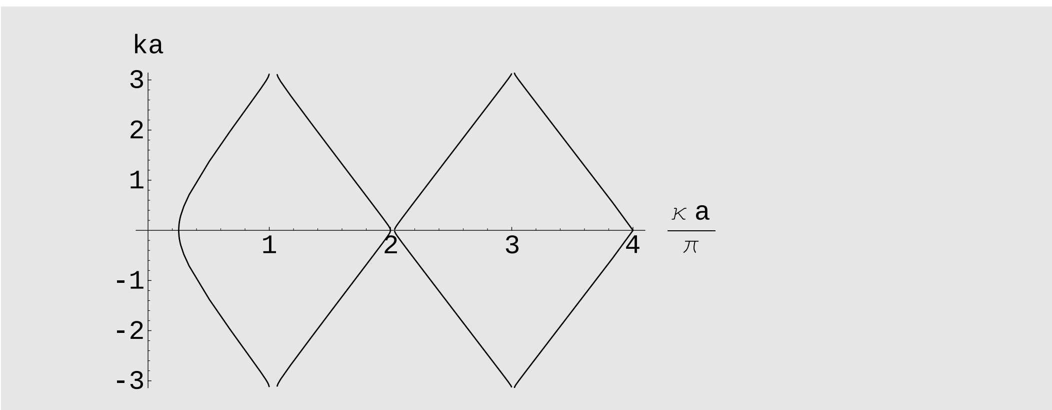
```
kplotcw1 = Plot[-I / a * Log[phase[[1]]] /. {a → 1, d → 3} /. κ → π * x,
   {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κ a/π", "ka"}];
```



```
kplotcw2 = Plot[-I / a * Log[phase[[2]]] /. {a → 1, d → 3} /. κ → π * x,
   {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κa/π", "ka"}];
```



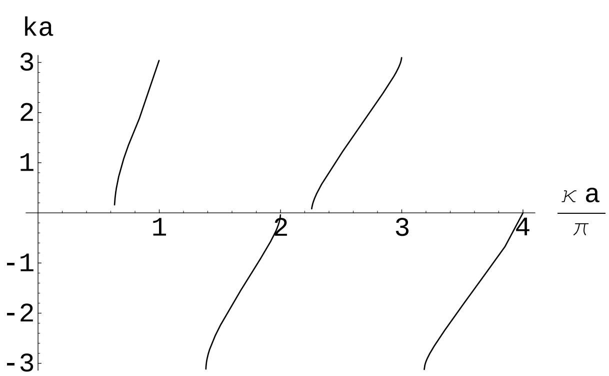

```
Show[kplotcw1, kplotcw2];
```



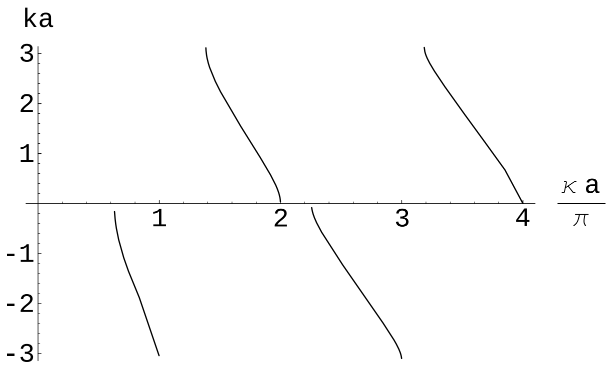
We see a big gap at $\kappa = 0$, a smaller one at $\kappa = \pi/a$, a yet smaller one at $\kappa = 2\pi/a$, and a gap you can barely see at $\kappa = 3\pi/a$. This is exactly what we predicted in part (c).

Now let's do the strong case $d = a/3$:

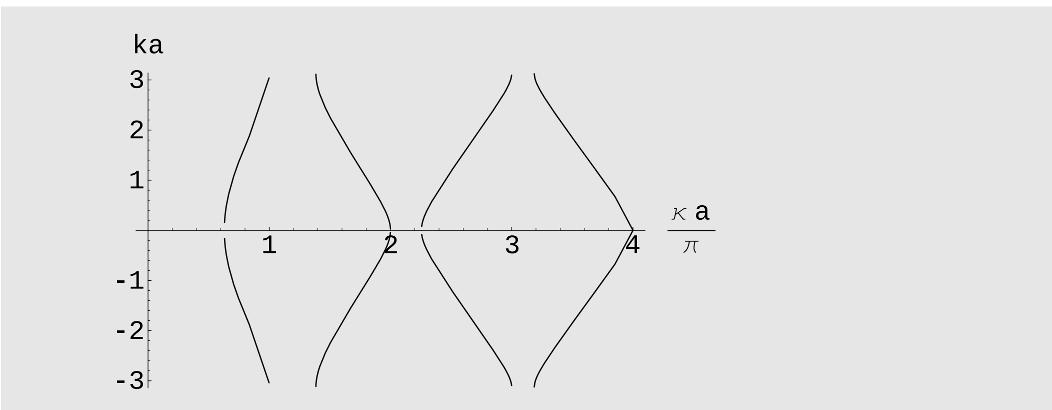
```
kplotcs1 = Plot[-I / a * Log[phase[[1]]] /. {a → 1, d → 1 / 3} /. κ → π * x,
   {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κa/π", "ka"}];
```



```
kplotcs2 = Plot[-I / a * Log[phase[[2]]] /. {a → 1, d → 1 / 3} /. κ → π * x,
   {x, 0, 4}, PlotRange → {-Pi, Pi}, AxesLabel → {"κ a/π", "ka"}];
```




```
Show[kplotcs1, kplotcs2];
```



Obviously, there is significant distortion from the free case in part (b), with gaps at $\kappa = n\pi/a$ much bigger than in the weak case above.

(e) $\boldsymbol{Z}_2$ symmetry in k

It is parity that changes the overall sign of k. This can be seen from the explicit form of the wave function,

$$\psi(x) = A\, e^{i\kappa x} + B\, e^{-i\kappa x} \qquad \text{for } -a < x < 0$$

$$\psi(x) = e^{i k a}\,(A\, e^{i\kappa(x-a)} + B\, e^{-i\kappa(x-a)}) \qquad \text{for } 0 < x < a\ .$$

The parity transformation gives

$$\begin{aligned}\psi(x) &= e^{i k a}\,(A\, e^{i\kappa(-x-a)} + B\, e^{-i\kappa(-x-a)}) \\ &= B\, e^{i(k+\kappa)a}\, e^{i\kappa x} + A\, e^{i(k-\kappa)a}\, e^{-i\kappa x} \\ &= A'\, e^{i\kappa x} + B'\, e^{-i\kappa x}\end{aligned}$$

and

$$\begin{aligned}\psi(x) &= B\, e^{i\kappa x} + A\, e^{-i\kappa x} \\ &= e^{-i k a}\,(B\, e^{i(k+\kappa)a}\, e^{i\kappa(x-a)} + A\, e^{i(k-\kappa)a}\, e^{-i\kappa(x-a)}) \\ &= e^{-i k a}\,(A'\, e^{i\kappa(x-a)} + B'\, e^{-i\kappa(x-a)})\end{aligned}$$

respectively. The two wave functions are related by the changes

$$A \to A' = B\, e^{i(k+\kappa)a}\ ,$$

$$B \to B' = A\, e^{i(k-\kappa)a}\ ,$$

$$e^{i k a} \to e^{-i k a}\ .$$